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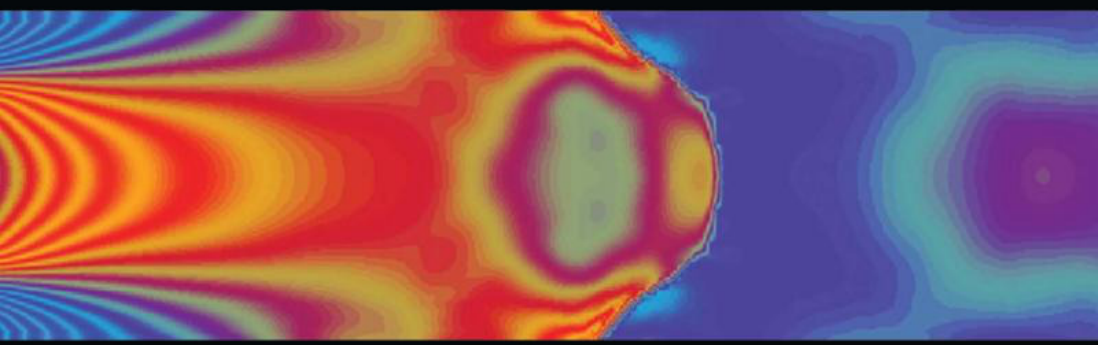
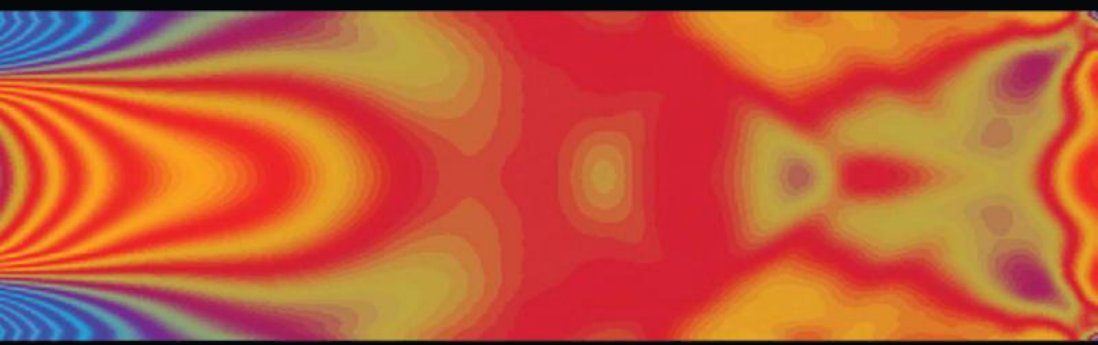
# CONFIGURATIONAL FORCES

## *THERMOMECHANICS, PHYSICS, MATHEMATICS, AND NUMERICS*



GÉRARD A. MAUGIN



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# CONFIGURATIONAL FORCES

## *THERMOMECHANICS, PHYSICS, MATHEMATICS, AND NUMERICS*

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*Dedicated to*

*the memory of Ekkehart Kröner,*

*Henryk Zorski, and Arnold M. Kosevich*

# *Contents*

# 1

# *Introduction*

## Object of the Chapter

Where advances made in the twentieth century in continuum mechanics and the recent developments in configurational mechanics are presented in a discursive and historical manner so as to introduce the subject matter of this book.

## 1.1 Continuum Mechanics in the Twentieth Century

Continuum mechanics in its simplest form has been the paragon of field theory and developed in parallel with the mathematical field of partial differential equations since the inception of this concept by d'Alembert in his studies of wave motion in a string and his elements of hydrodynamics in the mid-1700s, following Johann and Daniel Bernoulli. Then, after the successful modeling of standard behaviors by our great elders (Euler, Lagrange, Cauchy, Navier, Stokes, Kelvin, Kirchhoff, Helmholtz, Boussinesq, Boltzmann, von Mises, etc.), progress was relatively slow due to the mathematical difficulties in constructing appropriate solutions to boundary-value problems of complex geometries and finding the most appropriate functional classes to allow for the existence of the looked-for solutions. Now often considered, with some scorn—or at least condescension—as an "old" and closed science by some physicists, it is true that further progress at the conceptual level was also slow and perhaps not as spectacular as in other branches of "natural philosophy" such as electromagnetism. For example, the difficult notion of dissipation had to be grasped and mathematically formulated, whether in fluids in the form of viscosity or in solids in the form of plasticity and damage.

Until recently all these advances were made in the framework of three tenets of nineteenth-century physics: *linearity*, *isotropy*, and *homogeneity*. Of course, there are exceptions to these such as the early introduction of finite strains in elasticity by Cauchy in the 1820s and others (Piola, Kirchhoff, etc.) in following years,

and the inherent nonlinearity of some problems of fluid mechanics. *Anisotropy* was conquered next due to the consideration of crystals. Duhamel was among the pioneers along this line, but W. Voigt must be singled out in this framework in particular with his seminal introduction of tensorial concepts, while Gibbs and Heaviside were introducing dyadics and a true vectorial analysis. This became a landmark of the field to the point that, to many physicists, tensor analysis is practically synonymous with continuum mechanics (and general relativity). Much more recently, this notion of anisotropy even reached fluids in the form of liquid crystals, that is, media that can flow but still exhibit some ordering with direction-dependent properties akin to crystals. Considerations of *material heterogeneities* were to come last, as we shall briefly see.

Apart from mathematical advances with the introduction of new functional spaces (Sobolev spaces, distribution theory), the main advance that emerged after the rejuvenation (in fact a true "rebirth") of the field by authors such as C.A. Truesdell (e.g., Truesdell and Toupin, 1960; Truesdell and Noll, 1965) was the firm grounding of continuum mechanics in a thermomechanical framework, to the posthumous satisfaction of Pierre Duhem (see Maugin, 1999b). That very much helped scientists (i) to classify and logically arrange the field, although sometimes to a useless extreme ("bourbakism"), and also (ii) to incorporate some multiphysics effects (e.g., electromagnetism; see Eringen and Maugin, 1990), and to prepare the way for enlarging the categories of modeling, including multiscale continuum mechanics and the introduction of scale effects (characteristic internal lengths, nonsymmetric Cauchy stress, micropolar and micromorphic continua; gradient theories). In this regard, building on the early works of Duhem and the Cosserat brothers, scientists such as Eringen, Rivlin, Naghdi, Mindlin, Tiersten, Kroener, Sedov, and others (see Kroener, 1968) were instrumental in putting on solid grounds the essentials of such *generalized continuum mechanics* (cf. Maugin, 2010), with "generalized" often simply meaning "more complicated" than the now-standard models of Cauchy, Euler, and Navier and Stokes. The books of Eringen (1999, 2001, 2002) illustrate perfectly these generalizations, which call for new elements of the kinematics of deformation and, correspondingly, in agreement with the duality dear to us, new force concepts such as couple stresses, hyperstresses, and so on.

All these advances of the second half of the twentieth century are more generalizations than new conceptual thinking. Of course, we cannot ignore the very successful technique of *homogenization* (replacing a somewhat complicated microstructured—not necessarily periodic—medium by an effective medium, the building block of this being a representative volume element [RVE] made of rather simple—most often "classical"—material elements). Forest (2006), in a remarkable monograph, has established the relationship of the results of this powerful technique with generalized continuum mechanics, while the existence of the latter is also supported by long-wavelength limits of discrete models in so-called lattice dynamics.

Only at this point was more attention paid to a more original conceptual approach to *material heterogeneities*, whether in the case of composite materials

or that of polycrystals, and the necessary accompanying notion of *defects*. This, in our opinion, is the last great conceptual advance in continuum mechanics, in particular due to the recognition of the conceptual unity of the subfield of continuum mechanics related to the notion of *configurational force*, the subject matter of this book. Indeed, the first example of such "forces" is the Peach–Koehler (1950) force that drives a dislocation line, while the second is the force on a material elastic inhomogeneity (e.g., inclusion) and a field singularity in the pioneering work of J.D. Eshelby (1951), whom we consider the founding father of our field. The remarkable feature of these developments in a half century, which accelerated in the 1990s–2000s, has been the new interrelation of continuum mechanics with recent fields of mathematical physics, in particular insofar as invariances are concerned, and with some fields of solid-state physics and materials science insofar as the relationship between the two antagonistic views of the continuum and the discrete are concerned.

The basic thinking here is a typical Pavlovian reflex of a good "mechanician." Whatever apparently moves or progresses in the matter in an observable manner is thought of as being acted on by a "force" dual to the observed displacement of that "object." But here this is not a force of the Newtonian type (typically characterized per unit of matter), for the object can be a material defect of mathematically vanishing support, a dislocation line, a mathematical surface of discontinuity (e.g., a phase-transition front, a shock wave), a material inclusion, a hole, a field singularity such as a crack tip, a strongly localized mathematical field solution (e.g., structured shock waves, solitons), and so on. In the framework of continuum mechanics all these take place on the material manifold $M^3$, that is, the set of material points constituting the body in a more or less smooth manner. This is directly related to the notion of material heterogeneity since that feature describes the dependency of the material properties on the material point (not the point occupied in physical space), hence on the local configuration. The problem with such "configurational" forces is that they are not directly accessible, but what is shown in their theory is that they may be computed once more classical entities are obtained, and then further progress of their point of application can be envisaged depending on the implementation of a criterion of progress. One easily imagines the practical engineering interest for such a procedure in problems of fracture (progress of a crack tip) or phase transformations because of its predictive nature.

## 1.2 The Object of This Book

So-called *configurational forces*, also called *material forces* in modern continuum mechanics and, more generally, *energetic driving forces*, are those forces that are associated by duality with the displacement or motion of whatever may be considered a *defect* in a continuum field theory. Conceptually simple

examples of such defects are dislocations in ordered crystals, disclinations in liquid crystals, vortices in fluid mechanics, cracks and cavities in materials science, propagating fronts in phase-transition problems, shock waves in continuum mechanics, domain walls in solid-state science, and, more generally, all manifestations, smooth or abrupt, of changes in material properties. In such a framework, the material symmetry of the physical system is broken by the presence of a field singularity of a given dimensionality (point, line, surface, volume). Until very recently all these domains were studied separately but a general framework emerged essentially through the works of the present author and his coworkers, based initially on inclusive ideas of Eshelby (deceased 1981)—hence the coinage of *Eshelbian mechanics* by the author for the mechanics of such forces. In this framework, which is developed in a synthetic form in this book, all configurational forces appear as *forces of a non-Newtonian nature*, acting on the material manifold (the set of points building up the material, whether discrete or continuous) and *not* in physical space, which remains the realm of Newtonian forces and their more modern realizations, which usually act per quantity of matter (mass or electric charge). That is, configurational forces act on spatial gradients of properties, on field singularities, and so on. They acquire a true physical meaning only insofar as the associated expended power is none other than a *dissipation*; accordingly, configurational forces are essentially used to formulate *criteria of progress* of defects in accordance with the second law of thermodynamics. Within such a general vision, in fact, many irreversible properties of matter (e.g., damage, plasticity, magnetic hysteresis, phase transition) are seen as *irreversible local rearrangements* of matter (material particles in an ordered crystal, spin layout in a ferromagnetic sample, director network in a liquid crystal) that are represented by pure material mappings. This is where some elements of modern differential geometry enter the picture following earlier works by Kröner, Noll, and others.

Having recognized the *material* (also called sometimes *Lagrangian*—as opposed to *Eulerian*) nature of configurational forces, the main progress was to identify (i) that the energetic driving forces on material inhomogeneities—whether *true inhomogeneities*, as in recently developed gradient-materials and obviously in *composite materials* or *quasi-inhomogeneities*, as in field singularities or gradients in the solution of nonmechanical fields, such as temperature in conductors of heat—are generated by a change in *particle* and not a change in the placement of one particle in physical space, (ii) that the accompanying *flux* is none other than the "energy-momentum" tensor introduced by Eshelby in defect mechanics in the early 1950s (and obviously known in field theories since Hilbert), and, finally, (iii) that the associated *momentum* is a *material momentum*, also called *canonical momentum* in the nondissipative case but which we sometimes prefer to call *pseudomomentum* (after Peierls in optics). This kinetic quantity is a covector on the material manifold, and it includes, a priori, contributions from all fields. Its conservation or nonconservation relates to the fact that the physical system

as a whole may exhibit properties that generally depend *explicitly*—and not through the field solution—on the considered material point. In many applications this dynamic entity is not so much relevant (e.g., in fracture or phase transitions), but it plays an essential role in the linear dynamics of crystals (Brenig's so-called *crystal momentum*) and in the nonlinear dynamics of *solitonic structures* (wave momentum) and other nonlinear wave phenomena, as we proved in the dynamics of nearly integrable systems by using the notion of *quasiparticles.*

Although configurational forces do not live, if we may say so, in the real world, they are "visible" through the duality they enjoy with their thermodynamic partners, material displacements. For instance, a macrocrack in the protecting vessel of a nuclear reactor is observable; with changes in some external conditions (e.g., periodic thermal heating of the structure), we see the unfortunate crack progress. According to the classical reasoning of mechanics, a *force*—the said *configurational force*—is associated with this progress. The theory allows one to *compute* this force. Similarly, lines of dislocations can be observed by some techniques (x-rays). When a system of physical forces is applied to the specimen we see the dislocation lines "move." The configurational force associated with this movement, the *Peach–Koehler* force, can be computed. Finally, the same holds true of the tip of a crack, whose motion can be observed by infrared thermography in a transparent sample, or of domain walls in ferromagnets, which can be observed by Bitter's technique, or, further yet, of the propagation of a phase-transformation front during quenching of a Japanese sword! Configurational forces do not live in our world because they are not the direct manifestation at a point of a classical cause at the same point. They are the results of complex, in general cooperative, and most often dissipative phenomena, and they can only be the result of a computation, analytical in some cases, numerical in most cases. The *mechanics of configurational forces* or *Eshelbian mechanics*, as we like to call it, provides the means to perform this computation and gives us the tools to exploit them in decisive circumstances. It is a *true* mechanics of forces in the sense that these forces contribute in dynamics to a local "conservation" of momentum in the general manner of Newton, and they also combine, add, or subtract with one another, and they exhibit moments! Later on we will forcefully distinguish between "balance laws"—which in contemporary continuum physics are most often obtained by localization of global balance laws—and "conservation laws," which are deduced locally and would not correspond to the global balance of any a priori physically meaningful quantity.

The book presents the general framework for *configurational forces* along the above-described line of thought at a time when we consider this framework to have reached a sufficiently firm grounding and applications and to have embraced a sufficiently rich and varied range to justify this synthesis by an active proponent of the subject matter. The power of the concepts indeed resides in the many applications, which, in addition to the previously mentioned cases, involve as well the study of the perturbed motion of solitonic

structures (viewed as localized defects or quasiparticles) under the influence of external or coupled fields, and the accuracy of numerical computations in finite-difference schemes (FDS) and finite-element methods (FEM) where perturbing configurational forces appear if limit/boundary conditions are not exactly satisfied (in FDS) or simply due to a bad design of the grid of computation in FEM. Although it is based initially on field-theoretic concepts and a somewhat complex geometric vision, the theory of configurational forces is thus endowed with computational interests in addition to the obvious understanding and convenient tools that it brings to fields of engineering (e.g., in fracture, damage, plasticity) and condensed-matter physics. In our opinion, it constitutes one of the latest and most fruitful advances in macroscopic field theories, an area that many have considered a completely closed field of research offering no further progress, and therefore no true scientific interest, for quite a long time already.

## 1.3 The Contents of This Book

The present chapter is a discursive one presenting the most recent steps in the evolution of continuum mechanics—at the time of writing—and introducing the most relevant notions for our present purpose: *material inhomogeneities* and the allied notion of *material forces*. Although marked by the idiosyncrasies of the author, Chapter 2 presents in a rather condensed manner the fundamentals of accepted standard continuum mechanics with no effort at pure abstraction but still trying to keep a sufficient level of rigor. Special attention is paid to pull-back and push-forward operations between physical space and the material manifold. Unusual considerations are those pertaining to the so-called inverse motion. The basic thermomechanics are also formulated with an emphasis on the Cauchy format and the Piola–Kirchhoff format of local balance equations and recalling the role played by the principle of virtual power in modern continuum mechanics. Examples of standard linear and nonlinear, recoverable, and thermodynamically irreversible behaviors are given by way of illustration, including truly dissipative bulk mechanical behaviors treated by means of the notion of internal variable of state.

Chapter 3 inaugurates the truly original part of the book by introducing the notion of *Eshelby material stress*, the main ingredient in subsequent developments. This allows us to remind the reader of Eshelby's original works that relate to the evaluation of the "force" acting on an inhomogeneity or a material defect. Variational formulations of finite-strain elasticity are given on that occasion. In the absence of dissipative processes, Chapter 4 continues along the same line by introducing the reader to the general notions of field theory, variational formulations, and *Noether's theorem*, with resulting *conservation laws*. This subject matter is revisited in Chapter 5 in the general

case of complex continua admitting no variational formulation because of a present dissipation. Two viewpoints are contrasted here, the one classically associated with the names of B.D. Coleman and W. Noll and the other closer to the spirit of abstract field theory. Chapter 6 then introduces the reader to the important notion of *local structural rearrangement* and its relationship to the Eshelby stress as understood by Epstein and the author, following in the path of pioneering works by E. Kroener, W. Noll, and C.C. Wang. The *geometric theory of defects* is also dealt with in that chapter, where it is finally shown that three lines of research that were developed in the second half of the twentieth century unite in a single synthetic view, in particular unifying the line of thought of Eshelby with that of Kroener, Noll, and others and including the celebrated multiplicative decomposition of the total deformation gradient.

While previously mentioned chapters deal with rather smooth fields, Chapter 7 concerns the relevance of the notion of Eshelby stress in the thermodynamic description of *singular interfaces.* Applications concern shock waves, phase-transition fronts, and metallurgy problems involving a multitude of phases. Other singularity sets are those pertaining to the *fracture problem* and are examined in Chapter 8, with special attention paid to the consideration of *invariant integrals* and the exploitation of generalized functions. From here on the reader will find various applications of the already-introduced concepts to some complex cases that occur frequently in contemporary continuum mechanics. This concerns polar and other *microstructured media* (Chapter 9), systems with *mass exchanges*, such as in the phenomenon of growth or in solid–fluid mixtures (Chapter 10), and *electromagnetic deformable media* of different types (Chapter 11), a subject dear to the author. In each case attention is paid to the most relevant problems such as fracture and phase-transition fronts. Of course, the technicality of the exposition increases with the subsequent chapters, and we require here a good deal of patience and some previous knowledge from the readers. But the results are worth the effort as the whole simultaneously proves the richness, power, and efficiency of the approach from the application viewpoint.

Chapters 12 through 14 have a different nature than the previously described chapters. Chapter 12 deals with the exploitation of the canonical conservation law of momentum (where the involved flux is none other than the Eshelby stress) in *nonlinear wave propagation* as it captures the whole dynamic solution and therefore plays an obvious fundamental role in the dynamics of quasiparticles associated with some remarkable solutions such as solitary waves and solitons. A variety of examples based on generalized continuum mechanics are given. Chapter 13 deals with the application of the notions of canonical-momentum conservation law and material force in the implementation of *numerical schemes* of different types. The most original point here is the strategy of back-and-forth treatment between spatial and material configurations in the finite-element scheme, while FDS are directly related to the dynamic contents of Chapter 12, and finite-volume elements find a straightforward application in the numerical simulation of the

irreversible progress of phase-transition fronts in crystals. Finally, the conclusive Chapter 14 provides hints at analogies with some considerations of fluid mechanics and aerodynamics and really sets forth the general view of the world of material-configurational forces. A number of appendices have been added where necessary. I have been generous in giving an extended list of references, trying to be fair to most authors and providing access to a roster of works that can be useful to the reader, whether a graduate student or a professional researcher. Not all references are cited in the body of the text, but are listed in the Bibliography.

***The book is dedicated to Ekkehart Kroener, Henryk Zorski, and Arnold M. Kosevich. The chapter abstracts were written with the help of the late Jules Verne.***

## 1.4 Historical Note

The exposition that follows is a rationally ordered reconstruction of the field rather than a linear history of it. A short prejudiced personal historical perspective goes like this. Clearly, Eshelby's works were inspired by mathematical physics. The same can probably be said of the early work of Rogula (1977) and Golebiewska–Herrmann (1981, 1982). The latter strongly influenced engineering scientists at Stanford University, the late George Herrmann and his coworkers (e.g., Pak and Herrmann, 1986a, 1986b; Eischen and Herrmann, 1987). This was taken over very successfully by Reinhold Kienzler from Bremen, in collaboration with G. Herrmann, in their brilliant application of the concept of configurational forces to engineering mechanics (Kienzler and Herrmann, 1986) and the strength of materials, culminating in a book (Herrmann and Kienzler, 2000). In parallel, a more traditional school of mechanical engineering, following along the path opened by German scientists such as Günther (1962), studied in depth various path-independent integrals (Knowles and Sternberg, 1972; Fletcher, 1976; Bui, 1978) with a repeated interest in fracture and other problems whose solution exploits these integrals (see, e.g., Buggisch et al., 1981). Pioneers such as Cherepanov (1967; see also the collection of papers in the 1998 book edited by Cherepanov) and Rice (1968) must be cited as having been instrumental in the application of some path-independent integrals (e.g., the celebrated $J$-integral of fracture). We may say that the works of Abeyaratne and Knowles (1990) on interfaces follow this line as well, keeping simultaneously close contact with physical features (see their 2001 book). Along another line, it was natural for M.E. Gurtin, a pioneer in good mathematical approaches to fracture (Gurtin, 1979a, 1979b) and moving interfaces (Gurtin, 1993), to enter the domain of configurational forces with an original view (1995, 1999), which we cannot share for reasons repeatedly explained in the present book.

On our side, having devoted our previous research mostly to relativistic mechanics, the electrodynamics of deformable bodies, and nonlinear waves in solids while paying sustained attention to the general thermomechanics of continua, generalized media, and the theory of elastoplasticity, we entered the field in a pedestrian way by establishing first the relationship between the general geometric considerations of K. Kondo, E. Kröner, W. Noll, and C.C. Wang (e.g., Noll, 1967), and their theory of *material uniformity*, and the notion of *Eshelby stress tensor* (his energy-momentum tensor). This was achieved in collaboration with M. Epstein (Epstein and Maugin, 1990a, 1990b), while, in cooperation with C. Trimarco (Maugin and Trimarco, 1992), we revisited the relationship of the notion of Eshelby stress with that of the variational principle (obviously in the absence of dissipation in matter per se). Generalizations to electromagnetic materials of different types by the same group of three authors followed rapidly, while a small book (Maugin, 1993) written while I was a member of the Wissenschaftskolleg in Berlin set forth in a few pages general ideas on the subject with special emphasis on the differences between Newtonian mechanics and Eshelbian mechanics. This was complemented by a long review (Maugin, 1995). Both the book and the review were instrumental in attracting the attention of several researchers to the field. Particularly noteworthy was the important remark made by Manfred Braun (1997) on the possibility of exploiting the material momentum equation or its equilibrium version to the benefit of *finite-element computations*. This was to generate a series of works by R. Mueller and coworkers (in Darmstadt), including the present author (e.g., Maugin, 2000a; Mueller and Maugin, 2002) and the very active group of Paul Steinmann, then in Kaiserslautern (e.g., Steinmann, 2000, 2002a, 2002b; Steinmann et al., 2001). Steinmann and coworkers cleverly introduced in a systematic way the so-called Cauchy and Eshelby formats of a stress tensor and treated a number of numerical applications, in particular in the field of large-strain biomechanics.

In the meantime we established a kind of universality for the *canonical thermomechanics of continua*, including most intrinsically dissipative cases (Maugin, 1998b, 2000b). Before that, Epstein and I had introduced the notion of thermal material force in heat conductors (Epstein and Maugin, 1995a), a simple form of which had been introduced by Bui (1978). We also examined the geometric definition of the Eshelby stress in the case of finite-strain plasticity (Epstein and Maugin, 1995b, 1997) as well as in the theory of material growth (Epstein and Maugin, 2000). In this line I identified effects of pseudoinhomogeneity and pseudoplasticity by their resemblance to the Eshelbian type of inhomogeneity effects (Maugin, 2003). Many generalizations to the cases of electromagnetic materials of different classes and to generalized continuum mechanics were given by the author and coworkers between 1991 and 2005 (see the appropriate chapter in this book). An original approach to dissipative interfaces such as phase-transition fronts and shock waves was given in 1997–1998 (e.g., Maugin, 1997, 1998a). Applications

to the conservation laws and perturbation of soliton-like solutions were performed in cooperation with Christo I. Christov (e.g., Maugin, 1999a; Maugin and Christov, 2002)—after my work of 1992 published in the *Journal of the Mechanics and Physics of Solids* (Maugin, 1992a)—while an original thermodynamically admissible numerical scheme of the finite-volume type was conceived together with Arkadi Berezovski, with a special interest in moving interfaces (see Berezovski et al., 2008) and leaning heavily on the notion of material framework and configurational force.

Several authors have agreed that the work of Burton (1891) germinally contains the notion of "material space," but our own efforts to assess this fact have been unsuccessful due to that author's poetry and approximate statements. We rather like to toy with the idea that Nicole (Nicholas) Oresme (a French philosopher, mathematician, theologian, and economist, ca. 1320–1382, who received his doctorate from Paris University in 1356) could be our oldest precursor with his well-named *Tractatus de configuratione qualitatum et motuum*, who introduced a graphic representation of material inhomogeneity by plotting the variation of a characteristic material property along a direction and then generalizing this to three dimensions, inventing by the same token rectangular coordinate geometry long before Descartes. Indeed, he developed a universal theory explaining physical phenomena via the notion of geometric configuration (cf. Duhem, 1909; Taschow, 2003). This tells more or less the whole story in a nutshell.

A particular tribute must be paid to my main coworkers, in chronological order: Marcelo Epstein, Carmine Trimarco, Cristian Dascalu, Christo I. Christov, Anaclet Fomethe, Mohammed Sabir, Shoji Imatani, Liliana Restuccia, Arkadi Berezovski, Sara Quiligotti, Ralf Mueller, S. Cleja-Tigoiu, Vassilios Kalpakides, and Markus Lazar, all professionals of indispensable value. My friends George Herrmann and Henryk Zorski (both now deceased), Reinhold Kienzler, Wolfgang Muschik, Manfred Braun, Genady P. Cherepanov, Juri Engelbrecht, Paul Steinmann, and James Casey were also of great help in their sustained support and comprehension. I could also always count on my masters, Paul Germain, A. Cemal Eringen, and Ekkehart Kröner, all unfortunately now deceased.

# 2

# *Standard Continuum Mechanics*

## Object of the Chapter

Where we remind the reader of the formulation of deformation theory and thermomechanics principles accepted by most specialists in the period 1950–1990.

## 2.1 Theory of Motion and Deformation

First we have the notion of the material body.

### 2.1.1 Material Body

Here, a nondefective material body is a simply connected region $B$ of a three-dimensional Euclidean manifold $M$, or simply $M$, called the *material manifold*. The elements of this manifold are so-called material points $X$. In (possibly but not necessarily) curvilinear coordinates $X^K$, $K = 1, 2, 3$, this point is simply represented by the boldface letter $\mathbf{X}$. To each point $X$ on $M$ is attached a density, the matter density $\rho_0$, which is the density of matter at the reference configuration $K_R$. This may be a function of $\mathbf{X}$, as is the case in materially inhomogeneous bodies, and perhaps, but rarely, a function of Newtonian time $t$ itself. The latter scalar parameter belongs to an ordered one-dimensional continuum, the positive real line $R$, which presents no defects. That is, time itself cannot be "fractured." With this we have introduced the basic space–time parametrization of the classical mechanics of deformable solids, the set $(\mathbf{X}, t)$.

Next we have the definition of the motion.

### 2.1.2 Motion (or Deformation Mapping)

The motion (or deformation) of the material body $B$ of $M$ is the *time-ordered sequence* of the positions, sometimes called *placements*, occupied by the point $X$ in Euclidean *physical space* $E^3$, the arena of classical phenomenological

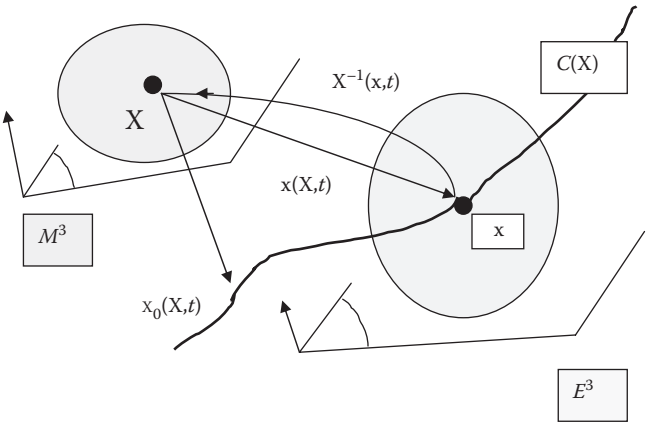


**FIGURE 2.1**
The classical view of finite transformations (direct and inverse motions).

physics. This is expressed by the sufficiently (as needed) regular space–time parametrized mapping (Figure 2.1).

$$\mathbf{x} = \chi\,(\mathbf{X},\, t). \tag{2.1}$$

This is often (but not necessarily) reported to a Cartesian system of coordinates $x^i$, $i = 1, 2, 3$. Note that physical space here is always Euclidean, since we work in Newtonian physics, while $M$ could be non-Euclidean (as would be the case in a *defective* material body). The set of geometric points $\mathbf{x}(B, t$ fixed) constitutes the *actual* or *current configuration* $K_t$ of the body at time $t$. Usually, an origin of time, say $t_0$, is chosen such that $t_0 < t$, and (2.1) then reads

$$\mathbf{x}_0 = \chi\,(\mathbf{X},\, t_0). \tag{2.2}$$

When both mappings (2.1) and (2.2) are sufficiently smooth, and in particular, invertible, we can rewrite (2.1) as

$$\mathbf{x} = \chi\left(\chi^{-1}\left(\mathbf{x}_0, t_0\right), t\right) = \bar{\chi}\left(\mathbf{x}_0, t\,; t_0\right) = \tilde{\chi}\left(\mathbf{x}_0, t\right). \tag{2.3}$$

This representation of the direct motion is called Lagrangian, the $\mathbf{x}_0$ being Lagrangian coordinates. The configuration $K_0 = K_t\,(t = t_0)$ of the body, the *initial configuration* at $t = t_0$, belongs to the sequence of "actual" configurations. This is the motion description preferred in fluid mechanics. Many authors identify the two representations (2.1) and (2.3) by identifying $\mathbf{X}$ and $\mathbf{x}_0$. But the motion representation (2.1) is somewhat more abstract and is essentially due to Gabrio Piola (1848) in a paper of far-reaching insight. Indeed, the consideration of the *material* configuration $K_R$ that corresponds to an ideally unstrained and unloaded configuration, corresponding usually to a minimizer of the energy (cf. Lardner, 1974), is essential in studying the material

symmetry of solid bodies and defining material properties in a general manner. While (2.1) is called the *direct-motion mapping* $K_R \to K_t$ *at* $t$, in the same smoothness conditions as above, the *inverse* motion is given by

$$\mathbf{X} = \chi^{-1}(\mathbf{x}, t). \tag{2.4}$$

The direct $\mathbf{F}$ and inverse $\mathbf{F}^{-1}$ motion **gradients** are defined thus

$$\mathbf{F} := \nabla_R \chi \equiv \frac{\partial \chi}{\partial \mathbf{X}}, \quad \mathbf{F}^{-1} := \nabla \chi^{-1} \equiv \frac{\partial \chi^{-1}}{\partial \mathbf{x}}. \tag{2.5}$$

It is immediately checked that

$$\mathbf{F}.\mathbf{F}^{-1} = \mathbf{1}, \quad \mathbf{F}^{-1}.\mathbf{F} = \mathbf{1}_R, \tag{2.6}$$

where the symbols $\mathbf{1}$ and $\mathbf{1}_R$ represent the unit dyadics in $E^3$ and on $M$, respectively. It must be emphasized that both $\mathbf{F}$ and $\mathbf{F}^{-1}$ are *not* tensors in the traditional sense because they are geometric objects defined on two different manifolds simultaneously. In picturesque language, we can say that they have one foot in $K_t$ and another in $K_R$. Such objects are so-called *two-point tensor fields*. They have components

$$\mathbf{F} = \left\{ F_K^i \equiv F_{iK} \right\}, \quad \mathbf{F}^{-1} = \left\{ \left(\mathbf{F}^{-1}\right)_i^K = \left(\mathbf{F}^{-1}\right)^{Ki} \right\}, \tag{2.7}$$

where the upward or downward position of the lower Latin indices is irrelevant by virtue of the Cartesian representation chosen in $K_t$. Speaking of an a priori symmetry of $\mathbf{F}$ and $\mathbf{F}^{-1}$ is a mathematical nonsense since one must specify with respect to what metric tensorial symmetry is defined. The Jacobian determinant of $\mathbf{F}$ is noted

$$J_F = \det \mathbf{F}. \tag{2.8}$$

Of course,

$$J_{F^{-1}} = \det \mathbf{F}^{-1} = \left(J_F\right)^{-1}.$$

**MATTER DENSITY:** If $\rho_0$, the matter density at $\mathbf{X}$, does not depend on time, the actual mass density $\rho$ is related to $\rho_0$ by the change of volume between configurations, that is,

$$\rho(\mathbf{x}, t) = \rho_0(\mathbf{X}) J_F^{-1}. \tag{2.9}$$

Since densities are always positive, only deformation mappings such that $J_F$ *is positive and never vanishes*, are considered. In physical terms this signifies the *impenetrability* of matter.

### 2.1.3 Some Deformation Measures

Deformation measures are typical "metrics" (truly symmetric tensors). Some of them can be defined thus (here the superscript $T$ denotes the operation of *transposition*, δ's are Kronecker symbols):

$$\mathbf{C}(\mathbf{X},t) := \mathbf{F}^T\mathbf{F} = \left\{C_{KL} = F^i_K \delta_{ij} F^j_L\right\}, \tag{2.10}$$

$$\mathbf{C}^{-1} := \left(\mathbf{F}^{-1}\right)\left(\mathbf{F}^{-1}\right)^T = \left\{\left(\mathbf{C}^{-1}\right)^{KL} = \left(\mathbf{F}^{-1}\right)^K_i \delta^{ij} \left(\mathbf{F}^{-1}\right)^L_j\right\}, \tag{2.11}$$

$$\mathbf{c}^{-1} := \mathbf{F}\mathbf{F}^T = \left\{\left(\mathbf{c}^{-1}\right)_{ij} = F_{iK}\delta^{KL}F_{jL}\right\}, \tag{2.12}$$

$$\mathbf{c} := \left(\mathbf{F}^{-1}\right)^T \mathbf{F}^{-1} = \left\{\left(\mathbf{F}^{-1}\right)^K_i \delta_{KL} \left(\mathbf{F}^{-1}\right)^L_j\right\}, \tag{2.13}$$

The first two, defined over $M$, are called the *Cauchy–Green* finite (material) strain tensor and the *Piola* finite (material) strain tensor, respectively. They are the inverse to one another. Similarly, the last two, defined in physical space, are the (unnamed) finite (spatial) strain tensor and the *Finger* finite (spatial) strain tensor, respectively, and they are inverses of one another. These four measures are *absolute* ones. They are not compared to an undeformed metric. Natural *relative* strain measures are given by

$$\mathbf{E} := \frac{1}{2}\left(\mathbf{C} - \mathbf{1}_R\right), \quad \mathbf{e} := \frac{1}{2}\left(\mathbf{1} - \mathbf{c}\right). \tag{2.14}$$

These two are shown to be related by

$$\mathbf{E} = \mathbf{F}^T\mathbf{e}\mathbf{F}, \quad \mathbf{e} = \mathbf{F}^{-T}\mathbf{E}\mathbf{F}^{-1}, \quad \mathbf{F}^{-T} \equiv \left(\mathbf{F}^{-1}\right)^T. \tag{2.15}$$

Equation 2.14 defines relative finite material and spatial strain measures. A more general definition than the first of (2.14) allows one to introduce a series of material strain measures such that, $m = \ldots, -2, -1, +1, +2, \ldots$,

$$\mathbf{E}^{(m)} := \frac{1}{m}\left(\mathbf{U}^m - \mathbf{1}_R\right). \tag{2.16}$$

Here **U** is the *right stretch (material) tensor* introduced in the polar decomposition of any nonsingular **F**—nonvanishing det **F**—according to a theorem due to Cauchy:

$$\mathbf{F} = \mathbf{RU} = \mathbf{VR}, \tag{2.17}$$

where **V** is the *left stretch (spatial) tensor*, and **R** is a rotation that belong to *SO*(3), that is,

$$\mathbf{R}^T = \mathbf{R}^{-1}, \quad \det \mathbf{R} = +1. \tag{2.18}$$

Both **U** and **V** are positive definite. We immediately check that

$$\mathbf{C} = \mathbf{U}^2, \quad \mathbf{c}^{-1} = \mathbf{V}^2; \quad J_F = \det \mathbf{U} = \det \mathbf{V} = \left(\det \mathbf{c}\right)^{-1/2}, \tag{2.19}$$

and thus from (2.16), in particular,

$$\mathbf{E}^{(2)} \equiv \mathbf{E}, \quad \mathbf{E}^{(-2)} = \frac{1}{2}\left(\mathbf{1}_R - \mathbf{C}^{-1}\right). \tag{2.20}$$

Note that there would be a difficulty with $m = 0$, so that the following *Hencky logarithmic strain measures* are of special interest by reason of their range of values:

$$\mathbf{E}_H = \frac{1}{2}\log \mathbf{C}, \quad \mathbf{e}_H = -\frac{1}{2}\log \mathbf{c}. \tag{2.21}$$

Also, finding **U** from **C**, or **V** from $\mathbf{c}^{-1}$, is an awkward operation (finding the square root of a tensor).

### 2.1.4 Displacement Field

This is the field $\mathbf{u}(\mathbf{X}, t)$ or $\bar{\mathbf{u}}(\mathbf{x}, t)$ defined by

$$\mathbf{x} = \mathbf{X} + \mathbf{u}(\mathbf{X}, t) \quad \text{or} \quad \mathbf{x} = \mathbf{X} + \bar{\mathbf{u}}(\mathbf{x}, t). \tag{2.22}$$

On taking the material gradient $\nabla_R$ of the first of these and the spatial gradient $\nabla$ of the second we obtain with (2.5),

$$\mathbf{F} = \mathbf{1} + \mathbf{H}, \quad \mathbf{H} \equiv \nabla_R \mathbf{u}; \quad \mathbf{F}^{-1} = \mathbf{1} - \mathbf{h}, \quad \mathbf{h} \equiv \nabla \bar{\mathbf{u}}. \tag{2.23}$$

It follows that we have the following *exact* formulas:

$$\mathbf{E} = \frac{1}{2}\left(\mathbf{H} + \mathbf{H}^T + \mathbf{H}^T\mathbf{H}\right), \quad \mathbf{e} = \frac{1}{2}\left(\mathbf{h} + \mathbf{h}^T - \mathbf{h}^T\mathbf{h}\right). \tag{2.24}$$

In *small-strain theory*, for which $\mathbf{H}$ and $\mathbf{h}$ are small in the sense that $|\mathbf{H}| \equiv (\text{trace } \mathbf{H}^T\mathbf{H})^{1/2}$ or $|\mathbf{h}| \equiv (\text{trace } \mathbf{h}^T\mathbf{h})^{1/2}$ is considered as an infinitesimal quantity of the first order, then neglecting terms of second order in the "small" displacement gradients, we obtain the following approximation:

$$\mathbf{E} = \mathbf{e} = \boldsymbol{\varepsilon} = \left(\nabla\mathbf{u}\right)_S \equiv \frac{1}{2}\left(\nabla\mathbf{u} + \left(\nabla\mathbf{u}\right)^T\right), \quad \mathbf{R} - \mathbf{1} = \boldsymbol{\omega} = \left(\nabla\mathbf{u}\right)_A \equiv \frac{1}{2}\left(\nabla\mathbf{u} - \left(\nabla\mathbf{u}\right)^T\right), \tag{2.25}$$

where the subscripts $S$ and $A$ denote the operations of symmetrization and skew (anti)- symmetrization, respectively. The true tensors $\boldsymbol{\varepsilon}$ and $\boldsymbol{\Omega}$ are called the infinitesimal strain and rotation. In Cartesian components in the actual configuration they have components

$$\varepsilon_{ij} = u_{(i,j)} \equiv \frac{1}{2}\left(u_{i,j} + u_{j,i}\right), \quad \omega = u_{[i,j]} \equiv \frac{1}{2}\left(u_{i,j} - u_{j,i}\right), \tag{2.26}$$

where a comma followed by an index $i$ means the partial derivative with respect to the spatial coordinate $x^i$. The reader will have noticed that in this small-strain approximation we no longer distinguish between material and spatial representations. To the same degree of approximation (tr = trace),

$$J_F \cong 1 + \text{tr}\boldsymbol{\varepsilon}, \quad J_F^{-1} \cong 1 - \text{tr}\,\boldsymbol{\varepsilon}. \tag{2.27}$$

QUESTION: Find a unique displacement $\mathbf{u}$ corresponding to a given deformed metric $\mathbf{C}$. Of course, there must exist six so-called *compatibility conditions* in order to extract the three components of $\mathbf{u}$ from the nine components of $\mathbf{C}$ or $\mathbf{E}$. These were originally derived in the nineteenth century by Navier and Saint-Venant in small-strain theory. For finite-strain theory, it is noticed that, in the absence of defects, the material manifold is *flat* (in the sense of Riemannian differential geometry) and must remain so in the course of the deformation. Accordingly, the Riemann curvature associated with $\mathbf{C}$ or $\mathbf{E}$ must always vanish (see, for instance, Maugin, 1993, pp. 54–57, for these developments). In three-dimensional space, which is our concern, the Riemann curvature tensor reduces to the so-called Einstein tensor. For small strains, this tensor, in term of the deformed metric $\boldsymbol{\varepsilon}$, is given by

$$S_{ab} = -\varepsilon_{ajk}\varepsilon_{bli}\varepsilon_{ki,jl}, \tag{2.28}$$

where $\varepsilon_{ijk}$ is the completely skewsymmetric Levi-Civita alternating symbol (equal zero when two indices are alike). The condition $S_{ab} = 0$ is the looked-for compatibility or integrability condition.

### 2.1.5 Convection, Pull Back, and Push Forward

Equation 2.15 gives examples of operations of *convection* of a tensorial object, called *pull back* or *push forward* depending on whether the operation carries a tensorial object from the actual configuration to the reference one, or from the latter to the former. They are tensorial transformations effected with the help of the motion mapping itself since these operations are conducted between two different manifolds. Historically first, but also endowed with a definite relevance in continuum mechanics, is the convection operation introduced by G. Piola, the *Piola transformation*. Let **A** be a vector field in the actual configuration. Then the material contravector defined by

$$\bar{\mathbf{A}} = J_F \mathbf{F}^{-1}\mathbf{A} = \left\{ \bar{A}^K = J_F \left(\mathbf{F}^{-1}\right)^{Ki} A_i \right\}. \tag{2.29}$$

is the *Piola transform* of **A**. Conversely,

$$\mathbf{A} = J_{\bar{F}}^{-1}\mathbf{F}\,\bar{\mathbf{A}} = \left\{ A^i = J_{\bar{F}}^{-1} F_K^i \bar{A}^K \right\}. \tag{2.30}$$

In this connection the reader will note the following two demonstrable identities:

$$\nabla_R \left(J_F \mathbf{F}^{-1}\right) = \mathbf{0}, \quad \nabla\left(J_{\bar{F}}^{-1}\,\mathbf{F}\right) = \mathbf{0}, \tag{2.31}$$

from which there follows that

$$\nabla_R . \bar{\mathbf{A}} = J_F \mathbf{F} . \left(\nabla_R \mathbf{A}\right) = J_F \nabla . \mathbf{A} \,. \tag{2.32}$$

Of course, this reminds us of the formula for the change of elementary volume, $dv$ and $dV$, between the actual and reference configurations:

$$dv = J_F dV,$$

so that

$$\left(\nabla_R . \bar{\mathbf{A}}\right) dV = \left(\nabla . \mathbf{A}\right) dv. \tag{2.33}$$

By the same token it is salient to remind the reader of the so-called Nanson's formula for the change between oriented surface elements $\mathbf{n}ds$ and $\mathbf{N}dS$ of

the same surface with respective unit normals **n** and **N** in the actual and reference configurations:

$$\mathbf{n}\,ds = J_F\,\mathbf{N}.\mathbf{F}^{-1}dS, \quad \mathbf{N}dS = J_F^{-1}\,\mathbf{n}.\mathbf{F}ds. \tag{2.34}$$

If $\sigma$ is a spatial tensor defined per unit area in $K_t$, then we readily check that

$$\mathbf{n}.\sigma ds = \mathbf{N}.\mathbf{T}dS, \tag{2.35}$$

where the two-point tensor field **T** is such that

$$\mathbf{T} = J_F\,\mathbf{F}^{-1}\sigma = \left\{T_i^K = J_F\left(\mathbf{F}^{-1}\right)^{Kj}\sigma_{ji}\right\}, \qquad \sigma = J_F^{-1}\mathbf{F}\mathbf{T}. \tag{2.36}$$

Note that Equation 2.35 still has a foot in the actual configuration (physical space). The object **T** is the Piola transformed of $\sigma$ but on the first index only. Of course, if one takes the material divergence to the left, noted $\mathrm{div}_R$ of **T**, one gets immediately (compare to (2.33)):

$$\mathrm{div}_R\,\mathbf{T} = J_F\mathrm{div}\,\sigma, \tag{2.37}$$

where the symbol $\nabla$ denotes the spatial divergence taken at the left of a tensorial object. Equation 2.37, just like (2.35), still has a foot in the actual configuration.

We have emphasized here the importance of the Piola transformation—compare the remarkable expressions (2.33), (2.35), and (2.37)—because most of this book is concerned with reference configurations while basic physical laws are first expressed in the physical frame (actual configuration; see Section 2.2).

### 2.1.6 Time Derivatives and Rates

Motion, as compared to statics and equilibrium, has to do with the *time* evolution of fields, whereas most of the operations mentioned before had to do with the spatial variation of fields. In this regards the basic notion in continuum mechanics is that of the velocity field. From the two descriptions (2.1) and (2.4) of the motion, we can define the *physical* velocity field **v** in $K_t$ and the *material* velocity field **V** in $K_R$ by

$$\mathbf{v}(\mathbf{X},t) := \left.\frac{\partial\chi}{\partial t}\right|_X, \quad \mathbf{V}(\mathbf{x},t) := \left.\frac{\partial\chi^{-1}}{\partial t}\right|_x, \tag{2.38}$$

where the second should not be mistaken for the right stretch tensor in spite of the notation. Please note the functional dependence indicated in Equation 2.38. We let the reader check by way of exercise the following two important relations between these two velocities:

$$\mathbf{v}+\mathbf{FV}=\mathbf{0},\quad \mathbf{V}+\mathbf{F}^{-1}\mathbf{v}=\mathbf{0}. \tag{2.39}$$

The derivatives used in (2.38) are called the material (or Lagrangian) time derivative and the spatial (Eulerian) time derivative since, depending on the case, they are taken at fixed material coordinates (particle) or fixed spatial coordinates. We clearly have the following operational definitions (prove these by way of exercise)

$$\left.\frac{\partial}{\partial t}\right|_{X\,\text{fixed}}=\left.\frac{\partial}{\partial t}\right|_{x\,\text{fixed}}+\mathbf{v}.\nabla,\quad \left.\frac{\partial}{\partial t}\right|_{x\,\text{fixed}}=\left.\frac{\partial}{\partial t}\right|_{X\,\text{fixed}}+\mathbf{V}.\nabla_R, \tag{2.40}$$

since we verify with (2.39) that

$$\mathbf{v}.\nabla=-\mathbf{V}.\nabla_R. \tag{2.41}$$

### 2.1.7 Rate of Deformation

This is now a pure question of computation given the basic definitions of the deformation field. First of all, we check that

$$\left.\frac{\partial \mathbf{F}}{\partial t}\right|_X=\left(\nabla_R\mathbf{v}\right)^T,\quad \left.\frac{\partial \mathbf{F}^{-1}}{\partial t}\right|_x=\left(\nabla\mathbf{V}\right)^T. \tag{2.42}$$

These are but compatibility conditions between second-order space–time derivatives. But this can also be written as

$$\left.\frac{\partial \mathbf{F}}{\partial t}\right|_X=\mathbf{LF},\quad \left.\frac{\partial \mathbf{F}^{-1}}{\partial t}\right|_x=\mathbf{M}.\mathbf{F}^{-1}, \tag{2.43}$$

where we defined the spatial and material rates, **L** and **M**, by

$$\mathbf{L}=\left(\nabla\mathbf{v}\right)^T,\quad \mathbf{M}=\left(\nabla_R\mathbf{V}\right)^T, \tag{2.44}$$

since

$$\nabla_R=\mathbf{F}^T\nabla,\quad \nabla=\mathbf{F}^{-T}\nabla_R. \tag{2.45}$$

We also have

$$\mathbf{L}=\dot{\mathbf{F}}\mathbf{F}^{-1},\quad \mathbf{M}=\left.\frac{\partial \mathbf{F}^{-1}}{\partial t}\right|_x\mathbf{F}, \tag{2.46}$$

where a superimposed dot is used as an alternate notation for the material time derivative. The symmetric and skewsymmetric parts of **L** are the *strain rate* (spatial) *tensor* and *rotation rate* (or vorticity) *tensor*, respectively, that is,

$$\mathbf{D} = \mathbf{L}_S = \frac{1}{2}\Big(\big(\nabla\mathbf{v}\big)^T + \nabla\mathbf{v}\Big), \quad \Omega = \mathbf{L}_A = \frac{1}{2}\Big(\big(\nabla\mathbf{v}\big)^T - \nabla\mathbf{v}\Big). \tag{2.47}$$

We could also define strain rates and rotation rates in material space. The denomination of **D** comes from the fact that a simple calculation yields

$$\mathbf{D} = \mathbf{F}^{-T}\dot{\mathbf{E}}\mathbf{F}^{-1}, \quad \dot{\mathbf{E}} = \mathbf{F}^T\mathbf{D}\mathbf{F}. \tag{2.48}$$

The following formulas are easily established:

$$\left.\frac{\partial J_F}{\partial t}\right|_X = J_F \mathrm{tr}\,\mathbf{L} = J_F\big(\nabla.\mathbf{v}\big), \quad \left.\frac{\partial\big(dv\big)}{\partial t}\right|_X = \big(\nabla.\mathbf{v}\big)dv, \tag{2.49}$$

since tr **L** = tr **D** = ∇.**v** and $\partial(dV)/\partial t\big|_X = 0$.

### 2.1.8 Rigid-Body Motions

This special class of motions is defined in geometry by Killing's equations for isometries (conservation of a metric in time), here, for instance,

$$\left.\frac{\partial\mathbf{E}\big(\mathbf{X},t\big)}{\partial t}\right|_X = \mathbf{0}. \tag{2.50}$$

For nonzero **F**, this is equivalent to the spatial expression

$$\mathbf{D}\big(\mathbf{x},t\big) = \mathbf{0}, \tag{2.51}$$

at all times *t*. The integral in space of this partial differential equation is shown to read (cf. Maugin, 1988, pp. 78–79)

$$\mathbf{v} = \Omega^* * \mathbf{x} + \mathbf{v}^*, \quad \nabla\Omega^* = \mathbf{0}, \quad \nabla\mathbf{v}^* = \mathbf{0}, \tag{2.52}$$

where Ω* is a skewsymmetric space-independent tensor (rotation rate) and **v*** is a space-independent velocity field, such that

$$\Omega^{*T} = \left(\frac{d\mathbf{P}}{dt}\right)^T \mathbf{P} = -\Omega^*, \quad \mathbf{v}^* = \frac{d\mathbf{a}^*}{dt} \tag{2.53}$$

after the space-to-space mapping

$$\mathbf{x} = \mathbf{P}^T(t)\mathbf{x}^* + \mathbf{a}(t), \tag{2.54}$$

where $\mathbf{P}(t) \in O(3)$ is a spatially uniform finite rotation, $\mathbf{x}^*$ is the position of a particular point in the material body in the reference frame, $\mathbf{a}(t)$ is a spatially uniform time-dependent vector, and $\mathbf{x}$ is the position of points of the solid in $R$. Equation 2.54 also represents a rigid change of frames in Newtonian mechanics, hence the use of rigid-body motions to define yardsticks for distance measurements in Newtonian–Galilean mechanics.

**REMARK 2.1:** In the case of a *deformable* body, quite similar to the first of (2.54), we would show that

$$\Omega = \left.\frac{\partial \mathbf{R}}{\partial t}\right|_X \mathbf{R}^T = -\Omega^T, \tag{2.55}$$

where $\mathbf{R}$ is the finite rotation involved in the polar decomposition (2.17).

**REMARK 2.2:** It is interesting to compute the material time derivative of a quantity defined by means of the Piola transformation. For instance, starting from (2.29), we let the reader show that

$$\left.\frac{\partial \bar{\mathbf{A}}}{\partial t}\right|_X = J_F \mathbf{F}^{-1}(\mathbf{A})^*,$$

where $(\mathbf{A})^*$ is the so-called *convected time derivative* of $\mathbf{A}$ given by

$$(\mathbf{A})^* := \dot{\mathbf{A}} + (\nabla \mathbf{A}).\mathbf{v} - \mathbf{A}(\nabla.\mathbf{v}) = \left.\frac{\partial \mathbf{A}}{\partial t}\right|_x + \nabla \times (\mathbf{A} \times \mathbf{v}) + \mathbf{v}(\nabla.\mathbf{A}). \tag{2.56}$$

This leads us to the question of so-called *objectivity* or *material-frame indifference*. A geometric object is said to be *objective* if it transforms *tensorially* with respect to changes of spatial frames (cf. (2.54)), that is, by purely spatial, spatially uniform rotations $Q(t)$, such that $\mathbf{Q}^T = \mathbf{Q}^{-1}$, $\det \mathbf{Q} = +1$. For instance, the rate of strain $\mathbf{D}$ is objective, while the velocity $\mathbf{v}$ itself and the vorticity are not objective**.** If a spatial vector field $\mathbf{A}$ is objective, then this is not the case of its material time derivative. However, we let the reader show that the convective time derivative defined by (2.56) is an objective field, hence the importance of this derivative in many problems of rheology (and electrodynamics of continua; cf. Eringen and Maugin, 1990), where constitutive equations in terms of velocities of fields are required to be

objective, a natural requirement for the description of matter properties independently of the observer. The perspicacious geometer will notice the close relationship of the derivative defined in (2.56) with the so-called *Lie derivative*, of which the left-hand side of Equation 2.56 may be the definition. Another useful objective time derivative is the so-called *corotational* or *Jaumann* derivative. Let $\mathbf{A}$ be a spatial vector field. Then its Jaumann derivative is defined by

$$D_J \mathbf{A} = \dot{\mathbf{A}} - \Omega \mathbf{A}, \tag{2.57}$$

where $\Omega$ is the vorticity tensor.

***EXERCISE:*** Prove the objectivity of the field $D_J\mathbf{A}$. As a matter of fact, define the following material vector by means of a *transport by rotation* (instead of standard pull back), $\tilde{\mathbf{A}} = \mathbf{R}^T\mathbf{A}$ and prove that

$$D_J \mathbf{A} = \mathbf{R}^{-T}\left( \left. \frac{\partial \tilde{\mathbf{A}}}{\partial t} \right|_X \right). \tag{2.58}$$

Generalization of the definition of convective and Jaumann derivatives to tensors of any order is straightforward.

**REMARK 2.3:** In the small-strain theory where the superimposed dot may be used for any of the two time derivatives defined in (2.40), we have the following reductions:

$$\mathbf{L} = \dot{\mathbf{F}} = \dot{\mathbf{H}} \quad \text{or} \quad v_{i,j} = \dot{u}_{i,j}, \tag{2.59}$$

$$\mathbf{D} = \dot{\varepsilon} \quad \text{or} \quad D_{ij} = \dot{\varepsilon}_{ij} = \dot{u}_{(i,j)}, \tag{2.60}$$

$$\Omega = \dot{\omega} \quad \text{or} \quad \Omega_{ij} = \dot{\omega}_{ij} = \dot{u}_{[i,j]}. \tag{2.61}$$

Of interest for future developments is also the approximation of an infinitesimally small rotation, as we can write in the first approximation (compare to the second of (2.25)):

$$\mathbf{P} = 1 + \eta\omega, \tag{2.62}$$

where $\eta$ is an infinitesimal parameter and $\omega = -\omega^T$ is finite. Equation 2.62 introduces the notion of infinitesimal generator of the rotation (orthogonal) group $O(3)$.

**REMARK 2.4:** The preceding introduction to the motion and kinematics of continua is necessary and sufficient for the purpose of this book. Of course, there exist more rigorous geometric approaches involving abstract manifolds, tangent spaces, fiber bundles, and so on. In this line we recommend the now-classic book by Marsden and Hughes (1975), as well as Ciarlet's (1988) book. But these are not really permeated by the true spirit of continuum mechanics. Along the present line we recommend the books of Eringen (1980) and Ogden (1984), with which we fully agree, and, of course, the classical treatises of Truesdell and Toupin (1960) and Truesdell and Noll (1965), the textbooks by Spencer (1976) and Chadwick (1976), the series *Continuum Physics* edited by Eringen (1971–1976), and our own books (Maugin, 1988, 1993) and Eringen and Maugin (1990).

## 2.2 Basic Thermomechanics of Continua

### 2.2.1 Balance Laws

It has become an established tradition in modern continuum physics to introduce the basic balance laws of continuum mechanics and thermodynamics in *global* form, that is, for a *whole* deformable body $B$. This applies even to Maxwell's equations in the electrodynamics of continua (cf. Eringen and Maugin, 1990). This can be achieved in two different formalisms—which are not fully independent of one another—whether the postulate of these balance laws is made in the actual configuration $K_t$ or on the material manifold (configuration $K_R$). To that purpose we note $B_R$ and $\partial B_R$ the open, simply connected region occupied by the body in $K_R$ and its regular boundary (in principle without edges and apices) with uniquely defined unit outward-pointing normal $\mathbf{N}$, and $B_t$ and $\partial Bt$, the image of these in the actual configuration, with uniquely defined outward-pointing normal $\mathbf{n}$, it being understood that the body still is simply connected in this configuration; that is, no holes have formed during the deformation mapping. The material bodies considered in this section are classical continua exhibiting no visible evolving microstructure, and they are acted on at most by body forces and surface forces. From the thermodynamic viewpoint, they may conduct heat and dissipate energy. They may also present body sources of energy and admit a flux of energy at their boundaries. They are submitted to the first and second laws of thermodynamics. We are thus led to introducing the following quantities:

- The mass density $\rho(\mathbf{x}, t)$ in $K_t$ and $\rho_0(\mathbf{X}, t)$ in $K_R$
- The body force $\mathbf{f}(\mathbf{x}, t)$ per unit mass in $K_t$
- An applied traction $\mathbf{T}^d(\mathbf{x}, t;\mathbf{n})$ at $\partial B_t$

- An internal energy $e$ per unit mass in $K_t$
- A body source of energy $h(\mathbf{x}, t)$ per unit mass in $K_t$
- An energy influx $q(\mathbf{x}, t; \mathbf{n})$ at $\partial B_t$
- An entropy $\eta$ per unit mass in $K_t$
- A body source of entropy $\hat{\eta}$ per unit mass in $K_t$
- An entropy influx $s(\mathbf{x}, t; \mathbf{n})$ at $K_t$
- An internal source of entropy $\tilde{\eta}$ per unit mass in $B_t$

Exchanging no mass with its exterior and with no mass being created internally in this modeling, the material body is endowed with an invariant mass measure $dm$, such that

$$dm = \rho dv = \rho_0 dV = \text{const.} \tag{2.63}$$

Then the following global balance laws hold true in the actual configuration.

- *Balance of mass*:

$$\frac{d}{dt}\int_{B_t} dm = 0 \tag{2.64}$$

- *Balance of linear (physical) momentum*:

$$\frac{d}{dt}\int_{B_t} \mathbf{v} dm = \int_{B_R} \mathbf{f} dm + \int_{\partial B_t} \mathbf{T}^d da \tag{2.65}$$

- *Balance of angular (physical) momentum*:

$$\frac{d}{dt}\int_{B_t} \mathbf{x} \times \mathbf{v} dm = \int_{B_t} \mathbf{x} \times \mathbf{f} dm + \int_{\partial B_t} \mathbf{x} \times \mathbf{T}^d da \tag{2.66}$$

- *First law of thermodynamics*:

$$\frac{d}{dt}\int_{B_t} \left(H^t/\rho\right) dm = P_{\text{ext}}\left(B_t\right) + \int_{B_t} h dm - \int_{\partial B_t} q da \tag{2.67}$$

- *Balance of entropy*:

$$\frac{d}{dt}\int_{B_t} \eta dm - \int_{B_t} \hat{\eta} dm + \int_{\partial B_t} s da = \int_{B_t} \tilde{\eta} dm \tag{2.68}$$

- *Second law of thermodynamics*:

$$\int_{B_t} \tilde{\eta} dm \geq 0 \tag{2.69}$$

Here we have defined the energy per unit volume or Hamiltonian density, the kinetic energy $E^t$, and the power expanded by external source $P_{\text{ext}}$ by

$$H^t = K^t + E^t, \quad K^t = \frac{1}{2}\rho(\mathbf{x},t)\mathbf{v}^2, \quad E^t = \rho e, \tag{2.70}$$

and

$$P_{\text{ext}}(B_t) = \int_{B_t} \mathbf{f}.\mathbf{v}dm + \int_{\partial B_t} \mathbf{T}^d.\mathbf{v}da. \tag{2.71}$$

Note that the balance law (2.66) contains no new notion; for example, there is no applied couple per unit volume in this modeling. The elementary surface area has been noted *da*.

Following a celebrated principle of Cauchy (cf. Truesdell and Toupin, 1960), the surface data ($\mathbf{T}^d$, $q$, $s$) are linear affine in the unit normal $\mathbf{n}$. Accordingly, we can write

$$\mathbf{T}^d(\mathbf{x},t;\mathbf{n}) = \mathbf{n}.\sigma, \quad q(\mathbf{x},t;\mathbf{n}) = \mathbf{q}.\mathbf{n}, \quad s(\mathbf{x},t;\mathbf{n}) = \mathbf{n}.\mathbf{s}, \tag{2.72}$$

where the second-order (spatial) tensor $\sigma$ is called the *Cauchy stress*, $\mathbf{q}$ is the (spatial) *heat* (in)*flux vector*, and $\mathbf{s}$ is the (spatial) *entropy* (in)*flux vector*. Equation 2.72 means that the "internal forces" introduced and their thermal analogs depend at most on the first-order description of the geometry of the limiting surface. This applies to any facet cut in the body. Accordingly, we are not considering here any generalized continuum mechanics (which call for the notions of hyperstresses, couple stresses, etc.).

In like manner, global balance laws can be postulated for material domains over *M*. To that purpose, we introduce the Piola transformation of several thermomechanical fields (stresses, heat flux, and entropy flux):

$$\mathbf{T} = J_F\mathbf{F}^{-1}\sigma, \quad \mathbf{Q} = J_F\mathbf{F}^{-1}\mathbf{q}, \quad \mathbf{S} = J_F\mathbf{F}^{-1}\mathbf{s}. \tag{2.73}$$

The first of these defines the *first Piola–Kirchhoff stress*. The transformation is performed only on the first index, so that the transformation is only partial, yielding a two-point tensor field and *not* a tensor in the classical sense. The second and third parts of (2.73) define the *material* heat and entropy fluxes. Then the postulate of the basic balance laws of thermomechanics in the Piola–Kirchhoff form is given by the following set of equations:

$$\frac{d}{dt}\int_{B_R} dm = 0, \tag{2.74}$$

$$\frac{d}{dt}\int_{B_R} \mathbf{p}_R dV = \int_{B_t} \rho_0 \mathbf{f} dV + \int_{\partial B_R} \mathbf{N}.\mathbf{T}dA, \tag{2.75}$$

$$\frac{d}{dt}\int_{B_R} H_R dV = \int_{B_R} \rho_0\left(h + \mathbf{f}.\mathbf{v}\right)dV - \int_{\partial B_R} \mathbf{N}.\left(\mathbf{Q} - \mathbf{T}.\mathbf{v}\right)dA, \tag{2.76}$$

$$\frac{d}{dt}\int_{B_R} S_R dV - \int_{B_R} \rho_0 \hat{\eta} dV + \int_{\partial B_R} \mathbf{N}.\mathbf{S} dA = \int_{B_R} \rho_0 \tilde{\eta} dV \geq 0. \tag{2.77}$$

Here we have not recalled the balance of angular momentum, which is a secondary notion, and we have defined a few new quantities by

$$\begin{aligned} &\mathbf{p}_R = \rho_0 \mathbf{v}, \quad \mathbf{p}^t = \rho \mathbf{v} = J_F^{-1}\mathbf{p}_R, \quad H_R = K^R + E^R, \\ &K^R = \frac{1}{2}\rho_0 \mathbf{v}^2, \quad E^R = \rho_0 e, \quad S_R = \rho_0 \eta. \end{aligned} \tag{2.78}$$

Because of the invariance of $dm$ and the fact that $dV$ and $B_R$ are material, it is immediately checked that we have the following obvious results for any $P$:

$$\frac{d}{dt}\int_{B_t} P dm = \int_{B_t} \frac{dP}{dt} dm, \quad \frac{d}{dt}\int_{B_R} P dV = \int_{B_R} \left.\frac{\partial P}{\partial t}\right|_X dV. \tag{2.79}$$

### 2.2.2 Cauchy Format of the Local Balance Laws of Thermomechanics

On using the first of (2.79), the divergence theorem, where it applies and enforcing the basic working continuity hypothesis of continuum physics according to which the final integrands must vanish for any spatial volume element and surface element, we obtain the following local balance laws from (2.64) through (2.69):

- *Balance of mass, also called the continuity equation*:

$$\dot{\rho} + \rho\left(\nabla.\mathbf{v}\right) = \left.\frac{\partial \rho}{\partial t}\right|_x + \nabla.\left(\mathbf{p}^t\right) = 0, \quad \mathbf{p}^t := \rho \mathbf{v} \tag{2.80}$$

- *Balance of linear (physical) momentum*:

$$\rho \dot{\mathbf{v}} - \mathrm{div}\sigma = \rho \mathbf{f} \tag{2.81a}$$

or

$$\left.\frac{\partial}{\partial t}\mathbf{p}^t\right|_x + \nabla.\left(\mathbf{p}^t \otimes \mathbf{v} - \sigma\right) = \rho \mathbf{f} \tag{2.81b}$$

- *Balance of angular (physical) momentum*:

$$\sigma = \sigma^T, \quad \text{i.e.,} \quad \sigma_{ij} = \sigma_{ji} \quad \text{or} \quad \sigma_{[ij]} = 0 \tag{2.82}$$

- *First law of thermodynamics*:

$$\rho \frac{d}{dt}\left(H^t/\rho\right) - \nabla.\left(\sigma.\mathbf{v} - \mathbf{q}\right) = \rho\left(h + \mathbf{f}.\mathbf{v}\right) \tag{2.83a}$$

or

$$\frac{\partial}{\partial t} H^t \Big|_x + \nabla.\left(\mathbf{p}^t \left(H^t/\rho\right) - \sigma.\mathbf{v} + \mathbf{q}\right) = \rho\left(h + \mathbf{f}.\mathbf{v}\right) \tag{2.83b}$$

- *Balance of entropy*:

$$\rho \frac{d}{dt}\left(S^t/\rho\right) + \nabla.\left(\rho\hat{\eta}\right) - \rho s = \rho\tilde{\eta} \tag{2.84a}$$

or

$$\frac{\partial}{\partial t} S^t \Big|_x + \nabla.\left(\mathbf{p}^t \eta - \mathbf{s}\right) - \rho s = \rho\tilde{\eta} \tag{2.84b}$$

- *Second law of thermodynamics*:

$$\rho\tilde{\eta} \geq 0. \tag{2.85}$$

Equation 2.82 means that the Cauchy stress is symmetric in the absence of microstructure and body couple. Equations 2.80, 2.81b, 2.83b, and 2.84b take the form of strict conservation laws in the spatial framework in the absence of any source.

### 2.2.3 Piola–Kirchhoff Format of the Local Balance Laws of Thermomechanics

In full parallelism with what was done for the Cauchy format, on using the second of (2.79), the material divergence theorem, where it applies and enforcing the basic working hypothesis of continuum physics according to which the final integrands must vanish for any material volume element

and surface element, we obtain the following local balance laws from (2.74) through (2.77):

- *Balance of mass, also called the continuity equation*:

$$\frac{\partial}{\partial t}\rho_0\Big|_X = 0 \tag{2.86}$$

- *Balance of linear (physical) momentum*:

$$\frac{\partial}{\partial t}\mathbf{p}_R\Big|_X - \mathrm{div}_R\mathbf{T} = \rho_0\mathbf{f} \tag{2.87}$$

- *Balance of angular (physical) momentum*:

$$\mathbf{FT} = \mathbf{T}^T\mathbf{F}^T \tag{2.88}$$

- *First law of thermodynamics*:

$$\frac{\partial}{\partial t}H_R\Big|_X - \nabla_R.\left(\mathbf{T}.\mathbf{v} - \mathbf{Q}\right) = \rho_0\mathbf{f}.\mathbf{v} \tag{2.89}$$

- *Balance of entropy*:

$$\frac{\partial}{\partial t}S_R\Big|_X + \nabla_R.\mathbf{S} - \rho_0\hat{\eta} = \Sigma_R := \rho_0\tilde{\eta} \tag{2.90}$$

- *Second law of thermodynamics*:

$$\Sigma_R \geq 0 \tag{2.91}$$

These equations are not independent of those deduced previously in the spatial frame. In particular, (2.88) is just a rewriting of (2.82) in the material framework. As for (2.87)—which still has components in physical space—it is readily shown to follow from (2.81) by multiplying the latter by $J_F$ and exploiting (2.9) and (2.31). Again, Equations 2.86, 2.87, 2.89, and 2.90 take the form of strict conservation laws in the material formalism ($\mathbf{X}$, $t$) in the absence of source terms. However, sometimes these equations are referred to as material equations, as compared to the spatial equations deduced in the Cauchy format. This is a misnomer because only the space–time parametrization and partial derivatives here refer to this framework while both Equations 2.87 and 2.88 still have components in the physical framework

(actual configuration $K_t$). We shall see in other chapters how one constructs equations that are completely in the material framework, in terms of both tensorial objects and space–time parametrization.

### 2.2.4 Thermodynamic Hypotheses

We denote by $\theta > 0$, *inf* $\theta = 0$, the thermodynamic temperature. Such a notion, as well as that of entropy, is well defined only in thermostatics (see my book on thermodynamics, Maugin, 1999), where $\theta$ is given by

$$\theta = \frac{\partial \bar{e}(.,\eta)}{\partial \eta} > 0, \quad e = \bar{e}(.,\eta), \tag{2.92}$$

where the missing argument may be any other variable of state such as strain in thermoelasticity. It is traditional to introduce another thermodynamic function, the *Helmholtz free energy* $\psi$, by the following Legendre transformation:

$$e + (-\psi) = \eta\theta, \quad \eta = \frac{\partial(-\psi)}{\partial\theta} = -\frac{\partial\,\psi}{\partial\theta}. \tag{2.93}$$

The first of these equations places $e$ and $\psi$ in *duality* in the sense of convex analysis (see Maugin, 1992). Since the Legendre transformation conserves convexity, if, as it should be, the internal energy $e$ is *convex* in $\eta$, then the free energy $\psi$ is *concave* in $\theta$, so that the specific heat $C_\theta$ is always positive:

$$C_\theta = -\theta\frac{\partial^2\psi}{\partial\theta^2} > 0. \tag{2.94}$$

Modern thermodynamics, in the manner of Coleman and Noll (cf. Truesdell and Noll, 1965), assumes that the notions of temperature and entropy are still defined in true thermo*dynamics*, that is, outside thermodynamic equilibrium. We shall assume the same as well as the fact that heat body source and heat flux and entropy body source and entropy flux are related by

$$\hat{\eta} = h/\theta, \quad \mathbf{s} = \mathbf{q}/\theta, \quad \mathbf{S} = \mathbf{Q}/\theta. \tag{2.95}$$

If necessary, the last two can be relaxed by considering more general expressions such as

$$\mathbf{s} = \frac{\mathbf{q}}{\theta} + \mathbf{k}, \quad \mathbf{S} = \frac{\mathbf{Q}}{\theta} + \mathbf{K}, \tag{2.96}$$

where **k** and **K** are so-called *extra fluxes of entropy*, in the spatial and material descriptions, respectively. These vanish most of the time, but there are exceptions (e.g., in fluid mixtures).

### 2.2.5 General Thermomechanical Theorems

We apply the working hypotheses enunciated in the preceding. Then we can establish the following theorems.

- *Kinetic energy theorem*: On taking the inner product of (2.81a) with **v**, we obtain that

$$\rho\frac{d\left(K^t/\rho\right)}{dt}-\nabla.\left(\sigma.\mathbf{v}\right)+\mathrm{tr}\left(\sigma.\left(\nabla\mathbf{v}\right)^T\right)=\rho\mathbf{f}.\mathbf{v}. \tag{2.97}$$

- *Internal energy theorem*: On expanding (2.84a) and combining with (2.97) we obtain that

$$\rho\frac{d\left(E^t/\rho\right)}{dt}-\mathrm{tr}\left(\sigma.\left(\nabla\mathbf{v}\right)^T\right)+\nabla.\mathbf{q}=\rho h. \tag{2.98}$$

- *Clausius–Duhem inequality*: Combining now (2.98), (2.84a), and (2.85) and introducing the free energy density $\psi = e - \eta\theta$, we obtain the following inequality:

$$-\rho\left(\dot{\psi}+\eta\dot{\theta}\right)+\mathrm{tr}\left(\sigma.\left(\nabla\mathbf{v}\right)^T\right)-\left(\mathbf{q}/\theta\right).\nabla\theta=\rho\theta\tilde{\eta}\geq 0, \tag{2.99}$$

while (2.98) takes also the alternate form

$$\rho\theta\dot{\eta}+\nabla.\mathbf{s}=\rho h+\rho\theta\tilde{\eta}. \tag{2.100}$$

Because of the symmetry of $\sigma$, we have here

$$\mathrm{tr}\left(\sigma.\left(\nabla\mathbf{v}\right)^T\right)\equiv\mathrm{tr}\left(\sigma.\mathbf{D}\right).$$

Ultimately, Equation 2.100 is the equation that will govern the temperature field.
In direct parallelism with these spatial equations, it is easy to establish the following equations in the *Piola–Kirchhoff* form:

- *Kinetic energy theorem*:

$$\left.\frac{\partial K_R}{\partial t}\right|_X-\nabla_R.\left(\mathbf{T}.\mathbf{v}\right)+\mathrm{tr}\left(\mathbf{T}.\left(\nabla_R\mathbf{v}\right)^T\right)=\rho_0\mathbf{f}.\mathbf{v} \tag{2.101}$$

- *Internal energy theorem*:

$$\left.\frac{\partial E_R}{\partial t}\right|_X - \mathrm{tr}\left(\mathbf{T}.\left(\nabla_R \mathbf{v}\right)^T\right) + \nabla_R.\mathbf{Q} = \rho_0 h \tag{2.102}$$

- *Clausius–Duhem inequality*:

$$\theta\Sigma_R = -\left(\dot{W} + S\dot{\theta}\right) + \mathrm{tr}\left(\mathbf{T}.\left(\nabla_R \mathbf{v}\right)^T\right) - \left(\mathbf{Q}/\theta\right)\nabla_R\theta \geq 0, \tag{2.103}$$

  where we introduced the free energy $W = E^t - S\theta$, per unit volume in the reference configuration.

- *Heat propagation equation*:

$$\theta\dot{S} + \nabla_R.\mathbf{S} = \rho_0 h + \theta\Sigma_R \tag{2.104}$$

**REMARK 2.5:** Had we kept the possibility of considering a nonzero extra entropy flux K, then the last two equations would be replaced by the following ones:

$$\theta\Sigma_R = -\left(\dot{W} + S\dot{\theta}\right) + \mathrm{tr}\left(\mathbf{T}.\left(\nabla_R \mathbf{v}\right)^T\right) + \nabla_R.\left(\theta\mathbf{K}\right) - \mathbf{S}.\nabla_R\theta \geq 0 \tag{2.105}$$

and

$$\theta\dot{S} + \nabla_R.\mathbf{S} = \rho_0 h + \theta\Sigma_R. \tag{2.106}$$

Equations 2.103 and 2.105 essentially mean that **S**, whatever its detailed form, is always the thermodynamic dual of the gradient of temperature.

**REMARK 2.6:** We already noticed that $e$ and $-\psi$ are dual to one another as regards Legendre transformations. But other, more general quantities are associated in the same way. In particular, this remark applies to the Hamiltonian and so-called Lagrangian densities (as usually conceived in analytical mechanics). As a matter of fact, as we shall find in some subsequent chapters, it may be of interest to consider the Hamiltonian built from the kinetic energy and the internal energy, while we may consider a Lagrangian built as the difference between a kinetic energy and a kind of potential energy—a most usual definition—but the latter may be the free energy. Accordingly, considering the material framework for the sake of example, we can write

$$H_R = K^R + E^R, \quad L_R = K^R - W^R, \tag{2.107}$$

We let the reader check that the Hamiltonian $H_R$ per unit volume in the reference configuration and the Lagrangian $L_R$ are related by

$$L_R = (\mathbf{p}_R.\mathbf{v} + S\theta) - H_R \quad \text{or} \quad H_R = (\mathbf{p}_R.\mathbf{v} + S\theta) - L_R, \tag{2.108}$$

with

$$\mathbf{p}_R = \frac{\partial L_R}{\partial \mathbf{v}}, \quad \mathbf{v} = \frac{\partial H_R}{\partial \mathbf{p}_R}; \quad S = \frac{\partial L_R}{\partial \theta}, \quad \theta = \frac{\partial H_R}{\partial S},$$

in agreement with the rules of analytical mechanics applied to a continuum. That is, Equation 2.108 represents a double Legendre transformation concerning simultaneously thermal processes and the dynamics of continua.

**REMARK 2.7:** The principle of virtual power

Consider Equation 2.81a and take its inner product by a vector field $\mathbf{v}^*$—with the dimension of a velocity field. On applying the divergence theorem and integrating, where fitted, over the volume $B_t$ or the surface $\partial B_t$, and accounting for the *natural boundary condition* $\mathbf{T}^d = \mathbf{n}.\sigma$, we obtain the following global expression that is referred to as the statement of the principle of virtual power:

$$P_{\text{inertia}}^*(B_t) = P_{\text{ext}}^*(B_t, \partial B_t) + P_{\text{int}}^*(B_t), \tag{2.109}$$

where we have defined the virtual power of inertial forces, of externally applied forces, and so-called "internal forces" (here stresses) by

$$P_{\text{inertia}}^*(B_t) = \int_{B_t} \mathbf{p}^t.\mathbf{v}^* \, dv, \tag{2.110}$$

$$P_{\text{ext}}^*(B_t, \partial B_t) = \int_{B_t} \rho \mathbf{f}.\mathbf{v}^* \, dv + \int_{\partial B_t} \mathbf{T}^d.\mathbf{v}^* \, da, \tag{2.111}$$

$$P_{\text{int}}^*(B_t) = -\int_{B_t} \text{tr}\left(\sigma.(\nabla \mathbf{v}^*)^T\right) dv = -\int_{B_t} \text{tr}(\sigma.\mathbf{D}^*) dv. \tag{2.112}$$

It is immediately noticed that the expressions in (2.110) and (2.111) are linear (continuous) functionals over the virtual velocity field $\mathbf{v}^*$, while (2.112) is a linear (continuous) functional over the spatial gradient of $\mathbf{v}^*$, or rather its

symmetric part $\mathbf{D}^*: = (\nabla \mathbf{v}^*)_s$, by virtue of the symmetry of the stress (in this case). For a special case for which $\mathbf{v}^*$ is none other than the actual (physical) velocity field $\mathbf{v}$, then (2.109) yields the global form of the kinetic energy theorem (cf. (2.97)):

$$\frac{d}{dt}\int_{B_t}\left(K^t\right)dv = P_{\text{ext}}\left(B_t, \partial B_t\right) + P_{\text{int}}\left(B_t\right). \tag{2.113}$$

Combining this with the global statement in (2.67), we shall obtain a global statement of the *internal energy theorem*. We can proceed along this line. Accordingly, this shows that instead of the global statements of the balance of linear and angular momenta, we may as well consider Equation 2.109 as an a priori statement in which the virtual power of internal forces (stresses) accounts for the objectivity of the stress tensor, hence the writing as a linear continuous functional over $\mathbf{D}^*$, an objective tensor, as is easily shown. This basic formulation of continuum thermomechanics is in the tradition of d'Alembert (notice the affiliation of the author) and presents the advantage of easy generalization to the case of generalized continuum mechanics by enlarging a priori the field of virtual velocities in agreement with the degree of fineness selected for the generalized velocity fields (see Maugin, 1980). Furthermore, it is already in the form of interest for the application of certain numerical schemes (e.g., finite elements) since $\mathbf{v}^*$ is none other than a test function in the appropriate functional space. Of course, a parallel formulation exists in the Piola–Kirchhoff formulation for which we would write

$$P_{\text{inertia}}{}^*\left(B_R\right) = P_{\text{ext}}{}^*\left(B_R, \partial B_R\right) + P_{\text{int}}{}^*\left(B_R\right), \tag{2.114}$$

wherein

$$P_{\text{inertia}}{}^*\left(B_R\right) = \int_{B_R} \mathbf{p}_R.\mathbf{v}^* dV, \tag{2.115}$$

$$P_{\text{ext}}{}^*\left(B_R, \partial B_R\right) = \int_{B_R} \rho_0 \mathbf{f}.\mathbf{v}^* dV + \int_{\partial B_R} \mathbf{T}_R^d.\mathbf{v}^* dA, \tag{2.116}$$

$$P_{\text{int}}{}^*\left(B_R\right) = -\int_{B_R} \text{tr}\left(\mathbf{T}.\left(\nabla_R \mathbf{v}^*\right)^T\right) dV. \tag{2.117}$$

Note here that because the Piola–Kirchhoff formulation is *not* completely material, the virtual velocity field $\mathbf{v}^*$ still is in the actual configuration.

Furthermore, this is also true of the body force **f** and the surface traction $\mathbf{T}_R^d$ that is related to the traction $\mathbf{T}^d$ via the change of area elements,

$$\mathbf{N}.\mathbf{T} = \mathbf{T}_R^d = \left(da/dA\right)\mathbf{T}^d,$$

with (cf. Truesdell and Toupin, 1960)

$$\frac{da}{dA} = J_F\left(\mathbf{N}.\mathbf{C}^{-1}.\mathbf{N}\right)^{1/2}.$$

## 2.3 Examples of Thermomechanical Behaviors

### 2.3.1 Thermoelastic Conductors

Apart from pure elasticity, this is the simplest thermomechanical behavior for deformable solids. It is simpler to present the derivation of the corresponding constitutive equations in the Piola–Kirchhoff formulation, for which the local form of the second law of thermodynamics takes on the form of (2.100), that is,

$$\theta\Sigma_R = -\left(\dot{W} + S\dot{\theta}\right) + \mathrm{tr}\left(\mathbf{T}.\left(\nabla_R\mathbf{v}\right)^T\right) - \left(\mathbf{Q}/\theta\right)\nabla_R\theta \geq 0. \tag{2.118}$$

The observable variables of state in this case are the deformation gradient **F** and temperature θ, so that we a priori write the following functional dependence for the thermodynamic dependent variables:

$$\mathbf{T} = \bar{\mathbf{T}}\left(\mathbf{F},\theta,\nabla_R\theta\right), \quad \mathbf{Q} = \bar{\mathbf{Q}}\left(\mathbf{F},\theta,\nabla_R\theta\right), \quad W = \bar{W}\left(\mathbf{F},\theta,\nabla_R\theta\right), \quad S = \bar{S}\left(\mathbf{F},\theta,\nabla_R\theta\right), \tag{2.219}$$

The same functional dependency is assumed just as a precautionary measure. Of course, computing the material time derivative of *W*, we have

$$\dot{W} = \mathrm{tr}\left(\frac{\partial\bar{W}}{\partial\mathbf{F}}.\left(\nabla_R\mathbf{v}\right)^T\right) + \frac{\partial\bar{W}}{\partial\theta}\dot{\theta} + \frac{\partial\bar{W}}{\partial\left(\nabla_R\theta\right)}.\nabla_R\dot{\theta}, \tag{2.120}$$

where we took advantage of the first of (2.42). On substituting this into the inequality (2.118) and, following a now-classical argument of B.D. Coleman and W. Noll, noting that the resulting inequality involves no terms linear affine in $\nabla_R\theta$ and $\nabla_R\dot{\theta}$ other than those already present in (2.118) or the term introduced by (2.120), and the coefficients of the time derivatives do

not depend on these, for any nonvanishing values of these derivatives (in particular, the motion of the body is not one of a rigid body), we necessarily arrive at the following constraints (a more rigorous proof is found in Maugin, 1988):

$$\frac{\partial \bar{W}}{\partial(\nabla_R \theta)} = \mathbf{0}, \quad \mathbf{T} = \tilde{\mathbf{T}}(\mathbf{F},\theta) = \left.\frac{\partial \tilde{W}}{\partial \mathbf{F}}\right|_{\theta}, \quad S = \tilde{S}(\mathbf{F},\theta) = -\left.\frac{\partial \tilde{W}}{\partial \theta}\right|_{\mathbf{F}}, \quad \mathbf{Q} = \tilde{\mathbf{Q}}(\mathbf{F},\theta;\nabla_R\theta), \tag{2.121}$$

with

$$W = \tilde{W}(\mathbf{F},\theta), \quad \lim \tilde{\mathbf{Q}}(\mathbf{F},\theta;\nabla_R\theta \to \mathbf{0}) = \mathbf{0}. \tag{2.122}$$

That is, entropy is formally defined just like in thermostatics, although there is thermal disequilibrium, and heat flux may still depend on deformation and temperature as parameters. The remaining dissipation inequality is of pure thermal origin and reads

$$\Phi_{\text{conduction}} \equiv -(\mathbf{Q}/\theta).\nabla_R\theta \geq 0. \tag{2.123}$$

A standard expression respecting the last of (2.122) is given by

$$\mathbf{Q} = -\mathbf{K}(\mathbf{F},\theta).\nabla_R\theta, \tag{2.124}$$

where the necessarily symmetric material tensor $\mathbf{K}$ is positive definite.

On using the push forward of $\mathbf{T}$ and $\mathbf{Q}$, we obtain the Cauchy stress and spatial heat flux as

$$\boldsymbol{\sigma} = J_F^{-1}\mathbf{F}\frac{\partial \tilde{W}}{\partial \mathbf{F}}, \quad \mathbf{q} = J_F^{-1}\mathbf{F}\tilde{\mathbf{Q}}. \tag{2.125}$$

Now, if we enforce the condition of objectivity on the function $W$ and the tensor $\mathbf{K}$, that is, form invariance under the finite *proper* orthogonal group of transformations in the actual configuration, this will reduce the functional dependency of $W$ and $\mathbf{K}$ on $\mathbf{F}$ on a material measure of strain, for example, $\mathbf{E}$, that is,

$$W = \hat{W}(\mathbf{E},\theta), \quad \mathbf{Q} = -\mathbf{K}(\mathbf{E},\theta).\nabla_R\theta. \tag{2.126}$$

One way to prove the first of these is to notice that the local balance of angular momentum here reads like (2.82) or (2.88). The latter can be viewed, on account of the second of (2.121), as a system of first-order partial differential

equations for $W$. According to the Monge–Ampère theory of such equations, the first of (2.126) is an admissible integral along the characteristics of this system. The identity between this result and (2.126) is due to the fact that the group of *proper* orthogonal transformations is connected, and, therefore, it is sufficient to study the invariance of the function $W$ under an infinitesimal generator of the group, as given by (2.62). At order $\eta^2$ of approximation, the resulting equation is none other than (2.88) with $\mathbf{T}$ given by the second of (2.121). This reasoning applies only to elasticity.

Now define the true symmetric material tensor, called the *second Piola–Kirchhoff stress* or *energy stress* in the case of elasticity, $\mathbf{S}$—*not to be mistaken for the material entropy flux*—by

$$\mathbf{S} = \mathbf{T}\mathbf{F} = J_F \mathbf{F}^{-1}\boldsymbol{\sigma}\mathbf{F}^{-T} = \left\{ S^{KL} = J_F \left(\mathbf{F}^{-1}\right)^{Ki} \sigma_{ij} \left(\mathbf{F}^{-1}\right)^{Lj} \right\}, \quad \boldsymbol{\sigma} = J_F^{-1}\mathbf{F}\mathbf{S}\mathbf{F}^T. \tag{2.127}$$

On account of (2.121) and (2.126), this yields

$$\mathbf{S} = \left. \frac{\partial \hat{W}}{\partial \mathbf{E}} \right|_{\theta}, \quad \boldsymbol{\sigma} = J_F^{-1}\,\mathbf{F} \left. \frac{\partial \hat{W}}{\partial \mathbf{E}} \right|_{\theta} \mathbf{F}^T, \tag{2.128}$$

where the first of these justifies the name of *energy stress*. Then a classical writing of the balance of linear momentum clearly is in components

$$\frac{\partial}{\partial X^K}\left[ S^{KL}\left(\delta_{iL} + u_{i,L}\right)\right] + \rho_0 f_i = \rho_0 \frac{\partial^2 u_i}{\partial t^2}. \tag{2.129}$$

**REMARK 2.8:** Material inhomogeneity

All the preceding developments still hold true when an explicit dependence of the function $W$ and of the tensorial coefficient $\mathbf{K}$ on the material point $\mathbf{X}$ exists, that is, when the thermoelastic material considered is *materially inhomogeneous*. It suffices to add the ignored dependency in the relevant functions, but none of the proofs is changed.

**REMARK 2.9:** Conjugate pairs or associated pairs of stresses and deformation measures

While proceeding we have shown that the power of internal stresses per unit mass is an invariant. By this we mean that, for example,

$$p_{\text{int}} = \rho^{-1}\text{tr}\left(\boldsymbol{\sigma}.\mathbf{D}\right) = \rho_0^{-1}\text{tr}\left(\mathbf{T}.\left(\nabla_R \mathbf{v}\right)^T\right). \tag{2.130}$$

In the present context these two formulations result from the consideration of the direct motion and directly derived finite-strain measures. There is no opposition in principle to considering formulations that account for the

*inverse motion* and associated finite-strain measures. Accordingly, we could envisage energy densities that depend on such arguments. For instance, making abstraction of the temperature dependence, we may consider the following energy densities:

$$W = W_{(1)}\left(\mathbf{F}^{-1}\right), \quad W = W_{(2)}\left(\mathbf{C}^{-1}\right), \quad W = W_{(3)}\left(\mathbf{E}^{(-2)}\right). \tag{2.131}$$

Then we verify that the following holds true:

$$-J_F p_{\text{int}} = \text{tr}\left(\mathbf{T}_{(1)}\cdot\left(\frac{\partial \mathbf{F}^{-1}}{\partial t}\right)^T\right) = \text{tr}\left(\tilde{\mathbf{S}}.\left(\frac{\partial \mathbf{C}^{-1}}{\partial t}\right)\right) = \text{tr}\left(\bar{\mathbf{S}}.\left(\frac{\partial \mathbf{E}^{(-2)}}{\partial t}\right)\right), \tag{2.132}$$

where the partial time derivatives are taken at actual placement **x** fixed, and we have set

$$\mathbf{T}_{(1)} = J_F^{-1}\left(\partial W_{(1)}/\partial \mathbf{F}^{-1}\right), \quad \tilde{\mathbf{S}} = 2J_F^{-1}\left(\partial W_{(2)}/\partial \mathbf{C}^{-1}\right), \quad \bar{\mathbf{S}} = J_F^{-1}\left(\partial W_{(3)}/\partial \mathbf{E}^{(-2)}\right). \tag{2.133}$$

We let the reader show that the Cauchy stress is then given by

$$\boldsymbol{\sigma} = -2\,\mathbf{F}^{-T}.\tilde{\mathbf{S}}.\mathbf{F}^{-1} = -\mathbf{F}^{-T}.\bar{\mathbf{S}}.\mathbf{F}^{-1}, \tag{2.134}$$

while the second and first Piola–Kirchhoff stresses are given by

$$\mathbf{S} = -2\mathbf{C}^{-1}.\tilde{\mathbf{S}}.\mathbf{C}^{-1} = -\mathbf{C}^{-1}.\bar{\mathbf{S}}.\mathbf{C}^{-1}, \quad \mathbf{T} = -J_F\mathbf{F}^{-1}.\mathbf{T}_{(1)}.\mathbf{F}^{-1}. \tag{2.135}$$

The proof of these identities exploits the following relations (written in components to facilitate the computations):

$$\frac{\partial\left(\mathbf{F}^{-1}\right)_j^L}{\partial F_K^i} = -\left(\mathbf{F}^{-1}\right)_i^L\left(\mathbf{F}^{-1}\right)_j^K \tag{2.136}$$

and

$$\frac{\partial\left(\mathbf{C}^{-1}\right)^{KL}}{\partial C_{MN}} = -\left(\mathbf{C}^{-1}\right)^{KM}\left(\mathbf{C}^{-1}\right)^{LN}. \tag{2.137}$$

We remark that $w = J_F^{-1}W$ is the free energy per unit volume in the actual configuration. Then we ask the reader to check that the Cauchy stress may be given the following form (Maugin and Trimarco, 1993):

$$\boldsymbol{\sigma} = w\mathbf{1} - \mathbf{F}^{-T}.\frac{\partial w\left(\mathbf{F}^{-1}\right)}{\partial \mathbf{F}^{-1}} = w\mathbf{1} - \mathbf{F}^{-T}.\mathbf{T}_{(1)}. \tag{2.138}$$

Although this is the Cauchy stress, for reasons to become clear in subsequent chapters, we say that (2.138) provides an *Eshelby format* of the Cauchy stress. In conclusion of this remark, we note that the various dependencies introduced in the preceding for the energy serve to illustrate the notion of *conjugate pairs* of associated stresses and deformation measures via the invariance of the specific power expanded by the various stresses (cf. (2.130) and (2.132); see also Ogden, 1984, p. 156).

**REMARK 2.10:** Isotropic thermoelasticity

The symmetry group of isotropy is the full orthogonal group in the reference configuration. Accordingly, in the isotropic case function $W$ and tensor $\mathbf{K}$ must be an isotropic scalar-valued function and an "isotropic" symmetric tensor-valued function of the finite strain $\mathbf{E}$, respectively. For instance, we shall have the following representations:

$$W = W(\mathbf{E},\theta) = W(\mathbf{P}\mathbf{E}\mathbf{P}^T,\theta) = W(I_\alpha,\ \alpha = 1,2,3,\theta), \quad \forall \mathbf{P} \in SO(3), \quad I_\alpha := \mathrm{tr}\mathbf{E}^\alpha$$

and

$$\mathbf{K} = K_0(I_\alpha,\theta)\mathbf{1}_R + K_1(I_\alpha,\theta)\mathbf{E} + K_2(I_\alpha,\theta)\mathbf{E}^2,$$

according to known representation theorems (cf. Eringen and Maugin, 1990, appendices).

**REMARK 2.11:** Anisotropic thermoelasticity

It is known, at least in special coordinate frames, how to represent *exactly* a scalar function and a material tensor in terms of a second-order tensor such as $\mathbf{E}$, for all crystallographic groups (cf. Eringen and Maugin, 1990, appendices). However, most times, it is sufficient to consider an expansion of the energy $W$ and of tensor $\mathbf{K}$ in terms of the "small" $\mathbf{E}$ and of a slight deviation $\tilde{\theta} = \theta - \theta_0$ from a uniform temperature field, for instance (the abbreviation h.o.t. stands for "higher-order terms"),

$$W(\mathbf{E},\tilde{\theta}) = -S_0\tilde{\theta} + \tilde{\theta}M^{KL}E_{KL} - \frac{\rho_0 C_\theta}{2\theta_0}\tilde{\theta}^2 + \frac{1}{2}C^{KLMN}E_{KL}E_{MN} + \text{h.o.t.}$$

and

$$K^{PQ}(\mathbf{E},\tilde{\theta}) = K_0^{PQ}(\mathbf{0},\theta_0) + \text{h.o.t.},$$

with the obvious tensorial symmetries

$$M^{KL} = M^{LK}, \quad C^{KLMN} = C^{(KL)(MN)} = C^{MNKL}, \quad K_0^{PQ} = K_0^{QP},$$

so that these two tensors have at most 21 and six independent components, respectively, and much less for many material symmetries. The first of these is called the tensor of *elasticity coefficients* of the second order since it corresponds to the second-order derivative of $W$, and $M_{KL}$ is the tensor of thermoelasticity coupling coefficients, that is,

$$M^{KL}(\theta_0) = \left.\frac{\partial^2 W}{\partial\theta\partial E_{KL}}\right|_{\mathbf{E}=\mathbf{0},\,\theta=\theta_0}, \quad C^{KLMN}(\theta_0) = \left.\frac{\partial^2 W}{\partial E_{KL}\partial E_{MN}}\right|_{\mathbf{E}=\mathbf{0},\,\theta=\theta_0}.$$

**REMARK 2.12:** Infinitesimal thermoelasticity

The way is already paved for this approximation, for which the higher-order terms noted h.o.t. in the preceding equations are discarded and the finite strain **E** can be replaced by the infinitesimal one, and we need not distinguish anymore between upper and lower Latin indices. The balance of linear physical momentum and the energy equation take on the following forms:

$$\sigma_{ij,j} + \rho_0 f_i = \rho_0 \ddot{u}_i, \quad \sigma_{ij} = C_{ijkl}\varepsilon_{kl} + M_{ij}\tilde{\theta}, \quad \varepsilon_{ij} = u_{(i,j)} \tag{2.139a}$$

and

$$\rho_0 C_\theta \dot{\tilde{\theta}} = \left(K_{0ij}\tilde{\theta}_{,j}\right)_{,i} + \theta_0 M_{ij}\dot{\varepsilon}_{ij} + \rho_0 h, \tag{2.139b}$$

where a superimposed dot stands for partial time derivative and the tensorial material coefficients may still be dependent on the point **x** for a materially inhomogeneous body. The expression of the tensorial material coefficients simplifies further in the case of *isotropy*, for which we have the following reduced representations:

$$C_{ijkl} = \lambda\delta_{ij}\delta_{kl} + \mu\left(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}\right), \quad M_{ij} = m\delta_{ij}, \quad K_{0ij} = K\delta_{ij},$$

where $\lambda$ *and* $\mu$ are Lamé constants (still dependent on $\theta_0$), $m$ is the remaining thermoelastic coefficient, and $K$ is the heat-conduction coefficient. The usual dilatation coefficient $\alpha$ is defined by $\alpha = -m/(3\lambda + 2\mu)$ since we have internal strains due to thermal processes defined by

$$\varepsilon_{0ij} = \varepsilon_{ij}\left(\sigma = \mathbf{0}, \tilde{\theta}\right) = \alpha\tilde{\theta}\delta_{ij}, \tag{2.140}$$

obtained by inversion of the *Hooke–Duhamel* linear constitutive equation in ($2.139a_2$). The elasticity coefficients introduced in the preceding correspond

to a situation of *isothermal* processes. We let the reader check that under the condition of *adiabatic* or isentropic processes, we have (anisotropic case)

$$\sigma_{ij} = C^{S}_{ijkl}\varepsilon_{kl}, \quad C^{S}_{ijkl} = C_{ijkl} + \left(\theta_0/\rho_O C_\theta\right) M_{ij} M_{kl}.$$

These are all the elements of thermoelasticity we need in further chapters.

### 2.3.2 A Sufficiently Large Class of Dissipative Solids

The elementary stress power (2.118) per unit reference volume can be written as

$$p^{R}_{(i)} = \mathrm{tr}\left(\mathbf{T}.\left(\nabla_R \mathbf{v}\right)^T\right) = \mathrm{tr}\left(\mathbf{S}.\dot{\mathbf{E}}\right). \tag{2.141}$$

If instead of (2.119) one assumes that a part of $\mathbf{T}$ or $\mathbf{S}$, say $\mathbf{S}^{\mathrm{v}}$, will also a priori depend on the strain rate $\dot{\mathbf{E}}$, for instance linearly, then we obtain for $\mathbf{S}^{\mathrm{v}}$ a tensor of stress much like what happens in the Newtonian model of viscous fluidity but for deformable solids. This provides the so-called *Kelvin–Voigt model of viscoelasticity*, which is not such a good model of solid viscosity (cf. Maugin, 1992). Fortunately, there is a much better way to obtain realistic models of dissipative solids, such as viscous, elastoplastic, viscoplastic, or damaging solids, models that also completely fulfill thermodynamic requirements while keeping some contact with physical bases. This is the due application of the *thermodynamics with internal variables of state* (Maugin and Muschik, 1994; Maugin, 1999). We remind the reader that both deformation and thermodynamic temperature are said to be observable state variables. They can be measured. They are also directly controlled by means of bulk and surface data. Accordingly, there are data associated with them in the bulk and at the bounding surface. This is even more visible on the expression of the principle of virtual power (for the mechanical part) where bulk and surface data are associated with the dual of deformations, stresses.

Of course, macroscopically observable dissipative effects result from intricate microscopic processes that are not directly controllable macroscopically, although they may be observed with the appropriate instrument (e.g., optical or electronic microscopes, x-ray, etc.). An example of this is the thermodynamically necessary presence of many dislocations (defects) in metals. Although the dislocations can be observed and some of their properties (e.g., density) can be measured, we have no means to act directly on them. We simply observe their evolution under the action of the local stress field, itself determined by bulk and surface force data applied to the body via a boundary-value problem solved by any means.

We have to acknowledge our relative ignorance of microscopic processes and remedy this in some way at the phenomenological level. The basic idea is to identify (a gifted experimentalist should do this identification) a new

set of thermodynamic variables, so-called *internal* ones, noted collectively by the symbol $\alpha$. This may have any tensorial nature depending on the phenomenon studied. According to a remark just made, there won't be any bulk and surface data associated with them, for example, neither contributions to the power of external forces in the principle of virtual power nor contributions to the statement of the first law of thermodynamics. These new variables are *purely dissipative*. This is the point of view forcefully advocated by Joseph Kestin that we adopted in previous works (Maugin and Muschik, 1994; Maugin, 1999). It has become a well-accepted point of departure in the description of many thermodynamically irreversible processes, whether in mechanics or in other fields of physics (e.g., electromagnetism; cf. Maugin, 1999). The result of this is that all basic statements are left unchanged compared to what was proposed in the foregoing paragraphs, save for the assumed dependence of the free energy density on $\alpha$; that is, instead of $(2.122_1)$ we shall a priori write

$$W = \bar{W}(\mathbf{F}, \theta, \alpha), \quad A = -\frac{\partial \bar{W}}{\partial \alpha}, \tag{2.142}$$

where $A$ is the thermodynamic force associated with $\alpha$, that is, its thermodynamic dual or conjugate. The associated (intrinsic) dissipated power is given by

$$p_{\text{intr}} = A.\dot{\alpha}. \tag{2.143}$$

If this is the only dissipative contribution to the Clausius–Duhem inequality (CDI), and its nonnegativity is required independently of thermal conduction dissipation (the most often considered hypothesis), then because of (2.142) and using an argument à la Coleman–Noll, we shall have the following results of the exploitation of the CDI:

$$\mathbf{T} = \frac{\partial \bar{W}}{\partial \mathbf{F}}, \quad S = -\frac{\partial \bar{W}}{\partial \theta}, \quad A.\dot{\alpha} \geq 0, \quad (\mathbf{Q}/\theta).\nabla_R \theta \leq 0. \tag{2.144}$$

The precise conditions in which these hold good, in particular, the second of these, are duly analyzed in Maugin and Muschik (1994); see the notion of *local accompanying state*. Examples of the exploitation of (2.144) are given in Maugin (1999) for both finite- and small-strain theories. It remains to exploit the third of (2.144), the simplest strategy consisting in considering the rate $\dot{\alpha}$ as being essentially determined by the conjugate "force" $A$ (Kestin and Rice, 1970), for example,

$$\dot{\alpha} = \bar{\alpha}(A; \mathbf{F}, \theta, \alpha). \tag{2.145}$$

Most of the physics related to $\alpha$ is contained in this evolution equation, which may have a very singular expression, as shown by some examples in the following. Indeed, a simple proportionality (linear affine) expression of $\dot{\alpha}$ in terms of $A$ involves a *time scale* typical of viscous and relaxation effects. But there exist dissipative effects, such as plasticity and magnetic hysteresis (at low frequencies), that are practically rate-independent; that is, they present *no* time scale. They may also exhibit a *threshold* in $A$ space. This must be dealt with more astutely.

### 2.3.3 Example: Elastoplasticity in Finite Strains

In general, deformation is characterized by the tangent map $\mathbf{F}$, a material gradient, between the reference configuration $K_R$ and the current configuration $K_t$. Such gradients, by their very nature, compose in a multiplicative manner. Accordingly, if there exist *elastic* (thermodynamically recoverable) finite deformations and *anelastic* (dissipative) deformations, they should compose the total, and only true, gradient $\mathbf{F}$ in a multiplicative manner. That is, with an obvious notation,

$$\mathbf{F} = \mathbf{F}^e\mathbf{F}^a, \tag{2.146}$$

where none of the contributors $\mathbf{F}^e$ and $\mathbf{F}^a$ of the decomposition is a true gradient. In geometric differential terms, they are only *Pfaffian forms*. The decomposition in (2.146) goes back to Bilby et al. (1957) but was made popular later on by Lee (1969) and his coworkers. A simple picturesque interpretation of this is given in Figure 2.2, where the first step, that is, $\mathbf{F}^a$, defines from $K_R$ a so-called *intermediate* or *elastically released configuration* $K_{\text{relax}}$, as it is also obtained from $K_t$ by applying the inverse elastic deformation $\left(\mathbf{F}^e\right)^{-1}$. Then it is clear that the decomposition in Equation 2.146 is invariant by rotations $\mathbf{Q} \in SO(3)$ of $K_{\text{relax}}$ as we can write

$$\mathbf{F}^e\mathbf{F}^a = \hat{\mathbf{F}}^e\hat{\mathbf{F}}^a, \quad \hat{\mathbf{F}}^e = \mathbf{F}^e\mathbf{Q}, \quad \hat{\mathbf{F}}^a = \mathbf{Q}^T\mathbf{F}^a, \tag{2.147}$$

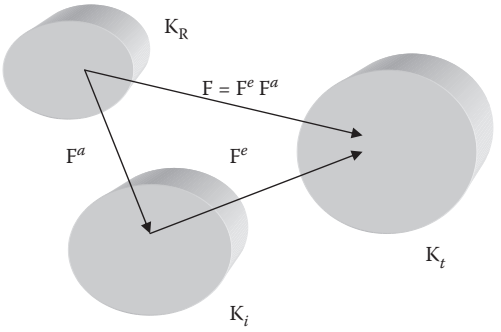


**FIGURE 2.2**
The multiplicative decomposition of finite strain.

with

$$\mathbf{Q}\mathbf{Q}^T = \mathbf{Q}^T\mathbf{Q} = \mathbf{1}, \quad \mathbf{Q}^T = \mathbf{Q}^{-1}, \quad \det\mathbf{Q} = \pm 1. \tag{2.148}$$

In practice a definite orientation can be granted to $K_{\text{relax}}$ through a particular crystal lattice (for this, see Mandel, 1971). Concerning constitutive equations all we note is that we may rewrite the inequality (2.118) in a specific form by introducing the following elements of kinematics and kinetics. For that purpose, on the basis of (2.142), noting that only $\mathbf{F}^e$ is observable by elastic unloading, we will set (an argument for this will be presented later on based on the notion of local structural rearrangement)

$$W = \bar{W}\left(\mathbf{F}^e, \alpha, \theta\right) \tag{2.149}$$

and

$$S = -\frac{\partial \bar{W}}{\partial \theta}, \quad \mathbf{T}^e := \frac{\partial \bar{W}}{\partial \mathbf{F}^e}, \quad A = -\frac{\partial \bar{W}}{\partial \alpha}. \tag{2.150}$$

Then we look for a convenient and suggestive expression for the residual dissipation inequality. To reach such an expression, first note that

$$\dot{\mathbf{F}}^e = \dot{\mathbf{F}}.\left(\mathbf{F}^a\right)^{-1} - \mathbf{F}^e.\dot{\mathbf{F}}^a.\left(\mathbf{F}^a\right)^{-1}, \tag{2.151}$$

obtained by computing $\dot{\mathbf{F}}$ on the basis of (2.145) and applying $\left(\mathbf{F}^a\right)^{-1}$ to the right of the result. Furthermore, setting

$$\bar{\mathbf{T}}^v := \mathbf{F}^a.\mathbf{T} - \mathbf{T}^e, \quad \bar{\mathbf{T}} := \mathbf{T}.\mathbf{F}, \tag{2.152}$$

it is readily checked on account of (2.118) and (2.150) that we obtain the following residual dissipation inequality:

$$\Phi = \Phi_{\text{intr}} + \Phi_{\text{th}} \geq 0, \tag{2.153}$$

with

$$\Phi_{\text{intr}} = \text{tr}\left\{\bar{\mathbf{T}}^v.\dot{\mathbf{F}}^e + \bar{\mathbf{T}}.\dot{\mathbf{F}}^a\right\} + A\dot{\alpha}, \quad \Phi_{\text{th}} = -\left(\mathbf{Q}/\theta\right).\nabla_R\theta. \tag{2.154}$$

Then we note that the original first Piola–Kirchhoff stress is recovered by computing

$$\mathbf{T} = \left(\mathbf{F}^a\right)^{-1}.\left(\bar{\mathbf{T}}^e + \bar{\mathbf{T}}^v\right) = \mathbf{T}^e + \mathbf{T}^a, \tag{2.155}$$

wherein

$$\mathbf{T}^e = \left(\mathbf{F}^a\right)^{-1}.\left(\partial \bar{W}/\partial \mathbf{F}^e\right), \quad \mathbf{T} = \left(\mathbf{F}^a\right)^{-1}.\bar{\mathbf{T}}^v. \tag{2.156}$$

The first of (2.154) is of interest because it clearly separates the dissipative effects related to $\dot{\mathbf{F}}^e$ and $\dot{\mathbf{F}}^a$ (cf. Maugin, 1994). Accordingly, the first is often related to pure viscous processes, hence the notation for $\mathbf{T}^v$, and the second to pure plasticity effects, so that the superscript *a* will now be replaced by *p*.

To proceed further we discard the "viscous" type of dissipation so that the first of (2.152) yields

$$\mathbf{T} = -\left(\mathbf{F}^p\right)^{-1}.\bar{\mathbf{T}}^e = \left(\mathbf{F}^p\right)^{-1}.\left(\partial \bar{W}/\partial \mathbf{F}^e\right). \tag{2.157}$$

It is salient to introduce strain measures in the configuration $K_{\text{relax}}$ by (compare to (2.10) and (2.14))

$$\mathbf{C}^e := \left(\mathbf{F}^e\right)^T \mathbf{F}^e, \quad \mathbf{E}^e = \frac{1}{2}\left(\mathbf{C}^e - 1_{\text{relax}}\right), \tag{2.158}$$

which are true covariant symmetric tensors in the configuration $K_{\text{relax}}$ equipped with unit $\mathbf{1}_{\text{relax}}$.

We introduce the Jacobian determinants

$$J^e = \det \mathbf{F}^e, \quad J^p = \det \mathbf{F}^p, \quad J_F = J^e J^p > 0. \tag{2.159}$$

The following *plastic strain rates* are also useful:

$$\mathbf{D}^p = \left\{\mathbf{F}^e.\mathbf{L}^p.\left(\mathbf{F}^e\right)^{-T}\right\}_S = \left(\mathbf{D}^p\right)^T \quad \text{in} \quad K_t, \quad \mathbf{L}^p = \dot{\mathbf{F}}^p\left(\mathbf{F}^p\right)^{-1} \tag{2.160}$$

and

$$\mathbf{D}^p_{\text{relax}} = \left\{\mathbf{C}^e.\mathbf{L}^p\right\}_S = \left(\mathbf{D}^p_{\text{relax}}\right)^T \quad \text{in} \quad K_{\text{relax}}, \tag{2.161}$$

while the second Piola–Kirchhoff stress relative to $K_{\text{relax}}$ reads as

$$\mathbf{S}_{\text{relax}} = J^e\left(\mathbf{F}^e\right)^{-1}.\sigma.\left(\mathbf{F}^e\right)^{-T}. \tag{2.162}$$

Then the *intrinsic* dissipation per unit volume reads

$$\Phi_{\text{intr}} = \text{tr}\left(\sigma.\mathbf{D}^p\right) + J_F^{-1} A\dot{\alpha} \quad \text{in} \quad K_t \tag{2.163}$$

and

$$\left(\Phi_{\text{intr}}\right)_{\text{relax}} = \text{tr}\left(\mathbf{S}_{\text{relax}}.\mathbf{D}^{p}_{\text{relax}}\right) + \tilde{A}\dot{\alpha} \quad \text{in} \quad K_{\text{relax}}, \tag{2.164}$$

together with the energy (per unit volume of $K_{\text{relax}}$)

$$W_{\text{relax}} = \tilde{W}\left(\mathbf{E}^{e}, \alpha, \theta\right), \tag{2.165}$$

and the laws of state

$$\mathbf{S}_{\text{relax}} = \frac{\partial \tilde{W}}{\partial \mathbf{E}^{e}}, \quad \tilde{A} = -\frac{\partial \tilde{W}}{\partial \alpha}, \quad S_{\text{relax}} = -\frac{\partial \tilde{W}}{\partial \theta}. \tag{2.166}$$

Here $\mathbf{E}^{e}$ is the *observable* mechanical variable of state.

A *finite-strain rate-independent theory of elastoplasticity* is now completed by assuming the existence of a *yield* (hyper-) *surface* $f\left(\mathbf{S}_{\text{relax}}, \tilde{A}\right) = 0$ bounding a convex set C in $\left(\mathbf{S}_{\text{relax}}, \tilde{A}\right)$ space, and considering the following plastic evolution equations

$$\mathbf{D}^{p}_{\text{relax}} = \dot{\lambda}\frac{\partial f}{\partial \mathbf{S}_{\text{relax}}}, \quad \dot{\alpha} = \dot{\lambda}\frac{\partial f}{\partial \tilde{A}}, \tag{2.167}$$

where $\dot{\lambda} \geq 0$, $\dot{\lambda}$ being a so-called plastic multiplier. Equation 2.167 means that the plastic evolution presents no time scale (there is a time derivative on both sides), and the corresponding intrinsic dissipation is mathematically homogeneous of degree one only in the time rates. Mechanical dissipation occurs possibly, but not necessarily, when a point on the surface *f* has been reached. The evolution, if any, then is directed along the outward unit normal to the yield surface. This is the very singular mechanical behavior exhibited by rate-independent plasticity. Finite-strain viscoplasticity would allow the working point in $\left(\mathbf{S}_{\text{relax}}, \tilde{A}\right)$ space to sit outside the convex set *C* but with a kind of elastic recall—related to a relaxation time—toward the hypersurface $f = 0$ (cf. Maugin, 1999).

**REMARK 2.13:** From (2.161) and (2.164), we note that the intrinsic dissipation due to stresses in the elastically released configuration is given by

$$\text{tr}\left(\mathbf{S}_{\text{relax}}.\mathbf{D}^{p}_{\text{relax}}\right) = \text{tr}\left(\mathbf{M}_{\text{relax}}.\mathbf{L}^{p}\right), \quad \mathbf{M}_{\text{relax}} := \mathbf{S}_{\text{relax}}.\mathbf{C}^{e}, \tag{2.168}$$

where $\mathbf{M}_{\text{relax}}$ is the Mandel stress relative to the configuration $K_{\text{relax}}$. This makes some say that the *Mandel stress is the driving force of plasticity* (cf. Mandel, 1971).

### 2.3.4 Small Strain Rate Independent Elastoplasticity

In this case we have $(\mathbf{F}-\mathbf{1})_{ij} = u_{i,j}$. The multiplicative decomposition in (2.146) translates into the additive decomposition

$$\varepsilon = \left(\nabla u\right)_S = \varepsilon^e + \varepsilon^a, \tag{2.169}$$

where neither the "elastic" strain $\varepsilon^e$ nor the "anelastic" strain are true gradients. There is no longer any distinction between various configurations. Following along the same line as for finite strains, we have the following expressions in that theory:

- Laws of state:

$$W = \bar{W}\left(\varepsilon^e, \alpha, \theta\right) \tag{2.170}$$

$$S = -\frac{\partial \bar{W}}{\partial \theta}, \quad \sigma^e = \frac{\partial \bar{W}}{\partial \varepsilon^e}, \quad A = -\frac{\partial \bar{W}}{\partial \alpha} \tag{2.171}$$

- Dissipation inequality:

$$\Phi = \Phi_{\text{intr}} + \Phi_{th} \geq 0 \tag{2.172}$$

$$\Phi_{\text{intr}} = \text{tr}\left(\sigma^v . \dot{\varepsilon}^e + \sigma . \dot{\varepsilon}^a\right) + A\dot{\alpha}, \quad \Phi_{th} = -\left(\mathbf{q}/\theta\right).\nabla\theta, \tag{2.173}$$

where $\sigma^v := \sigma - \sigma^e$. In the case where there is no viscous stress $\sigma^v$, we contemplate the case of pure elastoplasticity in small strains with $\varepsilon^a \equiv \varepsilon^p$. In close parallelism with the reasoning for finite strain, we shall have the following evolution equations for rate-independent plasticity:

$$\dot{\varepsilon}^p = \dot{\lambda}\frac{\partial f}{\partial \sigma}, \quad \dot{\alpha} = \dot{\lambda}\frac{\partial f}{\partial A}, \tag{2.174}$$

where $f(\sigma, A) = 0$ is the hypersurface in $(\sigma, A)$ space that represents the plasticity threshold limiting a convex set $C$ in that space. Points inside this convex set correspond to a purely elastic (thermodynamically reversible) behavior. Plasticity behavior (a possible nonzero evolution of $\varepsilon^p$) may occur when the working point is on the hypersurface $f = 0$. Examples of internal variables $\alpha$ and the mathematical developments of the small-strain theory are given in Maugin (1992). Variable $\alpha$ may be $\varepsilon^p$ itself or a more complex entity such as a work hardening variable accounting for the total past evolution of the plastic strain, in which case the convex set $C$ may become *mobile* during the time evolution.

# 3

# *Eshelbian Mechanics for Elastic Bodies*

## Object of the Chapter

Where we introduce the notion of Eshelby stress in elasticity and its direct generalizations, and witness its first applications to materially inhomogeneous bodies.

## 3.1 The Notion of Eshelby Material Stress

### 3.1.1 Quasistatic Eshelby Stress

For the sake of simplicity we consider the case of the quasistatics of *materially inhomogeneous* purely elastic bodies (no dissipation of any kind, inertial effects neglected). Then the balance of linear (physical) momentum in the Piola–Kirchhoff formulation reads:

$$\mathrm{div}_R\mathbf{T}+\rho_0\mathbf{f}=\mathbf{0},\quad \mathbf{T}=\frac{\partial W}{\partial \mathbf{F}},\quad W=\bar{W}\left(\mathbf{F};\mathbf{X}\right). \tag{3.1}$$

On applying $\mathbf{F}$ to the right of the first equation and noting that

$$\left(\mathrm{div}_R\mathbf{T}\right).\mathbf{F}=\mathrm{div}_R\left(\mathbf{T}.\mathbf{F}\right)-\mathbf{T}.\left(\nabla_R\mathbf{F}\right)^T=\mathrm{div}_R\left(\mathbf{T}.\mathbf{F}\right)-\nabla_R W-\mathbf{f}^{\mathrm{inh}}, \tag{3.2}$$

since

$$\nabla_R W=\frac{\partial \bar{W}}{\partial \mathbf{F}}.\left(\nabla_R\mathbf{F}\right)^T+\left.\frac{\partial \bar{W}}{\partial \mathbf{X}}\right|_{\mathbf{F}\,\mathrm{fixed}},\quad \mathbf{f}^{\mathrm{inh}}:=-\left.\frac{\partial \bar{W}}{\partial \mathbf{X}}\right|_{\mathrm{expl}}\equiv-\left.\frac{\partial \bar{W}}{\partial \mathbf{X}}\right|_{\mathbf{F}\,\mathrm{fixed}}, \tag{3.3}$$

we obtain the fully material equilibrium equation

$$\mathrm{div}_R\mathbf{b} + \mathbf{f}^{\mathrm{ext}} + \mathbf{f}^{\mathrm{inh}} = \mathbf{0}, \tag{3.4}$$

wherein we have set

$$\mathbf{b} := W1_R - \mathbf{T}.\mathbf{F}, \quad \mathbf{f}^{\mathrm{ext}} := -\rho_0\mathbf{f}.\mathbf{F} \tag{3.5}$$

The fully material stress tensor $\mathbf{b}$ is called the quasistatic *Eshelby stress tensor* in honor of J.D. Eshelby (cf. Maugin and Trimarco, 1992), who previously called it the elastic energy-momentum tensor or Maxwell stress tensor (but this denomination is somewhat misleading; see further developments in the following). This material tensor has no specific symmetry. However, on account of the local balance of angular momentum (2.82), we easily show that it satisfies the following symmetry condition with respect to the Cauchy–Green (or deformed) material metric **C:**

$$\mathbf{C}.\mathbf{b} = \left(\mathbf{C}.\mathbf{b}\right)^T = \mathbf{b}^T.\mathbf{C}. \tag{3.6}$$

The *material* forces $\mathbf{f}^{\mathrm{ext}}$ and $\mathbf{f}^{\mathrm{inh}}$ are the externally applied material force (obtained by the negative of the pull back of the prescribed body force) and the *material force of inhomogeneity.* According to its definition in (3.3), the latter captures the explicit dependence of the function $W$ on the material point (e.g., the dependence of the elasticity coefficients on $\mathbf{X}$). At all regular material points $\mathbf{X}$, (3.4) is an *identity* deduced from the basic balance law in (3.1). In field theory (see Section 4.2) this is called a *conservation law*, but here it is in fact a *non*conservation because of the lack of invariance of the physical system under material translation. In the absence of body force and material inhomogeneity, (3.4) reduces to a **strict** conservation law. In the case where (3.1) and (3.4) hold good, the preceding manipulation is equivalent to writing the following identity:

$$\left(\mathrm{div}_R\mathbf{T} + \rho_0\mathbf{f}\right).\mathbf{F} + \left(\mathrm{div}_R\mathbf{b} + \mathbf{f}^{\mathrm{ext}} + \mathbf{f}^{\mathrm{inh}}\right) = \mathbf{0}, \tag{3.7}$$

which may be referred to as the *Ericksen identity* of elasticity, as Ericksen (1977) gave it in the special case (no body force, no elastic inhomogeneity):

$$\left(\mathrm{div}_R\mathbf{T}\right).\mathbf{F} + \left(\mathrm{div}_R\mathbf{b}\right) = \mathbf{0}. \tag{3.8}$$

In field theory (Section 4.2), these are none other than special cases of the celebrated Noether's identity.

**REMARK 3.1:** On comparing the first of (3.5) and (2.138), we now understand why the latter was referred to as the Eshelby format of the Cauchy stress.

**REMARK 3.2:** Mandel stress

On using the definition of the second Piola–Kirchhoff stress, it is easily shown that the Eshelby stress **b** also reads

$$\mathbf{b} = W\mathbf{1}_R - \mathbf{S}.\mathbf{C} = W\mathbf{1}_R - \mathbf{M}, \quad \mathbf{M} := \mathbf{S}.\mathbf{C}, \tag{3.9}$$

where **M** is the so-called *Mandel stress* in the reference configuration (cf. Remark 2.13). This material true tensor plays an important role in finite-strain elastoplasticity (cf. Mandel, 1971; Lubliner, 1990). Just like **b**, **M** is symmetric with respect to **C**.

### 3.1.2 Dynamic Generalization

In this case we should start with the general equation of balance of linear (physical) momentum such as (2.87). We apply **F** to the right of the two sides of this equation for an inertially inhomogeneous material, noting the result in $(3.3_1)$, as well as the fact that

$$\left.\frac{\partial(\rho_0\mathbf{v})}{\partial t}\right|_X .\mathbf{F} = -\left.\frac{\partial \mathbf{P}}{\partial t}\right|_X - \nabla_R K^R + \left(K^R/\rho_0\right)\nabla_R\rho_0, \tag{3.10}$$

where we have set

$$\mathbf{P} := -\rho_0\mathbf{v}.\mathbf{F} = -\rho_0\mathbf{F}^T.\mathbf{v}, \quad K^R = \frac{1}{2}\rho_0(\mathbf{X})\mathbf{v}^2. \tag{3.11}$$

The first of these we called the *material momentum* or *pseudomomentum*. A short exercise consists in proving that this materially covariant vector can also be written as

$$\mathbf{P} = \rho_0\mathbf{C}.\mathbf{V} \quad \text{since} \quad \mathbf{v} = -\mathbf{F}\mathbf{V}, \tag{3.12}$$

if **V** is the material velocity field. Finally, we obtain the balance of material momentum in the form

$$\left.\frac{\partial \mathbf{P}}{\partial t}\right|_X - \mathrm{div}_R\mathbf{b} = \mathbf{f}^{\mathrm{ext}} + \mathbf{f}^{\mathrm{inh}}, \tag{3.13}$$

where, now,

$$\mathbf{b} := -\left(L^R\mathbf{1}_R + \mathbf{T}.\mathbf{F}\right) = -\left(L^R\mathbf{1}_R + \mathbf{M}\right), \quad \mathbf{f}^{\mathrm{inh}} := \left.\frac{\partial L^R}{\partial t}\right|_X, \tag{3.14}$$

if we define a density of *Lagrangian* $L^R$ by (cf. Chapter 2)

$$L^R = K^R - W \quad \text{with} \quad \left.\frac{\partial L^R}{\partial \mathbf{X}}\right|_{\text{expl}} = \left(K^R/\rho_0\right)\nabla_R\rho_0(\mathbf{X}) - \left.\frac{\partial W}{\partial \mathbf{X}}\right|_{\text{expl}}. \tag{3.15}$$

Accordingly, the material force $\mathbf{f}^{\text{inh}}$ captures both inertial (via $\rho_0$) and elastic (via $W$) inhomogeneities. Some authors (Gurtin, 1999) prefer to isolate the effect of inertial inhomogeneities. The dynamic Eshelby stress ($3.14_1$) satisfies the symmetry condition in Equation 3.6. The generalization of Ericksen's identity clearly reads

$$\left(\frac{\partial(\rho_0\mathbf{v})}{\partial t} - \left(\text{div}_R\mathbf{T} + \rho_0\mathbf{f}\right)\right).\mathbf{F} + \left(\frac{\partial \mathbf{P}}{\partial t} - \left(\text{div}_R\mathbf{b} + \mathbf{f}^{\text{ext}} + \mathbf{f}^{\text{inh}}\right)\right) = \mathbf{0}. \tag{3.16}$$

### 3.1.3 Weak Form of the Balance of Material Momentum

Equation 3.13 is a covectorial equation on the material manifold $M$. Let $\mathbf{V}^*$ be a virtual material velocity field, that is, a field at our disposal and not necessarily part of the solution of an actual problem. Taking the inner product of both sides of (3.13) by this $\mathbf{V}^*$ and integrating over the material volume $B_R$ bounded by $\partial B_R$, we arrive at the following expression:

$$\overline{P}_{\text{inertia}}{}^*(B_R) = \overline{P}_{\text{int}}{}^*(B_R) + \overline{P}_{\text{ext}}(B_R, \partial B_R) + \overline{P}_{\text{inh}}(B_R), \tag{3.17}$$

with the following definitions for the various virtual powers:

$$\overline{P}_{\text{inertia}}{}^*(B_R) = \int_{B_R} \left.\frac{\partial \mathbf{P}}{\partial t}\right|_X .\mathbf{V}^* dV, \tag{3.18}$$

$$\overline{P}_{\text{int}}{}^* = -\int_{B_R} \text{tr}\left(\mathbf{b}.\left(\nabla_R\mathbf{V}^*\right)^T\right) dV, \tag{3.19}$$

$$\overline{P}_{\text{ext}}{}^*(B_R, \partial B_R) = \int_{B_R} \mathbf{f}^{\text{ext}}.\mathbf{V}^* dV + \int_{\partial B_R} \left(\overline{\mathbf{T}}^d.\mathbf{v}^* - L^R(\mathbf{N}.\mathbf{V}^*)\right) dA, \tag{3.20}$$

$$\overline{P}_{\text{inh}}{}^*(B_R) = \int_{B_R} \mathbf{f}^{\text{inh}}.\mathbf{V}^* dV, \tag{3.21}$$

where we used the definition of $\overline{\mathbf{T}}^d := \mathbf{N}.\mathbf{T}$ and also the relation $\mathbf{v}^* + \mathbf{F}\mathbf{V}^* = \mathbf{0}$, which defines $\mathbf{v}^*$. Compared to (2.114), the weak formulation (principle of virtual power) in (3.17) is not altogether standard because of the intervention of (3.21) and of the energy contribution, via $L^R$, in the surface expression in (3.20). Such

a term (in quasistatics, hence with $L^R$ replaced by $-W$) is strangely postulated to exist by certain authors (cf. Gurtin, 1999) so as to recover essentially (3.13) after localization for any V* if the statement (3.17) is considered as primary.

## 3.2 Eshelby Stress in Small Strains in Elasticity

### 3.2.1 Reduced Form of the Eshelby Stress and Field Momentum

First, according to the introduction of this notion already given, we note that the Eshelby stress itself is less important than its divergence or its flux insofar as mechanics is concerned. This remark is to be taken seriously because such a tensor can then be defined up to a divergence-free tensor. This is what clearly occurs in the following consideration of the small-strain case. In the quasistatic case and in the absence of external body force, the Cauchy stress has a vanishing divergence. Abandoning the distinction between upper and lower Latin indices, from the preceding, we have for a materially inhomogeneous body

$$f_i^{\text{inh}} = -\left(\text{div}\,\mathbf{b}\right)_i = -b_{ji,j}, \quad \left(\text{div}\sigma\right)_i = \sigma_{ji,j}. \tag{3.22}$$

On account of the definition of the deformation gradient **F** in terms of the displacement gradient, we immediately have

$$b_{ji} = W\delta_{ji} - \sigma_{jk}\left(\delta_{ki} + u_{k,i}\right). \tag{3.23}$$

On substituting from this into the first of (3.22) and accounting for the second, we can write identically

$$f_i^{\text{inh}} = -b_{ji,j} \quad \text{with} \quad b_{ji} \equiv W\delta_{ji} - \sigma_{jk}u_{k,i} = \left(W1 - \sigma.\left(\nabla u\right)^T\right)_{ji}, \tag{3.24}$$

where the last expression is the one to be considered for the Eshelby stress in small strains. This procedure is *not* a linearization of **b**, a procedure that would have no meaning, because all elements of **b** should be of the energy type. Some authors, whom we will not cite, have mistakenly "linearized" the second contribution in the Eshelby stress, showing by that a lack of understanding of the notion. This remark has an importance in fracture studies. What about the *dynamic case*? For small strains we will have in components

$$\begin{aligned} P_i &= -\rho_0\dot{u}_j\left(\delta_{ji} + u_{j,i}\right) = -p_i + P_i^f, \quad p_i = \rho_0\dot{u}_i, \\ P_i^f &:= -\boldsymbol{\rho}_0\dot{u}_j u_{j,i} = -\left(\rho_0\dot{\mathbf{u}}.\left(\nabla\mathbf{u}\right)^T\right)_i, \end{aligned} \tag{3.25}$$

where the last equation defines the so-called *field momentum* (sometimes called *wave momentum*) as it appears in crystal physics (cf. Brenig, 1955). Of course, we note the remarkable identity

$$\mathbf{P}^f = \mathbf{p} + \mathbf{P}; \tag{3.26}$$

that is, field momentum is the sum of linear physical momentum and material momentum.

On account of the balance of linear physical momentum and of (3.25), we then check in the case of the presence of an external body force and of material inhomogeneities of both inertial and elastic origins that the balance of material momentum takes on the following form:

$$\dot{P}_i^f - b_{ji,j} = f_i^{\text{ext}} + f_i^{\text{inh}}, \tag{3.27}$$

wherein

$$b_{ji} = -\left(L\delta_{ji} + \sigma_{jk}u_{k,i}\right), \quad L = K - W, \quad K = \frac{1}{2}\rho_0(\mathbf{x})\dot{\mathbf{u}}^2, \quad f_i^{\text{ext}} = -\rho_0 f_{0j}u_{j,i}. \tag{3.28}$$

## 3.3 Classical Introduction of the Eshelby Stress by Eshelby's Original Reasoning

First, we note that if, by its very nature (components in the current configuration), (3.1) could be generated by a variation of the actual placement **x**, (3.4) would correspondingly be generated by an infinitesimal variation in the material point **X**. In order to respect the identity (3.7), these two variations should be related by

$$\delta\mathbf{x} + \mathbf{F}.\delta\mathbf{X} = \mathbf{0}, \quad \delta\mathbf{X} + \mathbf{F}^{-1}.\delta\mathbf{x} = \mathbf{0}, \tag{3.29}$$

where **F** and $\mathbf{F}^{-1}$ have their actual values. Mathematically, the elementary variations appearing in (3.29) should be defined by

$$\delta\mathbf{x} = \left.\frac{\partial\chi(\mathbf{X},t,\varepsilon)}{\partial\varepsilon}\right|_{\varepsilon=0}, \quad \delta\mathbf{X} = \left.\frac{\partial\chi^{-1}(\mathbf{x},t,\varepsilon)}{\partial\varepsilon}\right|_{\varepsilon=0}, \tag{3.30}$$

where ε is an infinitesimally small scalar. These variations, which may be referred to as material (at fixed **X)** and spatial or Eulerian (at fixed **x**) variations, were used by Maugin and Trimarco (1992). One way to establish any of the two parts of (3.29) is to notice that the material variation of **X** itself must vanish by definition, that is, with an improved notation,

$$\delta_X \mathbf{X} = \mathbf{0}, \quad \text{that is,} \quad \left.\frac{\partial \chi^{-1}(\chi(\mathbf{X},t,\varepsilon),\varepsilon)}{\partial \varepsilon}\right|_{\varepsilon=0} = \mathbf{0}.$$

The first part of (3.29) is but the variational version of (2.39). In terms of the displacement $\mathbf{u} = \mathbf{x} - \mathbf{X}$ and using only one coordinate system, the first of Equation 3.29 yields

$$\delta u_i = -u_{i,j}\delta X_j . \tag{3.31}$$

Then we cannot help but repeat in some detail the beautiful argument—a thought experiment—of J.D. Eshelby (1951, 1975), which this pioneer used to exhibit the notion of *material inhomogeneity force* in elasticity. (Note: Eshelby's collected works have been edited by Markenscoff and Gupta [2006].)

Consider to that effect Figure 3.1, representing an elastic body of finite extent with schematic boundary conditions in displacement and loading. The body is supposed to be perfectly elastic and made of a single material everywhere except perhaps at a "defect" *D* that creates a singularity in the elastic field and is symbolically represented by a small black region in the figure. We want to evaluate what we will now call the *configurational force* acting on that defect. In the spirit of d'Alembert and the principle of virtual work, to do so we must slightly move the defect in material space and

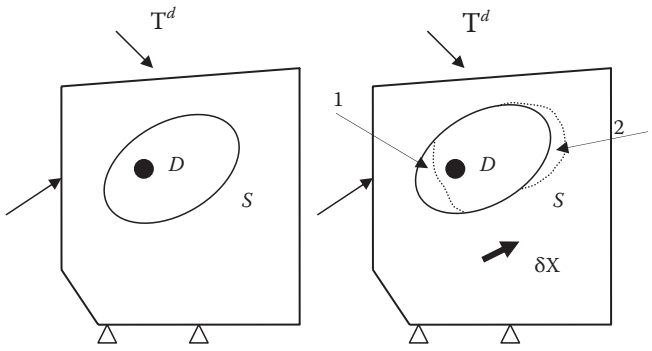


**FIGURE 3.1**
Evaluation of the force on a defect: (a) Original system, (b) replica. (Adapted from Maugin G.A. *Material inhomogeneities in elasticity*, London: Chapman & Hall, 1993.)

find out how the elastic field gets involved in this virtual material motion, hence the interest in the expression in (3.31). If, following Eshelby, we draw an arbitrary regular surface $S$ encircling the defect $D$ before its motion (Figure 3.1a), we also draw another surface $S'$ in the *replica* of Figure 3.1a (cf. Figure 3.1b), where $S'$ still encircles $D$ but is obtained from $S$ via a *uniform* infinitesimal displacement $-\delta\mathbf{X} = -\{\delta X_j;\ j = 1,2,3\}$ in the undeformed state of the body. Our aim is to compute the *energy change* from this rigid material displacement $\delta\mathbf{X}$ of the singularity. In the original system of Figure 3.1a, cut out the material inside $S$ and discard this material, thus creating a hole. We must apply suitable tractions on the surface of this hole to prevent any matter relaxation. In the replica in Figure 3.1b, we do the same but for the surface $S'$. The energy $E(S')$ inside $S'$ differs from that in $S$, $E(S)$, by the *addition* of the energy associated, schematically, with the crescent-shaped region $\omega_1$ and by the *removal* of the energy associated with the crescent-shaped region $\omega_2$, so that we can write

$$\delta E_1 := E(S') - E(S) = -\delta\mathbf{X}.\int_S W\mathbf{N}dA, \tag{3.32}$$

where $W$ is the elastic energy per unit volume in $K_R$. At this stage no change occurs outside the hole in the original system or in the energy of its loading mechanisms. Now, Eshelby tries to fit the body bounded by $S'$ into the hole $S$. Obviously, $S$ and $S'$ can be made to coincide by a simple translation in the undeformed state. But this is not true after deformation. The displacement on $S'$ differs from that on $S$ back to the original system by the amount given by (3.32). This is the displacement field that we shall apply to the surface of the hole. It corresponds to an amount of elementary work (remember that $\mathbf{n}.\sigma = \mathbf{T}^d$ at $S$):

$$\delta E_2 = -\int_S \delta\mathbf{u}.\mathbf{T}^d dA = -\int_S \delta\mathbf{u}.\sigma.\mathbf{N}dA, \tag{3.33}$$

where the minus sign is introduced because the unit normal $\mathbf{N}$ points outward of $S$. The subtlety now is as follows. Some of the energy variation (3.33) goes to raise the elastic energy in the material outside $S$ and some to increase the potential energy of the loading mechanisms. Now we can fit $S'$ into $S$ and weld across the interface. But though the displacement matches across the interface, the tractions on either side of this interface still differ by a quantity of the order of $|\delta\mathbf{X}|$. Accordingly, there exists a layer of body forces of the same order spread over the interface. As we relax this undesirable distribution of forces, the displacement changes by a quantity of the order of $|\delta\mathbf{X}|$. Therefore, an amount of energy of order $|\delta\mathbf{X}|^2$ is extracted. This will be negligible compared to (3.32) and (3.33). We are now in the situation where the system is as it was to begin with except that the defect has been shifted by the

material displacement $\delta\mathbf{X}$, as required in this thought experiment. Adding now (3.32) and (3.33) and accounting for (3.31), we obtain

$$\delta E = -\delta\mathbf{X}.\int_S (\mathbf{N}.\mathbf{b})\,dA, \tag{3.34}$$

where $\mathbf{b}$ is given by the second of (3.24). Because of the beauty of the argument Eshelby fully deserves to have his name associated with the material tensor $\mathbf{b}$ (to which he naturally gave a different name). The configurational force $\mathbf{F}^{\text{inh}}$ associated with the preceding calculation is such that

$$\delta E = \frac{\partial E}{\partial \mathbf{X}}.\delta\mathbf{X} = -\mathbf{F}^{\text{inh}}.\delta\mathbf{X}, \quad \mathbf{F}^{\text{inh}} = -\frac{\partial E}{\partial \mathbf{X}} = \int_S \mathbf{N}.\mathbf{b}\,dA. \tag{3.35}$$

This configurational force measures the negative of the change of energy in the rigid displacement of the defect $D$, in *material space.* This justifies the naming of "*mechanics on the material manifold*" or "*mechanics in material space*" used by some authors (e.g., Herrmann and Kienzler, 2000). This we personally christened *Eshelbian mechanics*.

## 3.4 Another Example Due to Eshelby: Material Force on an Elastic Inhomogeneity

This, if we may say so, is the example that started it all, with Eshelby's celebrated paper of 1951. Again we consider only small-strain elasticity and contemplate the material force acting on an inhomogeneity, such as a region of the material body where material properties, here elasticity coefficients, vary pointwise in the material. For instance, the components of the second-order tensor of elasticity coefficients $C^{ijkl}$ depend on three parameters $\xi_n$, $n = 1,2,3$, which may be the coordinates of a foreign inclusion in an otherwise uniform body. We write thus

$$C^{ijkl} = \bar{C}^{ijkl}\left(x_n - \xi_n\right) = C^{(ij)(kl)} = C^{klij}. \tag{3.36}$$

We assume that fixed surface tractions $\mathbf{T}^d$ are applied at the regular surface $\partial B$ of the body so that we can a priori state that

$$\frac{\partial}{\partial \xi_n}\left(n_j \sigma_{ji}\right) = 0 \quad \text{at} \quad \partial B. \tag{3.37}$$

In the same spirit as in the previous example, we envisage a slight variation of one of the $\xi_n$'s, say by the amount $\delta\xi_n$. This results in a variation of the external potential energy, assuming the absence of body force and quasistatics,

$$\frac{\partial E^{\text{ext}}}{\partial \xi_n} = -\frac{\partial}{\partial \xi_n}\int_{\partial B} \mathbf{u}.\mathbf{T}^d da = -\int_{\partial B} \frac{\partial \mathbf{u}}{\partial \xi_n}.(\boldsymbol{\sigma}.\mathbf{n})da, \tag{3.38}$$

on account of (3.37). Enforcing the balance of equilibrium in this special case (no body force, quasistatics), that is, $\sigma_{ji,j} = 0$ in $B$, and using the divergence theorem in (3.38), we obtain from (3.38) that

$$\frac{\partial E^{\text{ext}}}{\partial \xi_n} = -2\frac{\partial E^e}{\partial \xi_n}, \tag{3.39}$$

where $E^e$ is the total elastic energy given by

$$E^e(B) = \int_B \left(\frac{1}{2}C^{ijkl}\varepsilon_{ij}\varepsilon_{kl}\right)dv = \int_B \left(\frac{1}{2}\sigma_{ij}\varepsilon_{ji}\right)dv \tag{3.40}$$

in linear anisotropic (inhomogeneous or homogeneous) elasticity. We define the force acting on the inhomogeneity by

$$F_i^{\text{inh}} = \frac{\partial E^e}{\partial \xi_n}. \tag{3.41}$$

To evaluate this quantity we first consider finite differences and then take a limit. The difference of energy between two elastic bodies of the same shape and size acted on by the same surface tractions $\mathbf{T}^d$ but with different elasticity coefficients is obviously given by

$$\Delta W^e = \frac{1}{2}\int_B \left(\tilde{C}^{ijkl}\tilde{\varepsilon}_{ij}\tilde{\varepsilon}_{kl} - C^{ijkl}\varepsilon_{ij}\varepsilon_{kl}\right)dv = \frac{1}{2}\int_B \left(\tilde{\sigma}_{ij}\tilde{\varepsilon}_{ji} - \sigma_{ij}\varepsilon_{ji}\right)dv, \tag{3.42}$$

while there holds

$$\mathbf{n}.\boldsymbol{\sigma} = \mathbf{n}.\tilde{\boldsymbol{\sigma}} = \mathbf{T}^d \quad \text{at} \quad \partial B. \tag{3.43}$$

A simple consequence of this is that

$$\int_{\partial B} \left(\tilde{\sigma}_{ij} - \sigma_{ij}\right)n_i u_j da = 0 = \int_B \left(\tilde{\sigma}_{ij} - \sigma_{ij}\right)\varepsilon_{ji}dv, \tag{3.44}$$

where, we emphasize, $u_i$ is the elastic displacement pertaining to the solution without superimposed tildes. Combining now the last result with (3.42) provides the reduced expression

$$\Delta E^e = \frac{1}{2}\int_B \left(C^{ijkl} - \tilde{C}^{ijkl}\right)\tilde{\varepsilon}_{ij}\varepsilon_{kl}dv. \tag{3.45}$$

Thus

$$\frac{\Delta E^e}{\Delta\xi_n} = \frac{1}{2}\int_B \frac{\left(C^{ijkl} - \tilde{C}^{ijkl}\right)}{\Delta\xi_n}\tilde{\varepsilon}_{ij}\varepsilon_{kl}dv, \tag{3.46}$$

and passing to the limit for vanishingly small $|\Delta\xi_n|$, subscript $n$ fixed, delivers

$$F_n^{\text{inh}} = \frac{\partial E^e}{\partial\xi_n} = -\frac{1}{2}\int_B \frac{\partial C^{ijkl}}{\partial\xi_n}\varepsilon_{ij}\varepsilon_{kl}dv. \tag{3.47}$$

Then the relationship to the Eshelby stress follows from the evaluation of the derivative under the integral sign and noting that $\partial/\partial\xi_n = -\partial/\partial x_n$. We successively have

$$F_n^{\text{inh}} = \frac{1}{2}\int_B \left(\left(C^{ijkl}\varepsilon_{ij}\varepsilon_{kl}\right)_{,n} - 2C^{ijkl}u_{i,j}u_{,kln}\right)dv = \int_B \left(\left(W^e\right)_{,n} - \sigma_{kl}u_{k,ln}\right)dv, \tag{3.48}$$

or

$$F_n^{\text{inh}} = \int_B \left(\left(W^e\right)_{,n} - \left(\sigma_{mk}u_{k,n}\right)_{,m} + \sigma_{mk,m}u_{kn}\right)dv = \int_{\partial B}\left(\mathbf{n}.\mathbf{b}\right)_n da, \tag{3.49}$$

with a quasistatic Eshelby elastic stress given by (3.24).

## 3.5 Gradient Elastic Materials

The elementary material force associated with (3.47) is the inhomogeneity force given by

$$f_n^{\text{inh}} = -\left.\frac{\partial W^e}{\partial X_n}\right|_{\text{expl}} = -\frac{1}{2}\frac{\partial C^{ijkl}}{\partial X_n}\varepsilon_{ij}\varepsilon_{kl}, \tag{3.50}$$

where the strain (a field) is kept fixed. Imagine a simple variation of all elasticity coefficients in the same way, for example,

$$W^e(\varepsilon;\mathbf{X}) = \frac{1}{2}\left(C_0^{ijkl}\exp\left(-\alpha\mathbf{X}.\mathbf{e}_1\right)\right)\varepsilon_{ij}\varepsilon_{kl}, \quad \alpha > 0. \tag{3.51}$$

From (3.50) we have thus

$$f_1^{\text{inh}} = \mathbf{e}_1.\mathbf{f}^{\text{inh}} = \alpha W^e. \tag{3.52}$$

Since $\alpha$ is positive and $W^e$ is positive definite, the scalar $f_1^{\text{inh}}$ is positive in the direction of decrease in the value of the material constants. Accordingly, although it is not a force in the Newtonian sense, it provides an *indicator* of the *direction of variation of (here) elastic properties.* Here it is oriented *from the harder to the softer* part of the material. This will also hold with properties varying abruptly such as at the interface in layered composites.

## 3.6 Interface in a Composite

Both Equations 3.35 and 3.49 exhibit the fundamental role played by the Eshelby stress in the formulation of *configurational* or *material* forces driving singularities and/or material inhomogeneities. This can also be seen at an interface between two different elastic materials. Consider that the interface is an ideal mathematical surface $\Sigma$ of zero thickness obtained by the flattening of a regular region $B_T$ of transition. Let $x$ be the local coordinate orthogonal to this transition layer of thickness $(x_2–x_1)$ counted along the normal of the layer, which may be supposed to be flat locally without loss in generality. The material inhomogeneity force along $x$ per unit "surface" of this transition layer will be given by (cf. (3.47))

$$f^{\text{inh}} = \int_{x_1}^{x_2}\left(\frac{1}{2}\left(\frac{\partial C^{ijkl}}{\partial x}\right)\varepsilon_{ij}\varepsilon_{kl}\right)dv. \tag{3.53}$$

As the thickness of the transition layer goes to zero (the so-called *pill-box method* of engineers), it is easy to see that this expression will reduce to the singular expression

$$f^{\text{inh}}(\Sigma) = -\frac{1}{2}\left[C^{ijkl}\right]\varepsilon_{ij}\varepsilon_{kl}, \tag{3.54}$$

where we have introduced the jump [..] in elasticity coefficients at Σ by

$$[C] = C^{+} - C^{-}, \tag{3.55}$$

where $C^{\pm}$ are the uniform limits of $C$ in approaching Σ from its *plus* and *minus* sides, respectively, the unit normal being oriented from the *minus* to the *plus* side.

Accordingly, for hypothetical identical deformations on both sides of Σ, and for a one-dimensional model, we see that the "material force" $f^{\text{inh}}(\Sigma)$ is directed *from the harder to the softer side* of the surface Σ. It is not a force of the Newtonian type. We do not see it in the physical frame. It is none other than an *indicator* (a vectorial one in the truly three-dimensional case) of the manner in which material (here elastic) properties vary smoothly (cf. (3.53)) or abruptly (cf. (3.54)). On account of the continuity of tractions at Σ, $n.[\sigma] = 0$, we let the reader show that

$$\mathbf{f}^{\text{inh}}(\Sigma) = -\mathbf{n}.[\mathbf{b}]. \tag{3.56}$$

## 3.7 The Case of a Dislocation Line (Peach–Koehler Force)

In the preceding we examined successively the case of a localized singularity (in the *bulk*) and the case of smoothly or abruptly distributed material inhomogeneities, hence in the *bulk* or at a surface, so that we now conclude the *historical* contributions to this theory by the evaluation of a material force acting on one singular *line*. This was first developed by Peach and Koehler (1950) in a celebrated paper, a true landmark in dislocation theory. A dislocation line $L$ is seen in continuum physics as a line along which the displacement vector of elasticity suffers, in a certain sense, a finite discontinuity, called the *Burgers vector*, that we shall note $\tilde{\mathbf{b}}$ to avoid any confusion with Eshelby stress (although there exists a relation between these two notions). The magnitude and direction of $\tilde{\mathbf{b}}$ characterize the different types of dislocations (see Lardner, 1974). In a discrete crystal $\tilde{\mathbf{b}}$ can only be equal to a finite number of the vectors of the lattice. What exactly occurs is that in the presence of a dislocation line $L$, the displacement vector $\mathbf{u}$ is no longer a single-valued function of the coordinates: It receives a finite increment $\tilde{\mathbf{b}}$ in going along a circuit around the dislocation line $L$. With a definite choice of sign, this is expressed by

$$\oint_S d\mathbf{u} = \oint_S \frac{d\mathbf{u}}{ds} ds = -\tilde{\mathbf{b}}, \tag{3.57}$$

where $s$ is a line coordinate along the circuit $S$. A dislocation is called a screw dislocation when $\tilde{\mathbf{b}}$ is parallel to the unit tangent $\tau$ to $L$. It follows from this a singularity in the distortion $\beta = \nabla\mathbf{u}$. On subjecting an elastic crystal containing dislocations to an appropriate external loading, some of the atoms in the discrete view will move, and the dislocation line will seem to move in the opposite direction. The dislocation is thus subjected to a "displacement," and the true "mechanician" will associate with that motion a "force." This is the *driving force* on the dislocation, not a force in the classical Newtonian sense, since the dislocation line is not a massive object but a mathematical notion (a singularity of the field). This force is called the *Peach–Koehler force* after its creators, the qualification of *creators—not* discoverers—being justified here since this force does not belong to the physical space. However, this "force" can be computed if we know the field solution of the problem at hand outside the singularity. Its original derivation goes as follows.

In the continuum elastic description of a defective crystal, the interaction energy between a dislocation $D$ characterized by an elastic displacement field $\mathbf{u}^D$ and an applied stress field $\sigma^A$ is given by

$$E(D,A) = -\int_S \mathbf{n}.\sigma^A.\mathbf{u}^D da = -\int_S \mathbf{u}^D.\mathbf{T}^A da, \tag{3.58}$$

where $\mathbf{T}^A$ is the traction associated with stress $\sigma^A$ and $S$ is the boundary of the region containing the dislocation line L. Equation 3.58 is the expression of a *potential energy*. The dislocation itself is supposed to *not* produce any traction at $S$. Thus adding the vanishing contribution $-\mathbf{n}.\sigma^D.\mathbf{u}^A = -\mathbf{u}^A.\mathbf{T}^D$ to the integrand in (3.58), we obtain

$$E(D,A) = -\int_S \left(\mathbf{u}^D.\mathbf{T}^A - \mathbf{u}^A.\mathbf{T}^D\right) da. \tag{3.59}$$

According to the statement of the well-known *Rayleigh–Betti reciprocity theorem* of linear (isotropic or anisotropic) elasticity (cf. Maugin, 1992, p. 87, Equation A.16) for any closed surface $\partial\Omega$ that does not embrace any body force or singularity, we have

$$\int_{\partial\Omega} \left(\mathbf{u}^1.\mathbf{T}^2 - \mathbf{u}^2.\mathbf{T}^1\right) da = 0, \tag{3.60}$$

for two elastic solutions labeled 1 and 2. Accordingly, the vector

$$\mathbf{g} := \mathbf{u}^1.\sigma^2 - \mathbf{u}^2.\sigma^1, \tag{3.61}$$

is divergence free in that enclosed surface $\partial\Omega$. Applying this reasoning to our dislocation case, the surface $S$ can be replaced by any other surface enclosing

the line $L$, as the difference between (3.59) and the new integral will be zero. In particular, we may choose a surface such as that in Figure 3.2, made up of an open tube enclosing $L$ and the top $\Sigma_+$ and bottom $\Sigma_-$ of an arbitrary discontinuity surface $\Sigma$ leaning on the dislocation line $L$. Here Eshelby (1982, p. 211) proposes an ingenious argument that is often bypassed (compared to the treatments of Nabarro [1967, p. 83] or Kosevich [1979, p. 63]). Suppose, to simplify the reasoning (but this is really immaterial), that the cross-section of the small tube that provides a jacket for the loop is everywhere along $L$ a circle of radius $a$. Then divide the tube into a large number of short cylindrical beads threaded by the dislocation (i.e., somewhat like a necklace). While integrating the second contribution in (3.59) over one bead, we may take the comparatively slowly spatially varying field $\mathbf{u}^A$ outside the integral. The stress field $\sigma^D$ of a dislocation is of the order of the inverse, $1/r$, of the distance $r$ from the dislocation (for this, see Nabarro [1987] or Kosevich [1979]). Thus, the total traction exerted on the curved surface of the cylinder will be of the order of $a^2.a^{-1} = a$, while each bead is in static equilibrium. Accordingly, we are now sure that the second contribution in (3.59) will go to zero with $a$. As to the first contribution, according to a classical evaluation of dislocation theory (see Nabarro [1987] or Kosevich [1979]), we have $|\mathbf{u}^D| = \mathrm{O}(\ln r)$ for small $r$, so that this contribution causes no trouble. As a result, we shall be left in (3.59) with the integral over the two sides $\Sigma_+$ and $\Sigma_-$ of the cut $\Sigma$. The second contribution from (3.59) is continuous across $\Sigma$ while $\mathbf{u}^D$ has a discontinuity of the value equal to the Burgers vector $\tilde{\mathbf{b}}$. Therefore, the expression in (3.59) is now reduced to

$$E(D,A) = -\tilde{\mathbf{b}}.\int_{\Sigma=\Sigma_+} \mathbf{T}^A da, \tag{3.62}$$

where $\Sigma_+$ is oriented as $\Sigma$. To complete the proof we consider that when the dislocation loop $L$ suffers a little change of shape, say by an infinitesimal

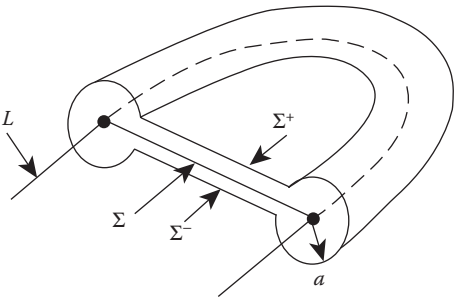


**FIGURE 3.2**
Shrinking of $S$ to a surface englobing the dislocation line $L$ and a singularity surface $\Sigma$. (Adapted from Maugin G.A. *Material inhomogeneities in elasticity*, London: Chapman & Hall, 1993.)

vectorial displacement $\delta\xi$ (cf. Figure 3.3), then the corresponding change in (3.62), $\delta E$, is just the value of the integral in the right-hand side of (3.62) taken over the freshly formed portion of the cut. This additional infinitesimal surface element can be written in vector form as

$$\delta\mathbf{a} = d\mathbf{X} \times \delta\boldsymbol{\xi}, \quad d\mathbf{X} \equiv \tau ds, \tag{3.63}$$

where $\tau$ is the unit tangent vector to $L$. We can now write $\delta E$ as

$$\delta E = -\int_L \mathbf{f}^{(PK)}.\delta\xi ds, \tag{3.64}$$

where the Peach–Koehler "force" acting on the dislocation line $L$ per unit length, due to an applied stress field $\sigma^A$, is given by

$$\mathbf{f}^{(PK)} = \left(\tilde{\mathbf{b}}.\sigma^A\right) \times \tau. \tag{3.65}$$

Like the material forces exhibited in previous paragraphs, the Peach–Koehler force is generated in a thought experiment by a displacement of the defect, the dislocation loop $L$, in material space.

Several remarks are in order. First, there exists a discussion whether it is the whole of $\sigma^A$ or just its deviatoric part that should be involved in the computation of $\mathbf{f}^{(PK)}$ (cf. Nabarro, 1967, p. 84). Second, the expression (3.65) is very similar to that of the force acting on a current-carrying wire in applied electromagnetism. Third, a generalization of (3.65) based on *nonlinear elasticity* was given by Zorski (1981). Finally, a dynamic equation was derived when velocities are involved. This was achieved by Kosevich (1962, 1964)

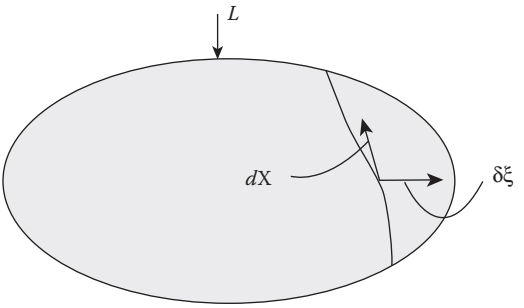


**FIGURE 3.3**
Slight change in the dislocation loop $L$ generating the Peach–Koehler force. (Adapted from Maugin G.A. *Material inhomogeneities in elasticity*, London: Chapman & Hall, 1993.)

using an analogy with Lorentz's derivation of the equation of motion of an electron accounting for its self-action (cf. Lorentz, 1952). The resulting equation reads

$$\mathbf{f}^{(PK)} = \left(\mathbf{p}.\tilde{\mathbf{b}}\right)\left(\mathbf{V}\times\boldsymbol{\tau}\right), \tag{3.66}$$

where the left-hand side is given by expression (3.65), $\mathbf{p} = \rho_0\mathbf{v}$ is the linear momentum corresponding to a displacement rate due to both the external field and the self-field of the dislocation, and $\mathbf{V}$ is the velocity field of the position of the dislocation loop $L$. A field-theoretic derivation of (3.66) was given by Rogula (1977, p. 709). The right-hand side of (3.66) can be further transformed to give it the appearance of the product of a "mass" (so-called effective mass of a dislocation) and an "acceleration," so that Equation 3.66 takes a "Newtonian" form—see Kosevich (1979, pp. 104–109) for this. Remarkably, the right-hand side of (3.66) is of second order jointly in the physical velocity of the material and the dislocation velocity. More recently, a connection between $\mathbf{f}^{(PK)}$ and the Eshelby stress has been established (cf. Denzer, 2006)—see also Section 3.11 and Chapter 9 for more complex media.

## 3.8 Four Formulations of the Balance of Linear Momentum

We already have at hand three "formulations" of the balance of linear momentum. These are given by (2.81a), (2.87), and (3.13). Consider the case of no external body force but a materially inhomogeneous body. These equations read:

$$\rho\frac{d}{dt}\mathbf{p}^t - \operatorname{div}\boldsymbol{\sigma} = \mathbf{0}, \tag{3.67}$$

$$\left.\frac{\partial}{\partial t}\mathbf{p}_R\right|_X - \operatorname{div}_R\mathbf{T} = \mathbf{0}, \tag{3.68}$$

and

$$\left.\frac{\partial}{\partial t}\mathbf{P}\right|_X - \operatorname{div}_R\mathbf{b} = \mathbf{f}^{\text{inh}}. \tag{3.69}$$

Equation 3.68 is deduced from (3.67) by multiplication by $J_F$. Then (3.69) follows from (3.68) after application of the deformation **F** to its right. Why not pursue the procedure by multiplying (3.69) by $J_F^{-1}$, constructing thus a material equation of momentum but per unit volume of the current configuration? We define thus $\hat{\mathbf{P}} = J_F^{-1}\mathbf{P} = \rho\mathbf{C}.\mathbf{V}$ and $\hat{\mathbf{f}}^{\text{inh}} = J_F^{-1}\mathbf{f}^{\text{inh}}$. Accounting now for obvious identities given in Chapter 2, we easily show that the result of this manipulation is the following balance of material momentum (cf. Maugin and Trimarco, 1992):

$$\frac{\partial}{\partial t}\hat{\mathbf{P}}\bigg|_x - div\left(\mathbf{B} - \mathbf{v}\otimes\hat{\mathbf{P}}\right) = \hat{\mathbf{f}}^{\text{inh}}, \tag{3.70}$$

where we have set (see (2.138))

$$\mathbf{B} := -\left(J_F^{-1}L\mathbf{F} - \mathbf{T}_{(1)}\right), \quad \mathbf{T}_{(1)} := J_F^{-1}\frac{\partial W_{(1)}}{\partial \mathbf{F}^{-1}}, \tag{3.71}$$

where the last stress has already been introduced in (2.133). Equation 3.70 is the Eulerian analog of (3.68) in the sense that its exploits the partial derivatives $\nabla$ and $\partial/\partial t$ at fixed placement **x**, but its components are in material space. **B** is a two-point tensor field with variance similar to that of **F**. It can also be written as

$$\mathbf{B} := -\left(J_F^{-1}L\mathbf{F} - \mathbf{T}_{(1)}\right) = -J_F^{-1}\mathbf{F}L + \mathbf{F}.\sigma, \tag{3.72}$$

where $\sigma$ is the *Cauchy stress in the Eshelby format* as defined by (2.138) (Maugin and Trimarco 1992). Furthermore, by factorizing out the actual density $\rho$, we arrive at the following expression:

$$\rho\frac{d}{dt}\left(\hat{\mathbf{P}}/\rho\right) - \text{div}\,\mathbf{B} = \hat{\mathbf{f}}^{\text{inh}}. \tag{3.73}$$

Now it is sufficient to check that by applying $\mathbf{F}^{-1}$ to the right of this equation, after some labor, one recovers the original Equation 3.67. We have thus completed the flowchart given in Figure 3.4. Just as in a legerdemain prowess, we have made the material inhomogeneity force appear and then disappear. The two formulations at the upper-left and lower-right corners involve two-point field stress tensors, while the others in the lower-left and upper-right corners involve true tensors in current and material configurations, respectively. This play with various representations of the same physically meaningful

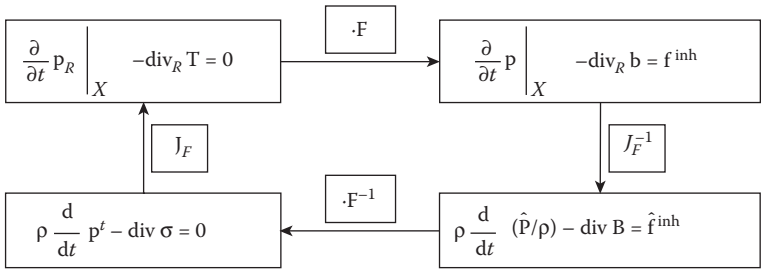


**FIGURE 3.4**
Flowchart exhibiting the four formulations of the linear momentum equation in the absence of physical forces. (Adapted from Maugin, G.A., *Material inhomogeneities in elasticity*, Figure 4.3, p. 86, Chapman & Hall, London, 1993.)

equation is systematically expressed in works by Steinmann et al. (2001 on). If these equations are mathematically equivalent (insofar as the fields considered are sufficiently smooth to allow for the different operations) at any bulk points **x** and **X** put in one-to-one correspondence through the deformation, the fact remains that data in the bulk and the bounding surface are only meaningful as Newtonian concepts, that is, in the current configuration in physical space. To end this paragraph, we note that the symmetry condition on $\sigma$ and **b** translate to the equations

$$\mathbf{B}.\mathbf{F}^{-1} = \mathbf{F}^{-T}.\mathbf{B}^{T}, \quad \mathbf{T}_{(1)}.\mathbf{F}^{-1} = \mathbf{F}^{-T}.\mathbf{T}_{(1)}^{T}. \tag{3.74}$$

The multiplicity of representations exhibited in the preceding for the balance of linear momentum necessarily requires, by duality, the existence of various variational statements using either the *direct*- or the *inverse*-motion description.

## 3.9 Variational Formulations in Elasticity

### 3.9.1 Variation of the Direct Motion

To simplify the presentation we consider the case of inhomogeneous finite-strain elasticity in quasistatics and no body force. The equilibrium equations in the bulk and at the boundary follow from the following "natural" variational principle:

$$\delta_X \left( \int_{B_R} W(\mathbf{F};\mathbf{X},\mathbf{x}) dV - \int_{\partial B_R} \bar{\mathbf{T}}^d(\mathbf{X}).\mathbf{x}\, dA \right) = 0, \tag{3.75}$$

where $\bar{\mathbf{T}}^d$ is a so-called dead loading and $\delta_X$ is a *material* variation (at fixed $\mathbf{X}$). The dependency of $W$ on $\mathbf{x}$ means that the contribution of an externally applied force has been included in that potential. The material variation conserves material volume and commutes with material space integration and gradient, so that (3.75) immediately yields

$$\int_{\partial B_R} \left( \left( \partial W / \partial \mathbf{F} \right).\mathbf{N} - \bar{\mathbf{T}}^d(\mathbf{X}) \right).\delta_X \mathbf{x}\, dA - \int_{B_R} \left( \mathrm{div}_R \left( \partial W / \partial \mathbf{F} \right) - \partial W / \partial \mathbf{x} \right).\delta_X \mathbf{x}\, dV = 0, \tag{3.76}$$

so that there follow the local equations

$$\mathrm{div}_R \mathbf{T} - \mathbf{f}^d = \mathbf{0} \quad \text{in} \quad B_R, \quad \mathbf{N}.\mathbf{T} = \bar{\mathbf{T}}^d \quad \text{at} \quad \partial B_R, \tag{3.77}$$

with

$$\mathbf{T} = \partial W / \partial \mathbf{F}, \quad \mathbf{f}^d = \partial W / \partial \mathbf{x}, \tag{3.78}$$

for an arbitrary variation and any material volume and surface elements. Here we can write

$$W(\mathbf{F};\mathbf{X},\mathbf{x}) = W^e(\mathbf{F};\mathbf{X}) - \rho_0(\mathbf{X})\varphi(\mathbf{x}), \tag{3.79}$$

separating thus the true elastic energy from the potential due to, for example, gravity. Then

$$\mathbf{f}^d = \frac{\partial W}{\partial \mathbf{x}} = -\rho_0 \frac{\partial \varphi}{\partial \mathbf{x}} = -\rho_0(\mathbf{X}) \nabla \varphi. \tag{3.80}$$

### 3.9.2 A Two-Fold Classical Variation: The Complementary Energy

In principle, the introduction of the *complementary energy* density $W_c$ through a Legendre transformation allows one to shift from strains to stresses as independent variables. But some caution must be taken in the case of finite strains. Indeed, as $\mathbf{T}$ can be viewed as the thermodynamic dual of $\mathbf{F}$, one could be tempted to choose $\mathbf{T}$ as the natural variable stresswise. This choice would even be additionally supported by the fact that $\mathbf{T}$ is naturally related to the traction. But for several reasons this would be an illegitimate choice. First, $\mathbf{T}$ being a two-point tensor field, it is not frame invariant as a tensor.

Second, **T** is not positive (or negative) definite, so that no polar decomposition applies to it. As a result, basing on **T** as the only variable, the complementary energy $W_c$ could not be made depending on material quantities, as constitutive laws are requested. Finally, a lack of uniqueness for the inversion with strains could emerge even in the presence of fixed tractions at the boundary and unique solution in stresses. This lack of uniqueness is due to the indeterminacy of the finite rotation **R** (see Ogden, 1984). For the appropriate choice of the stress tensor and for a detailed discussion of this problem, the reader is referred to Ogden (1984), Reissner (1953), Manacorda (1954), Hanyga and Seredynska (1983), Maugin and Trimarco (1993), and Knops et al. (2003). Indeed, following Reissner (1953)—who himself followed Hellinger (1914)—we may consider the second Piola–Kirchhoff stress **S** in such a way that the relevant Legendre transformation reads as follows for an elastic material in finite strains:

$$W(\mathbf{S},\mathbf{E}) = \mathrm{tr}(\mathbf{S}.\mathbf{E}) - W_c\,(\mathbf{S}). \tag{3.81}$$

Then we can state the following variational principle (Maugin and Trimarco, 1992b):

$$\begin{aligned}\delta_X\Big[\int_{B_R}\big(\mathrm{tr}(\mathbf{S}.\mathbf{E}) - W_c\,(\mathbf{S};\mathbf{X}) + \rho_0(\mathbf{X})\varphi(\mathbf{x})\big)dV \\ -\int_{\partial B_{R1}}(\mathbf{x}-\mathbf{x}_0)(\mathbf{FS}).\mathbf{N}d\,A - \int_{\partial B_{R2}}\bar{\mathbf{T}}^d.\mathbf{x}dA\Big] = 0.\end{aligned} \tag{3.82}$$

The variation now is a *two-fold* variation, as both **x** and **X** may vary independently, while the material particle **X** is fixed. It is not difficult to show that this variation results in the following set of equations:

$$\mathrm{div}_R(\mathbf{FS}) + \bar{\mathbf{f}}^d = \mathbf{0} \quad \text{in} \quad B_R, \tag{3.83}$$

$$\mathbf{FS} - \bar{\mathbf{T}}^d = \mathbf{0} \quad \text{on} \quad \partial B_{R1}, \tag{3.84}$$

$$\mathbf{x} - \mathbf{x}_0 = \mathbf{0} \quad \text{on} \quad \partial B_{R2}, \tag{3.85}$$

together with the reciprocal constitutive relation

$$\mathbf{E} - (\partial W_c / \partial\,\mathbf{S}) = \mathbf{0}. \tag{3.86}$$

Note that Equations 3.83 through 3.85, although expressed at material point $\mathbf{X}$, have components in the current configuration $K_t$. This naturally leads to considering the *inverse-motion* kinematic description.

### 3.9.3 Inverse Motion

This may be called the Piola description because we naturally consider the motion $\mathbf{X} = \chi^{-1}(\mathbf{x},t)$ and the related strain measures $\mathbf{C}^{-1}$ and $\mathbf{E}^{(-2)}$. Accordingly, we now consider the elastic energy density $w(\mathbf{F}^{-1},\mathbf{X})$ per unit volume of the current configuration $K_t$. The dependence of $w$ on $\mathbf{F}^{-1}$ has to be understood as through $\mathbf{C}^{-1}$ or $\mathbf{E}^{(-2)}$. Following the Piola procedure, we consider the following variational formulation (Maugin and Trimarco, 1993):

$$\delta_x\left[\int_B w\left(\mathbf{F}^{-1},\mathbf{X},\mathbf{x}\right)dv + \int_{\partial B}\tilde{\mathbf{T}}^d\left(\mathbf{x}\right).\mathbf{X}\,da\right] - \int_{\partial B} W\mathbf{N}.\delta_x\mathbf{X} = 0, \quad W = J_F w. \tag{3.87}$$

This entails the following local equations:

$$\operatorname{div}\left(\partial w/\partial \mathbf{F}^{-1}\right) - \partial w/\partial \mathbf{X}\big|_{\text{expl}} = \mathbf{0} \quad \text{in} \quad B, \tag{3.88}$$

$$\left(\left(\partial w/\partial \mathbf{F}^{-1}\right).\mathbf{F}^{-T} - w\mathbf{1}\right).\left(\mathbf{F}^T\mathbf{n}\right) + \tilde{\mathbf{T}}^d = \mathbf{0} \quad \text{on} \quad \partial B. \tag{3.89}$$

In contrast to (3.83) and (3.84), Equations 3.88 and 3.89 are expressed at the current placement $\mathbf{x}$, but their components are in the reference configuration $K_R$. This set of equations bears no relationship, in principle, with the classical equilibrium problem. As matter of fact, this set stands for the *balance among configurational forces* as shown by (3.88) and the expression of the second contribution in its left-hand side. The preceding computation and results call for various comments.

First, we note that (3.88) does not capture the spatial body force that would be given by $\partial w/\partial \mathbf{x} = \nabla w\big|_{\text{expl}}$ because $\delta_x\mathbf{x} = \mathbf{0}$ from its very definition (i.e., keeping $\mathbf{x}$ fixed). We may express this *verbatim* by "*the Eulerian variation is insensitive to the spatial (body) forces*." However, this variation does capture the force of inhomogeneity.

Second, we note that $\tilde{\mathbf{T}}^d\left(\mathbf{x}\right)$ is considered as a *dead loading* in the variation (3.87), although, of course, this traction cannot be a classical dead loading in the sense that it does change with configuration.

Third, the material variation $\delta_X\mathbf{x}$ can be interpreted as the most classical virtual infinitesimal displacement of a point in a continuum. Quite differently, the spatial or Eulerian variation $\delta_x\mathbf{X}$ has to be understood as a *re-placement* or *rearrangement of material points* on the material manifold. This remark suggests that the corresponding forces, related to this variation by conjugacy or

duality, are of *thermodynamic* nature. We shall return to this concept when examining the geometric meaning of the Eshelby stress (Chapter 6). As a matter of fact, (3.88) is none other than the equilibrium material equation involving the Eshelby stress but in a disguise. For the purpose of this identification, we let the reader check that one can write

$$\int_{\partial B}\left(\partial w/\partial \mathbf{F}^{-1}\right).\mathbf{n}\,da \equiv -\int_{\partial B_R}\mathbf{N}.\mathbf{b}\,dA = \int_{B_R}\left(\partial w/\partial \mathbf{X}\right)\big|_{\text{expl}}\,dv \equiv \int_{B_R}\left(\partial W/\partial \mathbf{X}\right)\big|_{\text{expl}}\,dV. \tag{3.90}$$

This is none other than the *global balance for the Eshelby stress and the material force of inhomogeneity*, either in a spatial region or in the corresponding material region. A similar approach can be found in works by Golebiewska and Herrmann (1983) and Pak and Herrmann (1986).

Finally, a complementary energy principle can also be stated in the framework of the inverse motion by proposing the following variational principle ($\bar{\mathbf{S}}$ is the stress dual of the strain measure $\mathbf{E}^{(-2)}$ ; cf. (2.133)):

$$\delta_x\left[\int_B w\left(\bar{\mathbf{S}},\mathbf{E}^{(-2)},\mathbf{X}\right)dv + \int_{\partial B_1}\bar{\mathbf{S}}.\mathbf{F}^{-1}\mathbf{n}.\left(\mathbf{X}-\mathbf{X}_0\right)da + \int_{\partial B_2}\tilde{\mathbf{T}}^d\left(\mathbf{x}\right).\mathbf{X}\,da\right]$$
$$-\int_{\partial B} W\mathbf{N}.\delta_x\mathbf{X}\,dA = 0, \tag{3.91}$$

where the fields $\mathbf{X}(\mathbf{x})$ and $\bar{\mathbf{S}}$ are "varied" independently (Maugin and Trimarco, 1993).

## 3.10 More Material Balance Laws

To illustrate this point we consider the dynamics of pure finite-strain elasticity in the presence of material inhomogeneities. We consider the following equations:

- *Balance of material momentum* (in the absence of body force):

$$\left.\frac{\partial \mathbf{P}}{\partial t}\right|_X - \text{div}_R\mathbf{b} = \mathbf{f}^{\text{inh}} \tag{3.92}$$

- *Energy equation* (no heat conduction, no dissipation, no heat supply):

$$\left.\frac{\partial H}{\partial t}\right|_X - \nabla_R.\left(\mathbf{T}.\mathbf{v}\right) = 0 \tag{3.93}$$

- *Definitions and constitutive equation*:

$$\mathbf{P} = -\rho_0 \mathbf{v}.\mathbf{F}, \quad \mathbf{b} = -\left(L\mathbf{1}_R + \mathbf{T}.\mathbf{F}\right), \quad L = K - W,$$
$$H = K + W, \quad K = \frac{1}{2}\rho_0(\mathbf{X})\mathbf{v}^2, \tag{3.94}$$

and

$$W = \bar{W}(\mathbf{F};\mathbf{X}), \quad \mathbf{T} = \frac{\partial \bar{W}}{\partial \mathbf{F}}, \quad \mathbf{f}^{\text{inh}} = \left.\frac{\partial L}{\partial \mathbf{X}}\right|_{\text{expl}}. \tag{3.95}$$

Equation 3.92 is *one* possible "material" field equation, a strict conservation law in the absence of inhomogeneities and applied body force. It relates to the notion of linear momentum but on the material manifold. There may exist other material balance laws, some of which we illustrate now by considering the so-called *divergence transformation* or gradient operation applied to a Lagrangian density. Indeed, consider a priori the material gradient of the "Lagrangian" density defined in ($3.94_3$). That is,

$$\nabla_R L = D, \tag{3.96}$$

where $D$ is the results of the evaluation of the left-hand side, so that (3.96) is an identity. It is an easy matter to show that this yields

$$\nabla_R L = \mathbf{f}^{\text{inh}} - \left.\frac{\partial \mathbf{P}}{\partial t}\right|_X - \text{div}_R\left(\mathbf{T}.\mathbf{F}\right). \tag{3.97}$$

But this is nothing but (3.92) in disguise. Now, (3.97), as its stands, is a material covectorial equation. We can operate on both of its sides by taking the *inner product* with $\mathbf{X}$ and the *vectorial product* with $\mathbf{X}$. Considering the first operation, we have, after some simple manipulations,

$$\left.\frac{\partial}{\partial t}\left(\mathbf{P}.\mathbf{X}\right)\right|_X - \nabla_R.\left(\mathbf{b}.\mathbf{X}\right) - \mathbf{f}^{\text{inh}}.\mathbf{X} - 3L - \text{tr}\left(\mathbf{T}.\mathbf{F}\right) = 0. \tag{3.98}$$

Now we would not know how to proceed further if we did not notice the parallelism between the deductions of Equations 3.92 and 3.93 from the linear (physical) momentum equation of the Piola–Kirchhoff formulation. Indeed, these two equations follow like identities from that equation simply noted $\mathbf{m} = \mathbf{0}$ by considering

$$\mathbf{m}.\left.\frac{\partial \chi}{\partial \mathbf{X}}\right|_t = \mathbf{0}, \quad \mathbf{m}.\left.\frac{\partial \chi}{\partial t}\right|_X = 0. \tag{3.99}$$

Thus, in parallel with the inner product $\mathbf{X}.\nabla_R L$, we propose to evaluate the scalar quantity $t(\partial H/\partial t)$. This yields

$$\frac{\partial}{\partial t}(Ht)\Big|_X - H - \nabla_R.(t\,\mathbf{T}.\mathbf{v}) = 0, \tag{3.100}$$

because $t$ and $\boldsymbol{X}$ are good independent variables in the $(\mathbf{X},t)$ space–time parametrization. We can also evaluate the inner product of the original balance of linear momentum with the placement $\mathbf{x}$, obtaining thus the identity

$$\frac{\partial}{\partial t}(\mathbf{p}_R.\mathbf{x})\Big|_X - \mathbf{p}_R.\mathbf{v} - \nabla_R.(\mathbf{T}.\mathbf{x}) + \mathrm{tr}(\mathbf{T}.\mathbf{F}) = 0. \tag{3.101}$$

On combining *plus* (3.98), *minus* (3.100), and *minus* (3.101), we are led to the following remarkable identity (Maugin, 1993, p. 91):

$$\frac{\partial}{\partial t}(\mathbf{P}.\mathbf{X} - Ht - \mathbf{p}_R.\mathbf{x})\Big|_X - \nabla_R.(\mathbf{b}.\mathbf{X} - t\mathbf{Q} - \mathbf{T}.\mathbf{x}) = \mathbf{f}^{\mathrm{inh}}.\mathbf{X} + 2L, \tag{3.102}$$

where $\mathbf{Q} = \mathbf{T}.\mathbf{v}$. The quantity of which the time derivative is taken in the left-hand side of this equation is not a commonly considered one in continuum mechanics. It is homogeneous to a so-called *action*, that is, the *product of time by energy* per unit volume. In particular, we shall see later on that

$$A := \mathbf{P}.\mathbf{X} - Ht, \tag{3.103}$$

is the *canonical action* in analytical continuum mechanics.

It remains now to take the *vector product* of (3.96) with $\mathbf{X}$. This is a much longer affair. We leave this to the reader by way of exercise. The result is as follows (Maugin, 1993):

$$\begin{aligned}&\frac{\partial}{\partial t}(\mathbf{X}\times\mathbf{P} - \mathbf{F}^T.(\mathbf{x}\times\mathbf{p}_R))\Big|_X - \mathrm{div}_R(\mathbf{X}\times\mathbf{b} - \mathbf{F}^T.(\mathbf{x}\times\mathbf{T}))\\ &\quad -\mathbf{X}\times(\mathbf{f}^{\mathrm{inh}} + \mathbf{f}^{\mathrm{ext}}) + \rho_0\mathbf{F}^T.(\mathbf{x}\times\mathbf{f}) = \mathbf{0},\end{aligned} \tag{3.104}$$

where the vector product with a tensor (first contribution in the divergence term) is to be understood with the first index of the tensor $\mathbf{b}$ . Equation 3.106 is a kind of *material* balance of moment of momentum. We have also trivially

accounted for the contribution due to an external body force. Adding the corresponding contributions in (3.92), (3.93), and (3.102) is also a trivial matter since their computation does not involve any space or time derivative. In particular, contributions $\rho_0\mathbf{f}$, $\rho_0\mathbf{f}.\mathbf{v}$, and $-\rho_0\mathbf{f}.(\mathbf{F}.\mathbf{X}+t\mathbf{v}+\mathbf{x})$ should be added to the right-hand side of (3.92), (3.93), and (3.102), respectively.

*Small-Strain Approximation*

In this case $\mathbf{X}$ is replaced by $\mathbf{x}$, $\mathbf{x}$ by $\mathbf{u}$, $\mathbf{P}$ by $\mathbf{P}^f$, $\mathbf{T}$ by $\sigma$, $\mathbf{F}$ by $\nabla\mathbf{u}$, and $\mathbf{b}$ takes its expression of small-strain theory, so that we obtain the following balance laws:

$$\frac{\partial}{\partial t}\mathbf{P}^f - \operatorname{div}\mathbf{b} - \mathbf{f}^{\text{inh}} + \rho_0\big(\nabla\mathbf{u}\big).\mathbf{f} = \mathbf{0}, \tag{3.105}$$

$$\frac{\partial}{\partial t}H - \nabla.\big(\mathbf{T}.\dot{\mathbf{u}}\big) - \rho_0\mathbf{f}.\dot{\mathbf{u}} = 0, \tag{3.106}$$

$$\frac{\partial}{\partial t}\Big(\mathbf{P}^f.\mathbf{x} - Ht - \mathbf{p}.\mathbf{u}\Big) - \nabla.\big(\mathbf{b}.\mathbf{x} - t\mathbf{T}.\dot{\mathbf{u}} - \sigma.\mathbf{u}\big) - \mathbf{x}.\mathbf{f}^{\text{inh}} + \rho_0\mathbf{f}.\big(\big(\nabla\mathbf{u}\big).\mathbf{x} + t\dot{\mathbf{u}} + \mathbf{u}\big) = 2L, \tag{3.107}$$

and

$$\begin{aligned}\frac{\partial}{\partial t}\big(\mathbf{x}\times\mathbf{P}^f - \mathbf{u}\times\mathbf{p}\big) - \operatorname{div}\big(\mathbf{x}\,\bar{\times}\,\mathbf{b} - \mathbf{u}\,\bar{\times}\,\sigma\big) - \sigma\,\dot{\times}\big(\nabla\mathbf{u}\big)\\ -\mathbf{x}\times\mathbf{f}^{\text{inh}} + \rho_0\mathbf{x}\times\big(\big(\nabla\mathbf{u}\big).\mathbf{f}\big) + \mathbf{u}\times\rho_0\mathbf{f} = \mathbf{0},\end{aligned} \tag{3.108}$$

where

$$\mathbf{P}^f = -\rho_0\big(\nabla\mathbf{u}\big).\dot{\mathbf{u}}, \quad \mathbf{p} = \rho_0\dot{\mathbf{u}}, \quad H = \frac{1}{2}\rho_0\big(\mathbf{x}\big)\dot{\mathbf{u}}^2 + \frac{1}{2}\operatorname{tr}\big(\sigma.\varepsilon\big), \tag{3.109}$$

$$b_{ji} = -\big(L\delta_{ji} + \sigma_{jk}u_{k,i}\big), \quad L = \mathbf{p}.\dot{\mathbf{u}} - H, \quad \sigma_{ij} = C^{ijkl}\big(\mathbf{x}\big)\varepsilon_{kl}, \tag{3.110}$$

along with the short-hand notation

$$\big(\mathbf{x}\,\bar{\times}\,\mathbf{b}\big)_{kn} \equiv \varepsilon_{kij}x_i b_{jn}, \quad \big(\sigma\,\dot{\times}\,\mathbf{a}\big)_k \equiv \varepsilon_{kij}\big(\sigma_{im}a_{jm} - \sigma_{jm}a_{mi}\big). \tag{3.111}$$

Equations 3.105 through 3.110 were essentially obtained by Eischen and Herrmann (1987). Delph (1982) had previously considered the preceding *divergence transformations* of the Lagrangian density function for linear elastostatics. We establish in the forthcoming chapter the relationship of the

divergence transformation and its results with generalized symmetries and Noether's theorem in field theory.

## 3.11 Eshelby Stress and Kröner's Theory of Incompatibility

We return to the notion of Peach–Koehler force but now within the framework of a continuous distribution of dislocations and Kröner's (1958) theory of incompatibility in small strains (Note: Kröner = Kroener). In these conditions the compatibility equations for integrating a displacement gradient (in general nine independent components) into a displacement vector (three components) are given by the vanishing of the Einstein tensor in (2.28), that is,

$$S_{ab} \equiv -\varepsilon_{ajk}\varepsilon_{bli}\frac{\partial^2 \varepsilon_{ki}}{\partial x_j \partial x_l} = 0, \tag{3.112}$$

where $\varepsilon_{ki} = \beta_{(ik)} = u_{(k,i)}$ or $\varepsilon = (\nabla \mathbf{u})_S$ in direct notation. Kroener (1958) introduced the source of elastic incompatibility $\eta$ as the negative of the quantity defined in the first part of (3.112), that is,

$$S_{ab} + \eta_{ab} = 0. \tag{3.113}$$

Accordingly, in the absence of elastic incompatibility, we recover the classical integrability condition given by the second part of (3.112). We may conceive of (3.113) as a *balance* equation between the Einstein *curvature* tensor (this is what is $S_{ab}$ in two dimensions) and Kroener's incompatibility tensor. But this is in fact related to a "defect of closure" and the concept of Burgers vector in a theory of continuous distributions of dislocations.

Indeed, in the theory of isolated dislocations, the Burgers vector $\tilde{\mathbf{b}}$ is introduced via the circuit integral (cf. (3.57))

$$\oint_S dx_j \beta_{ji} = -\tilde{b}_i\,, \tag{3.114}$$

where $\beta_{ji} = u_{i,j}$ is the distortion (displacement gradient). Using Stokes' theorem for a surface $A$ leaning on $S$, we can rewrite this for a single dislocation line $L$ as

$$\int_A da_p \varepsilon_{pmi}\beta_{ij,m} = -\int_A da_p \tau_p \tilde{b}_j \delta(\xi), \tag{3.115}$$

where $\delta(\xi)$ is Dirac's distribution and $\xi$ is the two-dimensional radius vector taken from the axis of the dislocation in the plane perpendicular to the unit tangent vector $\tau$ to the dislocation line at the given point. For arbitrary contour $S$ and surface $A$, (3.115) yields

$$\varepsilon_{pmi}\beta_{ij,m} = -\tau_p \tilde{b}_j \,\delta(\xi). \tag{3.116}$$

As $\xi$ goes to zero, this relation becomes meaningless due to the obvious singularity arising in the limit. Passing now to the *continuous theory of dislocations*, (3.115) is generalized by introducing a tensor of dislocation density $\alpha$, of components $\alpha_{ik}$, such that

$$\int_S da_i \,\alpha_{ik} = \tilde{b}_k\,, \tag{3.117}$$

so that (3.116) is replaced by

$$\varepsilon_{ilm}\beta_{mk,l} = -\alpha_{ik}\,, \tag{3.118}$$

after rearranging indices. From this there follows immediately a conservation law:

$$\operatorname{div}\alpha = \mathbf{0} \quad \text{or} \quad \frac{\partial \alpha_{ik}}{\partial x_i} = 0. \tag{3.119}$$

For a single dislocation this would be equivalent to the statement: "*The Burgers vector is constant along the dislocation line.*" Furthermore, applying the operator $\varepsilon_{jpk}\partial/\partial x_p$ to (3.117) and symmetrizing with respect to $i$ and $j$, we obtain (3.111) in the form

$$\eta_{ij} = \frac{1}{2}\left(\varepsilon_{ipl}\frac{\partial \alpha_{jl}}{\partial x_p} + \varepsilon_{jpl}\frac{\partial \alpha_{il}}{\partial x_p}\right). \tag{3.120}$$

Of course, dislocations are the source of the phenomenon of plasticity. One must therefore be able to relate the dislocation density just introduced to the plastic part of the distortion. Using the notation of Chapter 2 we have

$$\beta_{ji} = u_{i,j} = \beta^e_{ji} + \beta^p_{ji}\,, \quad \varepsilon_{ji} = u_{(j,i)} = \varepsilon^e_{ji} + \varepsilon^p_{ji}. \tag{3.121}$$

Only the total distortion and the total strain are compatible (integrable into a displacement). As a consequence, both "elastic" and "plastic" parts of the distortion have to satisfy "incompatibility conditions." This is what, according to Kroener, relates the density of dislocations and the plastic distortion, since we can write (cf. (3.118))

$$\alpha_{ji} = -\varepsilon_{jkl}\beta^{p}_{li,k}. \tag{3.122}$$

In Kroener's theory, the *dislocation density tensor* is identified with the linearized version of the *Cartan torsion* tensor $\tilde{T}_{ijk}$ according to (nine independent components)

$$\alpha_{ji} = \frac{1}{2}\varepsilon_{jkl}\tilde{T}_{ikl}. \tag{3.123}$$

But the torsion satisfies identically the so-called *Bianchi identity* of differential geometry; but here, on account of (3.122), this is the same as the "conservation law" in (3.118).

The driving force on a single dislocation is the celebrated Peach–Koehler force (3.65) such that

$$f_i^{(PK)} = \varepsilon_{ijp}\sigma_{jk}\tilde{b}_k\tau_p\delta(\xi). \tag{3.124}$$

For a continuous distribution of dislocation, this is replaced by

$$f_i^{(PK)} = \varepsilon_{ijp}\sigma_{jk}\alpha_{kp}. \tag{3.125}$$

We further note that the Eshelby stress reads under these conditions

$$b_{ji} = W\delta_{ji} - \sigma_{jk}\left(u_{k,i} - \beta^{p}_{ik}\right). \tag{3.126}$$

By direct calculation for a homogeneous elastic body endowed with a continuous distribution of dislocations (incompatible case), in quasistatics and in the absence of body force (i.e., there holds $\sigma_{ji,j} = 0$), we check that

$$b_{ji,j} = f_i^{(PK)}. \tag{3.127}$$

This shows that the Peach–Koehler force, a force driving a defect, just like the material inhomogeneity force is a *configurational force* that belongs in the mechanics of Eshelby on the material manifold.

# 4

# *Field Theory*

## Object of the Chapter

Where we discover the difference between field equations, balance laws, and conservation equations and where we see how engineering concepts fit nicely in abstract field theory and the two enrich one another as they should to the satisfaction of all, mathematical physicists and philistines.

## 4.1 Introduction

For many physicists the ultimate expression of a mathematical physical theory, that one that is most elegant and most "economical" in the sense of Ockham's razor and Ernst Mach, is the *variational* one, at least for those theories that do not involve dissipative processes. In this frame of mind a true analytical continuum mechanics can be formulated only for the two extreme cases of mechanical behavior of continua, that is, within the general landscape designed by W. Noll (1955) in a landmark paper on the "continuity of (mechanical) states," the *pure fluidity* of Euler, and the *pure elasticity*—of Cauchy, among others—whether the latter is linear or nonlinear, isotropic or anisotropic, homogeneous or inhomogeneous. In that framework the application of classical and generalized symmetries and related invariances is the most powerful tool for extracting the very substance of a theory called a *field theory*, for continuous fields in particular. We shall develop in the following the elements of such a theory for *elasticity in finite strains*, practically the most obvious application (just a change in notation), much more, say, than electrodynamics. This almost sacred faith in the power of variational principles in the manner of Lagrange, Hamilton, Jacobi, Lie, and others is well illustrated by the celebrated treatise on theoretical physics by Lev Landau and E.M. Lifshitz from which many benefited during the second half of the twentieth century. But we are close to believing the following: If we know how to formulate variationally a theory in the absence of dissipative processes, then the very structure of the deduced

field theory will suggest to us how to generalize the said theory to the case of dissipative processes. That is an interesting side benefit. For instance, it has long been thought that the notions of Eshelby stress and Eshelbian mechanics could be introduced and meaningfully interpreted only after their introduction in the framework of a variational field-theoretical formulation. But this is blatantly erroneous as these notions should always exist, as we shall show in further chapters. What is nonetheless true is that the field-theoretic formulation provides a hint for the formulatation of dissipative cases (in the same way as Lagrange analytical mechanics suggests to us how to introduce dissipative forces such as those related to friction). In what follows it is understood that "variation" means "infinitesimal variation," and the symmetries involved are generated by infinitesimally small variations and parameters.

## 4.2 Elements of Field Theory: Variational Formulation

### 4.2.1 Noether's Theorem

Here we are concerned with simple general features of field theories in a continuum with space–time parametrization $\{\mathbf{X},t\}$, where $\mathbf{X}$ stands for *material coordinates* of classical continuum mechanics (e.g., in Truesdell and Toupin, 1960) and $t$ for a time-like scalar variable (Newton's absolute time). We consider *Hamiltonian actions* of the type

$$A(\phi;V)=\int_{V\times I} L\left(\phi^{\alpha},\,\partial_{\mu}\phi^{\alpha},\,\partial_{\mu}\partial_{\nu}\phi^{\alpha},\ldots;X^{\mu}\right)d^{4}X, \tag{4.1}$$

where $\phi^{\alpha}$, $\alpha=1,2,\ldots,N$, denotes the ordered array of fields, say the independent components of a certain geometric object, and $d^4X = dV\,dt$. This is a Cartesian–Newtonian notation, with

$$\left\{\partial_{\mu}=\partial/\partial X^{\mu};\ \mu=1,2,3,4\right\}=\left\{\partial/\partial X^{K},\ K=1,2,3;\ \partial/\partial X^{4}=\partial/\partial t\right\}. \tag{4.2}$$

The summation over dummy indices (Einstein convention) is enforced.

In agreement with the rather general expression (4.1), we say that we envisage the construction of an *nth-order gradient theory* of the field $\phi^{\alpha}$ when gradients of order $n$ at most are considered in the functional dependence of the Lagrangian volume density $L$. Most of classical physics is based on first-order gradient theories (cf. Maugin, 1980). This is the case for classical elasticity, which considers gradients of placement or displacement, and electrodynamics, which considers gradients of electric and magnetic potentials—the basic "fields" in the latter theory are not, in fact, the quantities usually called fields, such as electric and magnetic fields. In Chapter 1 we have mentioned the recent attraction toward higher-order gradient theories in elasticity (a type of

generalized continuum). But historically, the first higher-order gradient theories based on a variational formulation are the Korteweg (1901) theory of dense liquids (including the gradient of density), Einstein's (1916) theory of gravitation (which is a second-gradient theory of the elasticity of curved space–time; space–time curvature is involved in $L$, and curvature is defined in terms of the second space–time gradient of the evolving space–time metric), and Le Roux's (1911, and following works) original theory of crystal elasticity.

From the expression (4.1), we can derive two types of equations: those relating to *each one* of the fields $\phi^\alpha$ and those that express a general conservation law of the system governing *all* fields simultaneously. The first group is obtained by imposing the requirement that the variation of the action $A$ be zero when we perform a *small* variation $\delta\phi^\alpha$ of the field under well-specified conditions at the boundary, $\partial V$, of $V$ (if $V$ is not the whole of space) and at the end points of the time interval $I = [t_0, t_1]$ if such limitations are considered. However, most field theories are developed for an infinite domain. The second group of equations is the result of the variation of the parametrization, and these results, on account of the former group, express the *invariance* or lack of invariance of the whole system under changes of this parametrization. To simplify the presentation we will assume an infinite domain $V$ with vanishing fields at infinity and an infinite time interval since our concern here is neither boundary conditions nor initial conditions.

To perform these variations we consider ε-parametrized families of transformations of *both* coordinates (parametrization) and fields such as

$$\left(X^\mu, \phi^\alpha\right) \to \left(\bar{X}^\mu, \bar{\phi}^\alpha\right), \tag{4.3}$$

with

$$\bar{X}^\mu = \kappa^\mu\left(\mathbf{X}, \varepsilon\right), \quad \bar{\phi}^\alpha\left(\bar{\mathbf{X}}\right) = \Phi^\alpha\left(\phi^\beta\left(\mathbf{X}\right), \bar{\mathbf{X}}, \varepsilon\right), \tag{4.4}$$

where ε is an infinitesimal parameter such that for $\varepsilon = 0$ we have identically $\kappa^\mu(\mathbf{X}, 0) = X^\mu$, $\Phi^\alpha(\phi^\beta, \mathbf{X}, 0) = \phi^\alpha$. We assume that the quantity $L$ in (4.1) transforms as a *scalar* quantity, that is,

$$L\left(\bar{\mathbf{X}}, \varepsilon\right) = \det\left(\partial\mathbf{X}/\partial\bar{\mathbf{X}}\right) L\left(\mathbf{X}\right). \tag{4.5}$$

We note that derivations with respect to $\mathbf{X}$ and ε commute, and the same holds true of integration in $\mathbf{X}$ space and derivation with respect to ε. The variation of a field $\phi^\alpha$ is then defined by

$$\delta\phi^\alpha := \partial\Phi^\alpha/\partial\varepsilon\big|_{\varepsilon=0}. \tag{4.6}$$

With vanishing fields at infinity in space and vanishing variations at the ends of the time intervals, limiting ourselves to a first-order gradient theory and applying an ε-parametrization to (4.1), we immediately have

$$\delta A = \int d^4X \left( \sum_\alpha \left\{ \frac{\partial L}{\partial \phi^\alpha} \delta\phi^\alpha + \frac{\partial L}{\partial \left( \partial_\mu \phi^\alpha \right)} \delta\left( \partial_\mu \phi^\alpha \right) \right\} + \frac{\partial L}{\partial X^\mu} \delta X^\mu \right). \tag{4.7}$$

In order that $\delta A$ vanish for all admissible $\delta\phi^\alpha(\mathbf{X})$, and any $\alpha$, with $\mathbf{X}$ *fixed*, a classical computation yields the following *Euler–Lagrange equations*:

$$E_\alpha \equiv \frac{\delta L}{\delta \phi^\alpha} = \frac{\partial L}{\partial \phi^\alpha} - \partial_\mu \frac{\partial L}{\partial \left( \partial_\mu \phi^\alpha \right)} = 0, \tag{4.8}$$

for each $\alpha = 1,2,\ldots,N$, at any space–time event $\mathbf{X}$. Equation 4.8 is a *strict* conservation law when $L$ does not depend explicitly on $\phi^\alpha$. We note that the result in (4.8) is left unchanged if we make the substitution

$$L \to L + \partial_\mu \Omega^\mu \left( \mathbf{X} \right),$$

that is, if we add to $L$ a four-divergence contribution in which $\Omega$ depends at most on the space–time coordinates, and *not* on the fields.

The second group of equations, called *conservation equations*, which can derive from (4.1) by variation, result from a simultaneous transformation of both the coordinates $X^\mu$ and the fields. We shall not repeat all the details of the derivation of the resulting theorem, known as *Noether's theorem* (Noether, 1918; Soper, 1976; Nelson, 1979), but we shall give the main steps. That theorem states that *to any symmetry of the system there corresponds the conservation (or lack of strict conservation) of a current* (cf. Maugin, 1993, pp. 99–103). For $L$ given in (4.1), such a current generally reads

$$J^\mu = L \frac{\partial \bar{X}^\mu}{\partial \varepsilon} + \sum_\alpha \frac{\partial L}{\partial \left( \partial_\mu \phi^\alpha \right)} \left[ \frac{\partial \bar{\phi}^\alpha}{\partial \varepsilon} - \partial_\nu \phi^\alpha \frac{\partial \bar{X}^\nu}{\partial \varepsilon} \right], \tag{4.9}$$

where $\varepsilon$ must be taken equal to zero. In spite of the notation, $J^\mu$ is not always simply a four-vector. It all depends on the group of transformations considered.

**PROOF OF NOETHER'S THEOREM (4.9)**

By invariance of the original action we mean that

$$\bar{A} = A(\varepsilon) = A(0), \quad \forall\varepsilon, \quad \forall\phi^\alpha. \tag{4.10}$$

Therefore, we need to find out the conditions in which $\partial A(\varepsilon)/\partial\varepsilon = 0$. Since

$$\delta A(\varepsilon) = \frac{\partial A}{\partial \varepsilon} \delta\varepsilon = \int d^4X \delta L, \quad \delta L \equiv \left. \frac{\partial L}{\partial \varepsilon} \right|_{\mathbf{X}\,\text{fixed}} \delta\varepsilon, \tag{4.11}$$

a *sufficient* condition for $\delta A$ to vanish is that $\delta L$ be the four-dimensional divergence of a certain quantity, noted $\delta B^{\mu}$, in such a way that

$$\delta L = \partial_{\mu}\left(\delta B^{\mu}\right). \tag{4.12}$$

It suffices now to make the variation $\delta L$ explicit when $L$ is a scalar such as in (4.5). In this case $\delta B^{\mu}$ has the following simple form:

$$\delta B^{\mu} = -L\frac{\partial X^{\mu}}{\partial \varepsilon}\delta\varepsilon. \tag{4.13}$$

Let us show that this is true. To do this we write explicitly

$$L(\mathbf{X},\varepsilon) = L\left(\phi^{\alpha}(\mathbf{X}), \partial_{\mu}\phi^{\alpha}, \mathbf{X}\right) \tag{4.14}$$

and

$$\bar{L}(\bar{\mathbf{X}}) = L\left(\bar{\phi}^{\alpha}(\mathbf{X}), \partial\bar{\phi}^{\alpha}/\partial\bar{X}^{\mu}, \bar{\mathbf{X}}\right), \tag{4.15}$$

where, here, $\mathbf{X}$ stands for ($X^K$, $t$). Accounting for (4.5), we have

$$A(\varepsilon) - A(0) = \int d^4X L(\mathbf{X},\varepsilon) - \int d^4X \bar{L}(\bar{\mathbf{X}}) = 0. \tag{4.16}$$

Now differentiate this with respect to $\varepsilon$, keeping $\mathbf{X}$ fixed. Assuming here that $L$ does not depend explicitly on $\mathbf{X}$, we obtain thus

$$\begin{aligned}\frac{\partial L}{\partial \bar{\mathbf{X}}}\frac{\partial \bar{\mathbf{X}}}{\partial \varepsilon} + \left(\frac{\partial L}{\partial \varepsilon}\right)\Big|_{\exp l} &= -\det\left(\partial\mathbf{X}/\partial\bar{\mathbf{X}}\right)\frac{\partial X^{\nu}}{\partial \bar{X}^{\mu}}\frac{\partial^2 \bar{X}^{\mu}}{\partial X^{\nu}\partial\varepsilon}L(\mathbf{X}) \\ &= -\det\left(\partial\mathbf{X}/\partial\bar{\mathbf{X}}\right)L\frac{\partial}{\partial \bar{X}^{\mu}}\left(\left(\frac{\partial \bar{X}^{\mu}}{\partial\varepsilon}\right)_{\mathbf{X}\text{ fixed}}\right)_{\varepsilon=\text{const}}\end{aligned} \tag{4.17}$$

or

$$\frac{\partial L}{\partial \bar{\mathbf{X}}}\frac{\partial \bar{\mathbf{X}}}{\partial \varepsilon} + \frac{\partial L}{\partial \varepsilon}\Big|_{\exp l} = -L\frac{\partial}{\partial \bar{X}^{\mu}}\left(\frac{\partial \bar{X}^{\mu}}{\partial\varepsilon}\right) \tag{4.18}$$

or else

$$\frac{\partial L}{\partial \varepsilon}\Big|_{\mathbf{X}\text{ fixed}} = -\frac{\partial}{\partial \bar{\mathbf{X}}}\left(\frac{\partial \bar{\mathbf{X}}}{\partial\varepsilon}L\right), \tag{4.19}$$

where the differential formula for a determinant has been used in the first part of (4.17). Finally, on comparing (4.19) and (4.12), we obtain (4.13). But we can also compute $\delta L$ directly. Using the second of (4.11), we have (omitting the $\alpha$'s)

$$\delta L = \frac{\partial L}{\partial \phi}\delta\phi + \partial_\mu\left(\frac{\partial L}{\partial(\partial_\mu\phi)}\delta\phi\right) \tag{4.20}$$

up to irrelevant terms. Comparing now this and (4.12) and accounting for (4.8), we are entitled to write

$$\left(\partial_\mu J^\mu\right)\delta\varepsilon = -\frac{\delta L}{\delta\phi^\alpha}\delta\phi^\alpha, \tag{4.21}$$

where the so-called *current* $J^\mu$ is such that

$$J^\mu\delta\varepsilon = -\delta B^\mu + \frac{\partial L}{\partial(\partial_\mu\phi^\alpha)}\delta\phi^\alpha. \tag{4.22}$$

If the Euler–Lagrange equations (4.8) hold good, then (4.21) tells us that the current is conserved. This is the contents of *Noether's theorem*. However, it remains to find the explicit expression of the current for each of the transformations involved in the set (4.3) and (4.4). This is, in general, obtained by evaluating

$$\delta\phi^\alpha(\mathbf{X}) = \left.\frac{\partial\bar{\phi}^\alpha}{\partial\varepsilon}\right|_{\bar{\mathbf{X}}\text{ fixed}}\delta\varepsilon = \left(\left.\frac{\partial\bar{\phi}^\alpha}{\partial\phi^\beta}\frac{\partial\phi^\beta}{\partial X^\mu}\frac{\partial X^\mu}{\partial\varepsilon}\right|_{\bar{\mathbf{X}}\text{fixed}} + \frac{\partial\phi^\alpha}{\partial\varepsilon}\right)\delta\varepsilon. \tag{4.23}$$

For $\varepsilon = 0$ we note that $\left.\partial X^\mu/\partial\varepsilon\right|_{\bar{\mathbf{X}}\text{ fixed}} = -\partial\bar{X}^\mu(\mathbf{X},\varepsilon)/\partial\varepsilon$. Accounting for this in (4.23) and (4.22), we obtain the following general expression for the current:

$$J^\mu = L\frac{\partial\bar{X}^\mu}{\partial\varepsilon} + \frac{\partial L}{\partial(\partial_\mu\phi^\alpha)}\left(\frac{\partial\phi^\alpha}{\partial\varepsilon} - \partial_\nu\phi^\alpha\frac{\partial\bar{X}^\nu}{\partial\varepsilon}\right). \tag{4.24}$$

The quantities within the last parentheses in this equation are called the *characteristics* $Q^\alpha$ of the transformation in group theory:

$$Q^\alpha = \frac{\partial\phi^\alpha}{\partial\varepsilon} - \partial_\nu\phi^\alpha\frac{\partial\bar{X}^\nu}{\partial\varepsilon} \quad \text{taken at} \quad \varepsilon = 0.$$

### 4.2.2 Example 1: Space–Time Translation

In this case the transformations in (4.3) and (4.4) reduce to a pure space–time transformation of the type

$$X^{\mu} \to \bar{X}^{\mu}(\mathbf{X},\varepsilon) = X^{\mu} + \varepsilon\delta^{\mu}_{.\lambda}, \tag{4.25}$$

where $\delta^{\mu}_{\lambda}$ is the Kronecker symbol; that is, it equals 1 only when $\mu$ takes the value granted to $\lambda$. There is no transformation of the fields themselves. On account of (4.24), we obtain the following current in components:

$$J^{\mu} \to J^{\mu}_{.\lambda} = T^{\mu}_{.\lambda} = L\delta^{\mu}_{.\lambda} - \sum_{\alpha} \partial_{\lambda}\phi^{\alpha} \frac{\partial L}{\partial(\partial_{\mu}\phi^{\alpha})}. \tag{4.26}$$

This is a mixed second-order space–time tensor called the *energy–momentum tensor*. This denomination is clearly understood when we separate space and time components. If $L$ does not depend explicitly on $\mathbf{X}$, then this tensor satisfies the following (four-dimensional) *strict conservation law*:

$$\partial_{\mu} T^{\mu}_{.\lambda} = 0, \quad \lambda = 1,2,3,4. \tag{4.27}$$

Had we considered an explicit dependence of $L$ on the space–time coordinates $X^{\mu}$, instead of the strict conservation law (4.27), we would have a source term

$$f_{\lambda} = -\left.\frac{\partial L}{\partial X^{\lambda}}\right|_{\text{expl}}, \tag{4.28}$$

on the right-hand side.

With the *Cartesian notation* introduced in (4.2), we see that the independence of $L$ on $t$, $\lambda = 4$, yields a *scalar* conservation law in the explicit form

$$\left.\frac{\partial H}{\partial t}\right|_{X} - \nabla_{R}.\mathbf{Q} = 0, \tag{4.29}$$

while the independence of $L$ on the spatial part of $\mathbf{X}$, $\{X^{K} = 1,2,3\}$, yields the *material balance law*:

$$\left.\frac{\partial \mathbf{P}}{\partial t}\right|_{X} - \operatorname{div}_{R}\mathbf{b} = \mathbf{0}, \tag{4.30}$$

where we defined the following canonical quantities:

- *Energy (Hamiltonian density)*:

$$H := \sum_{\alpha} \dot{\phi}^{\alpha} \left( \partial L / \partial \dot{\phi}^{\alpha} \right) - L, \quad \dot{\phi}^{\alpha} \equiv \partial \phi^{\alpha} / \partial t \tag{4.31}$$

- *Energy flux vector*:

$$\mathbf{Q} = \left\{ Q^{K} := - \sum_{\alpha} \dot{\phi}^{\alpha} \frac{\partial L}{\partial \left( \partial_{K} \phi^{\alpha} \right)} \right\} \tag{4.32}$$

- *Canonical (here material) momentum*:

$$\mathbf{P} = \left\{ P_{K} := - \sum_{\alpha} \frac{\partial \phi^{\alpha}}{\partial X^{K}} \frac{\partial L}{\partial \left( \partial \phi^{\alpha} / \partial t \right)} \right\} \tag{4.33}$$

- *Canonical stress tensor*:

$$\mathbf{b} = \left\{ b^{K}_{\cdot L} := - \left( L \delta^{K}_{\cdot L} - \sum_{\alpha} \frac{\partial \phi^{\alpha}}{\partial X^{K}} \frac{\partial L}{\partial \left( \partial \phi^{\alpha} / \partial X^{K} \right)} \right) \right\} \tag{4.34}$$

The "explicit" independence of $L$ from $t$—no right-hand side in (4.28)—stands for the *conservation of energy* in (4.28). The "explicit" independence of $L$ from $X^{K}$ signifies that the material body is *materially homogeneous*. But this is not a fundamental requirement of physics, so that, in general, (4.29) may contain a nonzero right-hand denoted

$$\mathbf{f}^{\text{inh}} = \left\{ f^{\text{inh}}_{L} = \left( \partial L / \partial X^{L} \right)_{\text{expl}} \right\}, \tag{4.35}$$

so that (4.29) would be replaced by the inhomogeneous equation

$$\left. \frac{\partial \mathbf{P}}{\partial t} \right|_{X} - \text{div}_{R} \mathbf{b} = \mathbf{f}^{\text{inh}}. \tag{4.36}$$

**REMARK 4.1:** Had we considered a Lagrangian depending explicitly on time, (4.29) would be replaced by

$$\left.\frac{\partial H}{\partial t}\right|_X - \nabla_R.\mathbf{Q} = h, \quad h = -\left.\frac{\partial L}{\partial t}\right|_{\text{expl}}. \tag{4.37}$$

What must be principally gathered from the preceding is the essentially different nature of the Euler–Lagrange equations (4.8) for which one such equation is written for *each field*—or, in a more mechanical jargon, *each degree of freedom*—and of the *canonical equations of energy and momentum* (e.g., (4.29) and (4.30)), which pertain to the whole physical system and by necessity consider all fields simultaneously (note the summations over $\alpha$ in the definitions (4.31) through (4.34)). In particular, in establishing (4.27), we have made use of the celebrated *Noether's identity*

$$\left(\partial_\mu J^\mu\right)\delta\varepsilon + \sum\nolimits_\alpha \left(E_\alpha \delta\phi^\alpha\right) = 0, \tag{4.38}$$

which emphasizes the remark already made but naturally implies (4.27) whenever all *field* equations (4.8) are satisfied simultaneously.

### 4.2.3 Relationship to Lie-Group Theory

The transformations in (4.3) and (4.4) can be written in the form

$$\bar{X}^\mu = X^\mu + \varepsilon \left.\frac{\partial \bar{X}^\mu}{\partial \varepsilon}\right|_{\varepsilon=0}, \quad \bar{\phi}^\alpha = \phi^\alpha + \varepsilon \left.\frac{\partial \bar{\phi}^\alpha}{\partial \varepsilon}\right|_{\varepsilon=0}. \tag{4.39}$$

In what follows it is understood that the partial derivatives are evaluated at $\varepsilon = 0$. Then the infinitesimal generator associated with the group of transformations in (4.39) is defined as

$$\mathbf{V} = \frac{\partial \bar{X}^\mu}{\partial \varepsilon}\frac{\partial}{\partial X^\mu} + \frac{\partial \bar{\phi}^\alpha}{\partial \varepsilon}\frac{\partial}{\partial \phi^\alpha}. \tag{4.40}$$

Then the so-called *first prolongation* of $\mathbf{V}$ is given by (cf. Ibragimov, 1985; Olver, 1986; Kalpakides and Maugin, 2004)

$$\mathbf{V}^{(1)} = \mathbf{V} + \left(\frac{\partial}{\partial X^\mu}\left(\frac{\partial \bar{\phi}^\alpha}{\partial \varepsilon}\right) - \frac{\partial \phi^\alpha}{\partial X^\beta}\frac{\partial}{\partial X^\mu}\left(\frac{\partial \bar{X}^\beta}{\partial \varepsilon}\right)\right)\frac{\partial}{\partial\left(\partial\phi^\alpha/\partial X^\mu\right)}. \tag{4.41}$$

The differential operators $\mathbf{V}$ and $\mathbf{V}^{(1)}$ are to be applied to $L$. Indeed, the equation

$$\mathbf{V}^{(1)}L + L\frac{\partial}{\partial X^{\mu}}\left(\frac{\partial \bar{X}^{\mu}}{\partial \varepsilon}\right) = 0 \tag{4.42}$$

is none other than the vanishing of $\delta L$ if we want to respect the invariance of the action $A$. The second contribution in the left-hand side of (4.42) accounts for the change of volume. In the same formalism, Noether's identity (4.38) reads

$$\partial_{\mu} J^{\mu} = 0 = E_{\alpha}\left(\frac{\partial \phi^{\alpha}}{\partial \varepsilon} - \frac{\partial \phi^{\alpha}}{\partial X^{\beta}}\frac{\partial X^{\beta}}{\partial \varepsilon}\right), \tag{4.43}$$

with

$$J^{\mu} = T^{\mu}_{.\beta}\frac{\partial \bar{X}^{\beta}}{\partial \varepsilon} + \frac{\partial L}{\partial\left(\partial \phi^{\alpha}/\partial X^{\mu}\right)}\frac{\partial \phi^{\alpha}}{\partial \varepsilon}, \quad T^{\mu}_{.\beta} := L\delta^{\mu}_{\beta} - \frac{\partial \phi}{\partial X^{\beta}}\frac{\partial L}{\partial\left(\partial \phi^{\alpha}/\partial X^{\mu}\right)} \tag{4.44}$$

This is entirely equivalent to the foregoing formulation.

**REMARK 4.2:** Had we considered a Lagrangian function $L$ depending on higher-order space-time gradients, for example, a second-order one,

$$L = L\left(\phi^{\alpha}, \partial_{\mu}\phi^{\alpha}, \partial_{\mu}\partial_{\nu}\phi^{\alpha}; \mathbf{X}\right), \tag{4.45}$$

we would have obtained longer expressions for $E_{\alpha}$, $J^{\mu}$, and Equation 4.9; for example, in place of (4.26) and (4.28),

$$T^{\mu}_{.\lambda} = L\delta^{\mu}_{\lambda} - \partial_{\lambda}\phi^{\alpha}\frac{\partial L}{\partial\left(\partial_{\mu}\phi^{\alpha}\right)} + 2\partial_{\nu}\partial_{\lambda}\phi^{\alpha}\frac{\partial L}{\partial\left(\partial_{\nu}\partial_{\mu}\phi^{\alpha}\right)} - \partial_{\nu}\left(\partial_{\lambda}\phi^{\alpha}\frac{\partial L}{\partial\left(\partial_{\nu}\partial_{\mu}\phi^{\alpha}\right)}\right) \tag{4.46}$$

and

$$\partial_{\mu} T^{\mu}_{.\lambda} = -\left.\frac{\partial L}{\partial X^{\lambda}}\right|_{\text{expl}}. \tag{4.47}$$

But apart for some paradoxical theories with strange inertial terms (see, e.g., Maugin and Christov, 1997, 2002), in classical theories $L$ depends at most on the first-order time derivatives, and the second-order gradients in (4.1) are purely spatial. When this is the case, the formal definitions of both $H$ and $\mathbf{P}$

are left unchanged, while **Q** and **b** take on the following more general component form including second-order space-like (here material) gradients:

$$Q^K = -\sum_\alpha \dot{\phi}^\alpha \left( \frac{\partial L}{\partial\left(\partial_K \phi^\beta\right)} - \partial_L \left( \frac{\partial L}{\partial\left(\partial_L \partial_K \phi^\alpha\right)} \right) \right) - \sum_\alpha \partial_L \dot{\phi}^\alpha \frac{\partial L}{\partial\left(\partial_L \partial_K \phi^\alpha\right)} \tag{4.48}$$

and

$$b^K_{\cdot L} = -\left( L\delta^K_L - \sum_\alpha \partial_L \phi^\alpha \frac{\partial L}{\partial\left(\partial_K \phi^\alpha\right)} \right) - \sum_\alpha 2\partial_L \partial_M \phi^\alpha \frac{\partial L}{\partial\left(\partial_M \partial_K \phi^\alpha\right)} + \sum_\alpha \partial_L \left( \partial_M \phi^\alpha \frac{\partial L}{\partial\left(\partial_M \partial_K \phi^\alpha\right)} \right). \tag{4.49}$$

Other symmetries, and thus other consequences of Noether's theorem, can be applied—for example, rotations, dilatation (change of scale), expansion, and so on (cf. Maugin, 1993, pp. 110–112).

### 4.2.4 Example 2: Rotations

An infinitesimal rotation of the material frame should generate some kind of material angular-momentum balance. Accordingly, we need to introduce infinitesimal four-dimensional rotations. For finite rotations we have (note these are *not* Lorentz transformations because our space–time is Euclidean)

$$X^\mu \to \bar{X}^\mu = \Lambda^\mu_{\cdot\nu} X^\nu, \quad \text{that is,} \quad \bar{\mathbf{X}} = \Lambda.\mathbf{X}, \tag{4.50}$$

with

$$\Lambda^{-1} = \Lambda^T, \quad \det \Lambda = +1. \tag{4.51}$$

We consider the following representation for $\Lambda$:

$$\Lambda = \exp(\mathbf{A}), \quad \mathbf{A} = -\mathbf{A}^T, \tag{4.52}$$

by which it is meant that

$$\exp(\mathbf{A}) = \mathbf{1} + \sum_{n=1}^{\infty} \frac{1}{n!} \mathbf{A}^n. \tag{4.53}$$

This satisfies the first of (4.51) identically, while the representation in (4.52) means that the finite transformation in (4.50) can be composed of the product

of many infinitesimal transformations (the corresponding group is connected). Accordingly, it suffices to study in detail the action of the *infinitesimal generators* of the transformations, that is, the matrices **A** that satisfy the second of (4.52), that is, that are skewsymmetric. Now, the last condition written as the equation

$$\mathbf{A} + \mathbf{A}^T = \mathbf{0}, \tag{4.54}$$

has *six* linearly independent solutions, that we label $\mathbf{M}_{\alpha\beta}$ so that (the $\mathbf{M}_{\alpha\beta}$ are $4 \times 4$ matrices)

$$\mathbf{M}_{\alpha\beta} = \mathbf{0} \quad \text{if} \quad \alpha \neq \beta, \quad \mathbf{M}_{\alpha\beta} = -\mathbf{M}_{\beta\alpha}, \quad \alpha > \beta. \tag{4.55}$$

The elements of these matrices are given by

$$\left(\mathbf{M}_{\alpha\beta}\right)^{\mu}_{.\nu} = \delta^{\mu}_{\beta}\delta_{\alpha\nu} - \delta^{\mu}_{\alpha}\delta_{\beta\nu} = 2\delta^{\mu}_{.[\beta}\delta_{.\alpha]\nu}. \tag{4.56}$$

A finite rotation is now written as a linear combination of the **M**'s by

$$\Lambda = \exp\left(\frac{1}{2}\omega^{\alpha\beta}\mathbf{M}_{\alpha\beta}\right), \tag{4.57}$$

where $\omega^{\alpha\beta}$ are the components (six in all) of the linear combination, the sum being effected on $\alpha$ and $\beta$ and the ½ factor accounting for the second of (4.55) to avoid counting the same elements twice. In a transformation such as (4.57), a four-dimensional vector **V** and a four-dimensional second-order tensor **T**, respectively, transform as

$$\bar{V}^{\mu} = \Lambda^{\mu}_{.\nu} V^{\nu} = \left(\exp\left(\frac{1}{2}\omega^{\alpha\beta}\mathbf{M}_{\alpha\beta}\right)\right)^{\mu}_{.\nu} V^{\nu}, \tag{4.58a}$$

$$\bar{T}^{\mu\nu} = \Lambda^{\mu}_{.\kappa}\Lambda^{\nu}_{.\rho} T^{\kappa\rho} = \left(\exp\left(\frac{1}{2}\omega^{\alpha\beta}\bar{\mathbf{M}}_{\alpha\beta}\right)\right)^{\mu\nu}_{..\kappa\rho} T^{\kappa\rho}, \tag{4.58b}$$

where we have introduced the following $16 \times 16$ generating matrices:

$$\left(\bar{\mathbf{M}}_{\alpha\beta}\right)^{\mu\nu}_{..\kappa\rho} = \left(\mathbf{M}_{\alpha\beta}\right)^{\mu}_{\kappa}\delta^{\nu}_{\rho} + \delta^{\mu}_{.\kappa}\left(\mathbf{M}_{\alpha\beta}\right)^{\nu}_{.\rho}. \tag{4.59}$$

This works because of the exponential property

$$\mathbf{M} = \mathbf{M}_1 + \mathbf{M}_2, \quad \exp\left(\mathbf{M}_1 + \mathbf{M}_2\right) = \exp\left(\mathbf{M}_1\right)\exp\left(\mathbf{M}_2\right). \tag{4.60}$$

Equation (4.58) can be generalized to any geometric object. Therefore, we can agree to work in a general manner for coordinates *and* fields with the transformations

$$X^{\mu} \rightarrow \bar{X}^{\mu} = \left( \exp\left( \frac{1}{2} \omega^{\alpha\beta} \mathbf{M}_{\alpha\beta} \right) \right)^{\mu}_{\cdot\nu} X^{\nu}, \tag{4.61a}$$

$$\phi^{\lambda}(\mathbf{X}) \rightarrow \bar{\phi}^{\alpha}(\bar{\mathbf{X}}) = \left( \exp\left( \frac{1}{2} \omega^{\alpha\beta} \mathbf{M}_{\alpha\beta} \right) \right)^{\lambda}_{\cdot\sigma} \phi^{\sigma}(\mathbf{X}). \tag{4.61b}$$

The generating matrices $\bar{\mathbf{M}}_{\alpha\beta}$ have a general block diagonal form so their components are zero unless $\bar{\phi}^{\lambda}$ and $\phi^{\sigma}$ are components of the *same* tensorial field.

If our original Lagrangian density is to be invariant under the transformations in (4.50), then according to Noether's theorem, there exist *six* independent conserved quantities noted $S^{\alpha\beta}$, one for each of the $\omega_{\alpha\beta}$. The corresponding current will be noted $\tilde{S}^{\mu\alpha\beta}$. Noting that in our formalism

$$\left. \frac{\partial \bar{X}^{\mu}}{\partial \varepsilon} \right|_{\varepsilon, \omega^{\alpha\beta}} = \left( \mathbf{M}_{\alpha\beta} \right)^{\mu}_{\cdot\nu} X^{\nu}, \quad \left. \frac{\partial \bar{\phi}^{\lambda}}{\partial \varepsilon} \right|_{\varepsilon, \omega^{\alpha\beta}} = \left( \bar{\mathbf{M}}_{\alpha\beta} \right)^{\lambda}_{\cdot\sigma} \phi^{\sigma}, \tag{4.62}$$

we can evaluate the currents $\tilde{S}^{\mu\alpha\beta}$ by using the general formula (4.9). After some computation we obtain

$$\tilde{S}^{\mu\alpha\beta} = \tilde{S}^{\mu[\alpha\beta]} = \left( X^{\alpha} T^{\mu\beta} - X^{\beta} T^{\mu\alpha} \right) + S^{\mu\alpha\beta}, \tag{4.63}$$

where the first contribution within parentheses to this *angular-momentum current* is called the *orbital spin*, and the remainder is the *spin tensor*, per se, such that

$$S^{\mu\alpha\beta} = \frac{\partial L}{\partial\left( \partial_{\mu} \phi^{\lambda} \right)} \left( \bar{\mathbf{M}}_{\alpha\beta} \right)^{\lambda}_{\cdot\sigma} \phi^{\sigma}. \tag{4.64}$$

The conservation of the current yields

$$\partial_{\mu} \tilde{S}^{\mu\alpha\beta} = 0 \quad \text{or} \quad \partial_{\mu} S^{\mu\alpha\beta} = T^{\alpha\beta} - T^{\beta\alpha}. \tag{4.65}$$

Thus, in general, $T^{\alpha\beta}$ is *not* symmetric. A symmetrization procedure was proposed by Belinfante (1940) and Rosenfeld (1940), to replace $\mathbf{T}$ by a symmetric energy–momentum tensor $\Theta^{\alpha\beta}$ defined by

$$\Theta^{\alpha\beta} = T^{\alpha\beta} + \partial_{\mu} G^{\mu\alpha\beta}, \tag{4.66}$$

where $G^{\mu\alpha\beta}$ is itself defined by

$$G^{\mu\alpha\beta} = \frac{1}{2}\left(S^{\mu\alpha\beta} + S^{\alpha\beta\mu} - S^{\alpha\mu\beta}\right). \tag{4.67}$$

Due to the skewsymmetry of $S^{\mu\alpha\beta}$ in its last two indices, it is checked that this is also true of $G^{\mu\alpha\beta}$ while the four-divergence of $\Theta^{\alpha\beta}$ indeed vanishes. Such a procedure of symmetrization is common in the study of materials involving a microstructure (cf. Maugin, 1978).

### 4.2.5 Example 3: Change of Scale

Consider the special case of transformations in (4.3) and (4.4), for which fields are unchanged but material space–time coordinates suffer the transformation

$$X^{\mu} \to \bar{X}^{\mu} = \left(1+\eta\right)X^{\mu}, \tag{4.68}$$

where $\eta$ is an infinitesimally small parameter. This is a simple case. Noether's theorem directly yields the following conservation law (in fact with a source term when $L$ depends explicitly on the $X^{\mu}$'s):

$$\partial_{\mu} J^{\mu} = \left.\frac{\partial L}{\partial X^{\mu}}\right|_{\text{expl}} X^{\mu}, \tag{4.69}$$

with

$$J^{\mu} = LX^{\mu} - \frac{\partial L}{\partial\left(\partial_{\mu}\phi^{\alpha}\right)} D\phi^{\alpha}, \quad D \equiv X^{\mu}\partial_{\mu}. \tag{4.70}$$

Other conservation laws will be introduced in the application to elasticity.

## 4.3 Application to Elasticity

### 4.3.1 Direct-Motion Formulation for Classical Elasticity

In this formulation the fields $\phi^{\alpha}$ are none other than the physical components of the current placement. In a general manner we can consider the following Lagrangian density per unit volume of $K_R$:

$$L = \bar{L}\left(\mathbf{v},\mathbf{F};\mathbf{X},\mathbf{x},t\right) = \bar{K} - \bar{W} - \mathbf{\Phi}_R, \tag{4.71}$$

where

$$\bar{K}(\mathbf{v};\mathbf{X},t)=\frac{1}{2}\rho_0(\mathbf{X},t)\mathbf{v}^2,\quad W=\bar{W}(\mathbf{F};\mathbf{X},t),\quad \Phi_R=\rho_0(\mathbf{X},t)\varphi(\mathbf{x},t). \tag{4.72}$$

This is indeed quite general because it includes a potential for *physical* body forces, via $\Phi_R$, where the potential $\varphi$ per unit mass is necessarily dependent on the current placement, while both the reference matter density and the elasticity potential remain dependent on both the material point $\mathbf{X}$ and Newtonian time $t$. Dependence on $\mathbf{X}$ means material inhomogeneity; that is, whenever

$$\left.\frac{\partial\rho_0}{\partial\mathbf{X}}\right|_t\neq\mathbf{0},\quad \left.\frac{\partial\bar{W}}{\partial\mathbf{X}}\right|_{\text{expl}}\neq\mathbf{0}. \tag{4.73}$$

Explicit dependence on time $t$ is a much rarer occurrence in books on continuum mechanics. Indeed the condition (cf. Epstein and Maugin, 2000)

$$\left.\frac{\partial\rho_0}{\partial t}\right|_X\neq 0, \tag{4.74}$$

would mean that the reference density may evolve in time by addition or subtraction of matter by some means. This would account for the phenomenon of *growth* or *resorption* of matter. We shall return to this in due time. As to the condition (cf. Maugin, 2009)

$$\left.\frac{\partial\bar{W}}{\partial t}\right|_{\text{expl}}\neq 0, \tag{4.75}$$

it would mean a possible evolution in time of elastic properties, hence the phenomenon of *aging*. This is seldom considered in view of the large time scales involved in the process for normal physical conditions for inert matter. From the point of view of analytical mechanics, systems in which the Lagrangian density depends explicitly on time are said to be *rheonomic*, according to a classification originally due to Boltzmann (cf. Lanczos, 1962). In contrast, systems in which $L$ does not depend explicitly on time are called *scleronomic* systems. Most systems considered are scleronomic.

**REMARK:** A typical example of a rheonomic system is one in which a time-dependent spring constant yields a Mathieu differential equation with a time-dependent characteristic frequency.

A last remark concerning the Lagrangian density for the direct-motion description is that neither the kinetic energy nor the elasticity potential

energy involve the field **x** itself but only its space and time derivative in the parametrization (**X**,*t*). The reason is that elasticity is a *gauge theory*, as *Galilean invariance* (translation in physical space) eliminates this possible dependence on **x** (or displacement **u** in small strains).

To account for both natural boundary conditions at the boundary $\partial B$ and initial conditions (this specifies the physical momentum, the position being **X** at $t = 0$), we envisage a Hamiltonian variational principle in the following form:

$$\delta_X \int_0^t \int_{B_R} L dV dt + \int_0^t \int_{\partial B} \mathbf{T}^d . \delta_X \chi \, da dt - \int_{B_R} \left( \mathbf{p}_R(t) - \mathbf{p}_R(0) \right) . \delta_X \chi dV = 0, \quad (4.76)$$

where the surface term corresponding to the datum of a physical traction is expressed at the deformed (actual) boundary. The variation effected in (4.76) with simple calculations immediately yields the *field* equation, which is none other than the Piola–Kirchhoff form of the local balance of linear (physical) momentum:

$$\left. \frac{\partial \mathbf{p}_R}{\partial t} \right|_X - \mathrm{div}_R \mathbf{T} = \rho_0 \mathbf{f}, \quad \mathbf{f} = -\nabla \varphi \quad \text{in} \quad B_R, \quad (4.77)$$

$$\mathbf{N}.\mathbf{T} = \left( da/dA \right) \mathbf{T}^d = \bar{\mathbf{T}}^d \quad \text{at} \quad \partial B_R, \quad (4.78)$$

$$\mathbf{p}_R(t = 0) = \mathbf{p}_R(0), \quad \mathbf{p}_R(t = t) = \mathbf{p}_R(t), \quad (4.79)$$

of which the last one is a mere identity.

On applying now Noether's identity, we can write down the accompanying conservation laws that follow for space–time translations $\lambda = 4$ and $\lambda = K$, $K = 1,2,3$,

- *Conservation of energy*:

$$\left. \frac{\partial H}{\partial t} \right|_X - \nabla_R . \mathbf{Q} = h \quad (4.80)$$

- *Conservation of material momentum*:

$$\left. \frac{\partial \mathbf{P}}{\partial t} \right|_X - \mathrm{div}_R \mathbf{b} = \mathbf{f}^{\mathrm{inh}} + \mathbf{f}^{\mathrm{ext}}, \quad (4.81)$$

where the have defined the following quantities:

$$\mathbf{p}_R = \rho_0 \mathbf{v}, \quad \mathbf{T} = \partial \bar{W} / \partial \mathbf{F}, \quad H = K + W, \quad \mathbf{Q} = \mathbf{T}.\mathbf{v}, \quad (4.82)$$

$$\mathbf{P} = -\rho_0 \mathbf{v}.\mathbf{F}, \quad \mathbf{b} = -\left(L\mathbf{1}_R + \mathbf{T}.\mathbf{F}\right), \tag{4.83}$$

and

$$h = -\left(K/\rho_0\right)\left.\frac{\partial \rho_0}{\partial t}\right|_X + \left.\frac{\partial \bar{W}}{\partial t}\right|_{\text{expl}}, \tag{4.84}$$

$$\mathbf{f}^{\text{inh}} = \left(K/\rho_0\right)\left.\frac{\partial \rho_0}{\partial \mathbf{X}}\right|_t - \left.\frac{\partial \bar{W}}{\partial \mathbf{X}}\right|_{\text{expl}}. \tag{4.85}$$

In view of (4.81) we may say that material momentum is not *strictly* conserved for a materially inhomogeneous elastic material and in the presence of an external body force. As to (4.80), it tells us that energy is not strictly conserved for rheonomic materials, whether they suffer growth or aging. However, the very form of the source term in the right-hand side of (4.80) provides some hint at a simple and naïve approach to deal with these *dissipative* effects. Indeed, we would have energy conservation if the right-hand side of (4.80) would vanish. Without introducing any thermal processes, this could be accomplished by adding from the outside ("out of the blue") a term that makes this right-hand side vanishe. This will be a dissipation rate $\Phi_d$. Thus we would have

$$\Phi_d = -\left(-\left.\frac{\partial L}{\partial t}\right|_{\text{expl}}\right) = \Phi_{\text{growth}} + \Phi_{\text{age}}, \tag{4.86}$$

with (cf. (4.84))

$$\Phi_{\text{growth}} = K\Pi_0/\rho_0, \quad \Phi_{\text{age}} = -\left.\frac{\partial W}{\partial t}\right|_{\text{expl}}, \tag{4.87}$$

where $\Pi_0$ is the right-hand side of (4.74). This right-hand side will typically be of the form (see Epstein and Maugin, 2000)

$$\Pi_0 = R_0 + \nabla_R.\mathbf{M}, \tag{4.88}$$

where $R_0$ is an external supply (e.g., via some biophysical process, nutriments) and $\mathbf{M}$ is an influx of mass. Since both $K$ and $\rho_0$ are obviously positive, $\Pi_0$ must be also to guarantee a positive $\Phi_{\text{growth}}$.

As to $\Phi_{\text{age}}$ a simplistic case exemplifies the situation. We may assume that the explicit time dependence of $W$ is only through material functions (with certain tensorial properties, a set of scalars being the simplest case) $\alpha(t)$. Then,

using a notation intentionally akin to that of the thermodynamics of irreversible processes with internal variables (cf. Chapter 2), we will set and have

$$A := -\frac{\partial W}{\partial \alpha}, \quad \Phi_{\text{age}} = A\dot{\alpha}, \tag{4.89}$$

where the appropriate inner product must be used in the last expression, which is classically written as a *bilinear* form, the product of a thermodynamic force, $A$, and a time rate. The total expression must be nonnegative according to the second law of thermodynamics. We do not pursue here these considerations and consider from here on only the case of *scleronomic* elastic systems.

***Change of scale***: Let us apply the formalism in (4.68) through (4.70). This is a simple case that yields immediately

$$\frac{\partial}{\partial t}\left( tL - \frac{\partial L}{\partial \mathbf{v}}.(D\mathbf{x}) \right) + \nabla_R.\left( \mathbf{X}L - \frac{\partial L}{\partial \mathbf{F}}.(D\mathbf{x}) \right) = \mathbf{X}.\mathbf{f}^{\text{inh}}, \tag{4.90}$$

where $\mathbf{X}$ now stands only for the usual material coordinates. Expanding (4.90), we are led to

$$\frac{\partial}{\partial t}\left(\mathbf{P}.\mathbf{X} - tH - \rho_0 t\varphi\right) - \nabla_R.\left(\mathbf{b}.\mathbf{X} - t\mathbf{Q}\right) - \mathbf{X}.\mathbf{f}^{\text{inh}} = 0. \tag{4.91}$$

Exploiting the fact that $\partial\varphi/\partial t = -\mathbf{f}.\mathbf{v}$, we could as well write

$$\frac{\partial}{\partial t}\left(\mathbf{P}.\mathbf{X} - tH\right) - \nabla_R.\left(\mathbf{b}.\mathbf{X} - t\mathbf{Q}\right) - \mathbf{X}.\mathbf{f}^{\text{inh}} - \rho_0\varphi + \rho_0 t\,\mathbf{f}.\mathbf{v} = 0. \tag{4.92}$$

The scalar quantity $A = \mathbf{P}.\mathbf{X} - Ht$ is identified as the *action* per unit reference volume. The material (contra-) vector $\mathbf{b}.\mathbf{X} - t\mathbf{Q}$ could also be called the dilatational (or scaling) flux. In structural static mechanics this is sometimes called the *virial*.

Although this has many elements in common with (3.99), (4.92) is not exactly the same. The reason for this discrepancy is that we have assumed here, following (4.68) through (4.70), that time was dilated by the same amount as the material coordinates, whence time may be changed in a different amount to obtain a so-called divergence symmetry. In particular, we can note that

$$\frac{\partial}{\partial t}\left(\mathbf{p}_R.\chi\right) - \nabla_R.\left(\mathbf{T}.\chi\right) - \rho_0\mathbf{f}.\chi = \left( \frac{\partial \mathbf{p}_R}{\partial t} - \text{div}_R\mathbf{T} - \rho_0\mathbf{f} \right).\chi$$

$$+\mathbf{p}_R.\mathbf{v} - \text{tr}\left(\mathbf{T}.\mathbf{F}\right) + \rho_0\frac{\partial\varphi}{\partial\mathbf{x}}.\mathbf{x} \tag{4.93}$$

or

$$\frac{\partial}{\partial t}\left(\mathbf{p}_R.\chi\right)-\nabla_R.\left(\mathbf{T}.\chi\right)-\rho_0\mathbf{f}.\chi=\mathbf{p}_R.\mathbf{v}-\mathrm{tr}\left(\mathbf{T}.\mathbf{F}\right)+\rho_0\frac{\partial\varphi}{\partial\mathbf{x}}\mathbf{x}. \tag{4.94}$$

**REMARK:** In the case where $W$ is a homogeneous function of *degree two* with respect to $\mathbf{F}$ and $\varphi$ is also a function homogeneous of degree two in $\mathbf{x}$, K being already such a function in terms of $\mathbf{v}$, so that

$$\begin{aligned}\mathbf{p}_R.\mathbf{v}-\mathrm{tr}\left(\mathbf{T}.\mathbf{F}\right)+\rho_0\frac{\partial\varphi}{\partial\mathbf{x}}.\mathbf{x}&=\frac{\partial K}{\partial\mathbf{v}}.\mathbf{v}-\mathrm{tr}\left(\frac{\partial W}{\partial\mathbf{F}}.\mathbf{F}\right)+\rho_0\frac{\partial\varphi}{\partial\mathbf{x}}.\mathbf{x}\\&=2K-2W=2L,\end{aligned} \tag{4.95}$$

we note that (4.93) yields

$$\frac{\partial}{\partial t}\left(\mathbf{p}_R.\chi\right)-\nabla_R.\left(\mathbf{T}.\chi\right)-\rho_0\mathbf{f}.\chi=2L. \tag{4.96}$$

Accordingly, *in the absence of body force and material inhomogeneities*, subtracting (4.96) from (4.93), we obtain the identity

$$\frac{\partial}{\partial t}\left(\mathbf{P}.\mathbf{X}-Ht-\mathbf{p}_R.\mathbf{x}\right)\Big|_X-\nabla_R.\left(\mathbf{b}.\mathbf{X}-t\mathbf{Q}-\mathbf{T}.\mathbf{x}\right)=2L, \tag{4.97}$$

to be compared to the weighted sum

$$\mathbf{X}.\left(\frac{\partial\mathbf{P}}{\partial t}-\mathrm{div}_R\mathbf{b}\right)-t\left(\frac{\partial H}{\partial t}-\nabla_R.\mathbf{Q}\right)-\mathbf{x}.\left(\frac{\partial\mathbf{p}_R}{\partial t}-\mathrm{div}_R\mathbf{T}\right)\equiv 0,$$

obviously an identity by its very construction.

***Rotation of the material frame***: Here we would have to apply the formalism in (4.50) through (4.65), specializing to the material space. In the direct-motion description, the motion itself is seen as scalar invariant belonging to a different world insofar as material coordinate transformations are concerned. Accordingly, (4.65) is reduced to the symmetry of the space part of the energy–momentum tensor. We let the reader show that this boils down to comparing the torque exerted by the "convected" quantity with the "convected" part of the torque exerted by that quantity. This is clearly seen in the result, which reads

$$\frac{\partial}{\partial t}\left(\mathbf{X}\times\mathbf{P}-\mathbf{F}^{T}.\left(\chi\times\mathbf{p}_{R}\right)\right)-\operatorname{div}_{R}\left(\mathbf{X}\times\mathbf{b}-\mathbf{F}^{T}.\left(\chi\times\mathbf{T}\right)\right)$$
$$-\left(\mathbf{X}\times\left(\mathbf{f}^{\text{inh}}+\mathbf{f}^{\text{ext}}\right)+\mathbf{F}^{T}.\left(\chi\times\rho_{0}\mathbf{f}\right)\right)=\mathbf{0}. \tag{4.98}$$

This is not exactly the same as the symmetry of **b** with respect to the deformed metric **C**, or the symmetry of **b** with respect to $\mathbf{C}^{-1}$, or the very symmetry of the second Piola–Kirchhoff stress since

$$\mathbf{b}.\mathbf{C}^{-1}=-L\mathbf{C}^{-1}-\mathbf{S}.\mathbf{C}.\mathbf{C}^{-1}=-\left(L\mathbf{C}^{-1}+\mathbf{S}\right), \tag{4.99}$$

and the symmetry of **S** is equivalent to that of the Cauchy stress.

***Other conservation laws***: Additional conservation laws useful in structural mechanics hold good only in the *linear theory of elasticity*. In effect, linearity allows for the superposition of solutions. "Addition of solutions" can in fact be cast in the framework of group theory if we notice that this "symmetry" is a consequence of the linearity of the system *S* of field equations and a divergence symmetry for *L*, that is, the case where the relevant Lie group of transformations *G* is such that (4.42) is replaced by

$$\mathbf{v}^{(1)}L+L\frac{\partial\bar{X}^{\mu}}{\partial X^{\mu}}=\partial_{\mu}B^{\mu}, \tag{4.100}$$

where $B^{\mu}$ is an appropriate analytic function. The case $B^{\mu}=0$, which has already been studied, corresponds to a variational symmetry of *L* generated by the infinitesimal generator **v**. Every variational or divergence symmetry of the function *L* is also a symmetry of the associated Euler–Lagrange (i.e., field) equations. But not every symmetry of these latter equations is a variational or divergence symmetry. "Addition of solutions" requires the construction of the relevant $B^{\mu}$. In small strains and quasistatics, the spatial part of $B^{\mu}$, $B_i$, $i=1,2,3$, is given by

$$B_i=u_j\sigma_{ji}\left(\mathbf{s}\right), \tag{4.101}$$

where the notation introduced within parentheses stands for a replacement of **u** by any solution **s** of the linear system *S*. The corresponding generator and conserved vector flux are given by

$$v^{(4)}=s_i\left(\mathbf{x}\right)\frac{\partial}{\partial u_i},\quad J_i=s_j\sigma_{ji}\left(\mathbf{u}\right)-u_j\sigma_{ji}\left(\mathbf{s}\right). \tag{4.102}$$

In the absence of body force, this results in the *Rayleigh–Betti reciprocity theorem* that we already expressed in integral form in (3.60) and local form in (3.61), which yields the divergence-free nature of $J_i$.

We do not repeat the other conservation laws (e.g., for energy, field momentum, and material angular momentum) associated with small-strain linear elasticity on the basis of group theory. They are just those obtained previously via more naïve methods.

### 4.3.2 Inverse-Motion Formulation for Classical Elasticity

In that case, assuming for the sake of simplicity that there is no physical body force present and the system is scleronomic, we naturally consider a Lagrangian density $L$, still per unit volume of $K_R$ but as

$$L = L(\mathbf{X},\mathbf{V},\mathbf{F}^{-1}) = L\left(\mathbf{X},\left.\frac{\partial \mathbf{X}}{\partial t}\right|_x,\left.\frac{\partial \mathbf{X}}{\partial \mathbf{x}}\right|_t\right) = \frac{1}{2}\rho_0(\mathbf{X})\mathbf{V}.\mathbf{C}.\mathbf{V} - \hat{W}(\mathbf{F}^{-1};\mathbf{X}), \quad (4.103)$$

as we easily verify that $\mathbf{v}^2 \equiv \mathbf{V}.\mathbf{C}.\mathbf{V}$, so that the deformed metric (hence **F**) is involved in the kinetic energy contributing to $L$. The situation with (4.103) is quite different from that in Equation 4.71 since we cannot avoid the direct presence of the field $\mathbf{X} = \chi^{-1}$ itself in (4.103) if the body is materially inhomogeneous. We then consider the following *natural Hamiltonian principle*:

$$\delta_x \int_0^t \int_{B_R} L dV dt + \int_0^t \int_{\partial B} (\mathbf{F}^T.\mathbf{T}^d).\delta_x \mathbf{X}\, da dt - \int_0^t \int_{\partial B} L(\mathbf{N}.\delta_x \mathbf{X}) dA dt = 0 \quad (4.104)$$

The variation is Eulerian and has to be performed at fixed placement **x**. This variation commutes with spatial integration. Thus,

$$\delta_x \int_{B_R} L dV = \delta_x \int_B (J_F^{-1} L) dv = \int_{B_R} J_F \delta_x (J_F^{-1} L) dV, \quad (4.105)$$

and we can prove that

$$\delta_x (J_F^{-1}) = J_F^{-1} \nabla_R . \delta_x \chi^{-1}, \quad (4.106)$$

$$\delta_x \left(\frac{1}{2}\rho_0 \mathbf{V}.\mathbf{C}.\mathbf{V}\right) = \left(\frac{1}{2}\mathbf{v}^2\right)(\nabla_R \rho_0).\delta_x \chi^{-1} + \mathbf{P}.\frac{\partial}{\partial t}(\delta_x \chi^{-1}) + \mathbf{P}.(\mathbf{v}.\nabla)\delta_x \chi^{-1}, \quad (4.107)$$

and

$$\delta_x \hat{W} = \left(\nabla_R \hat{W}\right)_{\text{expl}} .\delta_x \chi^{-1} + J_F \overline{\mathbf{T}}^{(1)T} .\nabla(\delta_x \chi^{-1}), \overline{\mathbf{T}}^{(1)} = \frac{\partial \hat{W}}{\partial \mathbf{F}^{-1}} = \frac{\partial W^{(1)}}{\partial \mathbf{F}^{-1}} \quad (4.108)$$

The last contribution in (4.107) arises as a result of the presence of the deformed metric in the kinetic energy and the fact that $\delta_x \mathbf{C} \neq \mathbf{0}$ as

$$\delta_x \mathbf{F} = -\nabla_R \left(\delta_x \mathbf{X}\right).\mathbf{F}^T. \tag{4.109}$$

Now the proof is completed by showing that (4.105) yields

$$\begin{aligned}\delta_x \int_{B_R} L dV \equiv \int_{B_R} J_F \left( \hat{\mathbf{f}}^{\text{inh}} + \text{div}\left(\mathbf{B} - \mathbf{v} \otimes \hat{\mathbf{P}}\right) - \left.\frac{\partial \hat{\mathbf{P}}}{\partial t}\right|_x \right).\delta_x \chi^{-1} dV \\ + \int_{B_R} J_F \left( \nabla.\left(\left(\mathbf{B} - \mathbf{v} \otimes \hat{\mathbf{P}}\right).\delta_x \chi^{-1}\right) + \frac{\partial}{\partial t}\left(\hat{\mathbf{P}}.\delta_x \chi^{-1}\right)\right) dV,\end{aligned} \tag{4.110}$$

where (see (3.70) and (3.71))

$$\hat{\mathbf{P}} = J_F^{-1}\mathbf{P} = \rho \mathbf{C}.\mathbf{V}, \quad \hat{\mathbf{f}}^{\text{inh}} = J_F^{-1}\mathbf{f}^{\text{inh}}, \quad \mathbf{B} = -\left(J_F^{-1} L\mathbf{F} - \overline{\mathbf{T}}^{(1)}\right). \tag{4.111}$$

The localization of (4.104) on account of (4.110) yields, for arbitrary $\delta_x \chi^{-1}$ at any material point $\mathbf{X} \in B_R$, the local form of the linear-momentum balance equation per unit current volume as

$$\left.\frac{\partial \hat{\mathbf{P}}}{\partial t}\right|_{x \text{ fixed}} - \text{div}\left(\mathbf{B} - \mathbf{v} \otimes \hat{\mathbf{P}}\right) = \hat{\mathbf{f}}^{\text{inh}}. \tag{4.112}$$

Therefore, Equation 3.70 is directly derivable from Hamilton's principle applied to the inverse-motion description. Obviously, the $\delta_x$-variation effected at fixed current point $\mathbf{x}$ automatically captures the material inhomogeneities by extracting the material force $\hat{\mathbf{f}}^{\text{inh}}$, but the latter is per unit current volume. Then Equation 3.70 is deduced from (4.112), and Equation 3.73 is recovered by multiplication by $J_F$ and appropriate manipulations. In this procedure one must take notice of the following useful identities:

$$\text{div}\left(\mathbf{v} \otimes \hat{\mathbf{P}}\right) = -J_F^{-1}\text{div}_R\left(\mathbf{V} \otimes \mathbf{P}\right), \tag{4.113}$$

$$J_F \left.\frac{\partial \hat{\mathbf{P}}}{\partial t}\right|_{x \text{ fixed}} = \left.\frac{\partial \mathbf{P}}{\partial t}\right|_{\mathbf{X} \text{ fixed}} + \text{div}_R\left(\mathbf{V} \otimes \mathbf{P}\right), \tag{4.114}$$

and

$$\text{div}\,\mathbf{B} \equiv J_F^{-1}\,\text{div}_R\,\mathbf{b}. \tag{4.115}$$

If we now apply Noether's theorem to the inverse-motion description for space–time translations, but this time with spatial coordinates $x^i$, we shall

obtain the energy equation for $\hat{L} = J_F^{-1}L$ not depending explicitly on time $t$, and the linear (physical) momentum balance law. Thus, as noted by the most penetrating observers of the continuum mechanics scene (Rogula, 1977; Edelen, 1981; Golebiewska-Herrmann, 1981), there are situations where linear physical momentum is strictly conserved (no body force), while material momentum is *not* conserved (presence of material inhomogeneities), and others where the situation is clearly reversed. What about body forces in the formulation just given? The inverse-motion description misses body forces in the $\delta_x$-variation. Indeed, assume that these forces are derivable for a potential $\varphi(\mathbf{x})$. Then the missing term in the principle in (4.104) would give

$$\delta_x \int_{B_R} \rho_0(\mathbf{X})\varphi(\mathbf{x})dV = \delta_x \int_B \left(J_F^{-1}\rho_0(\mathbf{X})\varphi(\mathbf{x})dv = \delta_x \int_B \rho(\mathbf{x},t)\varphi(\mathbf{x})dv \equiv 0, \quad (4.116)$$

from the very definition of an Eulerian variation.

**EXERCISE 4.1:** In the absence of body force, show that Equation 4.29 can also be written as

$$\frac{\partial H}{\partial t} - \nabla_R.\left(\left(\mathbf{b} + L\mathbf{1}_R\right).\mathbf{V}\right) = 0; \quad (4.117)$$

and that this is also a consequence of the following identity:

$$\left(\frac{\partial H}{\partial t} - \nabla_R.\mathbf{G}\right) - \left(\frac{\partial \mathbf{P}}{\partial t} - \left(\mathrm{div}_R\mathbf{b} + \mathbf{f}^{\mathrm{inh}}\right)\right).\mathbf{V} = 0, \quad (4.118)$$

which is the time-like counterpart of the identity obtained by multiplying the identity in (3.16) by $\mathbf{F}^{-1}$ to the right.

### 4.3.3 Second-Gradient Elasticity

Many of the results stated in the preceding can be generalized to the case of a field theory of elasticity that is a *second-gradient theory*, that is, whenever (4.71) and (4.72), ignoring the presence of a body force and its potential, are replaced by the more general expressions:

$$L = \bar{L}(\mathbf{v},\mathbf{F},\nabla_R\mathbf{F};\mathbf{X}) = \bar{L}\left(\frac{\partial\chi}{\partial t},\frac{\partial\chi}{\partial\mathbf{X}},\frac{\partial^2\chi}{\partial\mathbf{X}\otimes\partial\mathbf{X}};\mathbf{X}\right), \quad (4.119)$$

and

$$L = \frac{1}{2}\rho_0(\mathbf{X})\mathbf{v}^2 - \bar{W}(\mathbf{F},\nabla_R\mathbf{F};\mathbf{X}). \quad (4.120)$$

The kinetic energy is left unchanged for there is no additional microstructure here, just a finer description of stress effects. Elastic media of the type of those governed by a Lagrangian in (4.120) were considered by Toupin (1962, 1964) for finite strains and Mindlin and Tiersten (1962) and Mindlin and Eshel (1968) for the small-strain approximation for which Le Roux's (1911) work seems to be a pioneer. In the 1960s and 1970s, theories of this complexity (also called second-grade or strain-gradient theories) were expected to bring some satisfactory answer to the question raised by the appearance of local singularities in some elasticity problems (e.g., those involving corners, edges, etc.). This was not so successful. But gradient theories are also relevant to the elasticity theory of crystals, where long-range interactions and the associated wave-dispersion effects cannot be neglected (cf. Maugin, 1999). This appears of necessity because scale effects are present (e.g., coherence length), and theories such as (4.120) include *internal length* scales.

We are just in the framework of the variational formulation. The field (Euler–Lagrange) equations are the spatial components of the local balance of linear (physical) momentum in the Piola–Kirchhoff formulation:

$$\left.\frac{\partial \mathbf{p}}{\partial t}\right|_{\mathbf{x}} - \mathrm{div}_R \mathbf{T}^{\mathrm{eff}} = \mathbf{0}, \tag{4.121}$$

wherein

$$\mathbf{p} = \rho_0 \mathbf{v}, \quad \mathbf{T}^{\mathrm{eff}} = \mathbf{T} - \mathrm{div}_R \mathbf{M}, \tag{4.122}$$

$$\mathbf{T} = \frac{\partial \bar{W}}{\partial \mathbf{F}}, \quad \mathbf{M} = \frac{\partial \bar{W}}{\partial (\nabla_R \mathbf{F})}, \tag{4.123}$$

where the last introduced quantity has components

$$M_{.i}^{LK} = \frac{\partial \bar{W}}{\partial (F_{K,L}^{i})} = M_{.i}^{KL}. \tag{4.124}$$

Here $\mathbf{T}^{\mathrm{eff}}$ is an *effective* first Piola–Kirchhoff stress, and $\mathbf{M}$ is a new *internal force* that may be referred to as the Piola–Kirchhoff *hyperstress*. The latter has at most 18 independent components due to the symmetry on the two material indices. This large number of components will unfortunately be accompanied by a large number of new material coefficients to be determined by appropriate experiments or by comparison with the long-wave limits of a microscopic model or a procedure of homogenization (cf. Forest, 2006). The application of Noether's theorem to the case of material space–time translations for scleronomic systems in the absence of body force systems yields the *conservation of material momentum* and that of *energy* in the form

$$\left.\frac{\partial \mathbf{P}}{\partial t}\right|_{\mathbf{x}} - \mathrm{div}_R \mathbf{b}^{\mathrm{eff}} = \mathbf{f}^{\mathrm{inh}}, \tag{4.125}$$

and

$$\left.\frac{\partial H}{\partial t}\right|_{\mathbf{x}} - \nabla_R . \mathbf{G}^{\mathrm{eff}} = 0, \tag{4.126}$$

where we have defined the following quantities:

$$\mathbf{P} = -\mathbf{p}.\mathbf{F}, \quad \mathbf{b}^{\mathrm{eff}} = \mathbf{b} - \mathrm{div}_R\left(\mathbf{M}.\mathbf{F}\right), \tag{4.127}$$

$$\mathbf{b} = -\left(L\mathbf{1}_R + \mathbf{T}.\mathbf{F} + \mathbf{M}:\left(\nabla_R \mathbf{F}\right)^T\right), \tag{4.128}$$

$$H = K + W, \quad L = K - W, \quad \mathbf{G}^{\mathrm{eff}} = \mathbf{G} - \left(\mathrm{div}_R \mathbf{M}\right).\mathbf{v}, \quad \mathbf{G}=\mathbf{T}.\mathbf{v} + \mathbf{M}:\left(\nabla_R \mathbf{v}\right)^T, \tag{4.129}$$

and

$$\mathbf{f}^{\mathrm{inh}} = \left.\frac{\partial L}{\partial \mathbf{X}}\right|_{\mathrm{expl}}. \tag{4.130}$$

This shows very little variance with the first-gradient theory. But two remarks are in order. First, we must express the rotational invariance of *W*. This can be obtained by performing an infinitesimal rotation in the current configuration, the result of which is a generalization of (2.88), as

$$\mathrm{skew}_{[ij]}\left(\mathbf{FT} + 2\left(\nabla_{\mathrm{R}}\mathbf{F}\right)^T : \mathbf{M}\right) = 0, \tag{4.131}$$

which shows that the Cauchy stress is *not* symmetric in this description since it is proportional to **F.T**. Equation 4.131 is automatically satisfied if, for instance, for an anisotropic inhomogeneous material, we take

$$W = \bar{W}\left(\mathbf{C}, \left(\nabla_R \mathbf{F}\right) : \left(\nabla_R \mathbf{F}\right)^T, \left(\nabla_R \mathbf{F}\right)^T . \mathbf{F}; \mathbf{X}\right). \tag{4.132}$$

The second remark concerns *boundary conditions*, which must accompany (4.121) and (4.125) for a body of finite extent, as the theory clearly becomes of higher degree in space derivatives. This, however, is much better evidenced in the corresponding small-strain theory as developed by, for example, Mindlin and Eshel (1968)—obviously without the concepts of inhomogeneity, material momentum (field momentum), and Eshelby stress—to whom

we refer the reader. In terms of "forces," **N**.**M** must be specified in addition to **N**.**T**. In terms of displacements, their **curvature** should be specified in order to match the duality of data in terms of forces.

***Small-strain strain-gradient theory***: From the preceding this is trivially given by

- *Balance of linear (physical) momentum*:

$$\rho_0 \ddot{u}_i - \sigma_{ji,j} = \rho_0 f_i \quad \text{in} \quad B \tag{4.133}$$

- *Balance of energy*:

$$\dot{W} = \bar{\sigma}_{ji}\, \dot{u}_{i,j} + m_{kji} \dot{\varepsilon}_{ij,k} \tag{4.134}$$

- *Balance of field momentum*:

$$\dot{P}_i^f - b_{ji,j} = f_i^{\text{inh}} - \rho_0 f_j\, u_{j,i} \tag{4.135}$$

- *Constitutive equations*:

$$\sigma = \frac{\delta \bar{W}}{\delta \varepsilon} = \bar{\sigma} - \text{div}\, \mathbf{m}, \tag{4.136}$$

$$W = \bar{W}(\varepsilon, \nabla\varepsilon; \mathbf{x}), \quad \bar{\sigma} = \frac{\partial \bar{W}}{\partial \varepsilon}, \quad \mathbf{m} = \frac{\partial \bar{W}}{\partial (\nabla \varepsilon)}, \tag{4.137}$$

- *Definitions*:

$$P_i^f = -\rho_0 \dot{u}_j u_{j,i}, \quad b_{ji} = -\left(L\delta_{ji} + \bar{\sigma}_{jk} u_{i,k} + m_{jkp} u_{i,kp}\right) - \left(m_{kjp} u_{i,p}\right)_{,k},$$

$$f_i^{\text{inh}} = \left.\frac{\partial L}{\partial \mathbf{x}}\right|_{\text{expl}}, \tag{4.138}$$

  where $\sigma$ is the Cauchy stress, the symmetric tensor $\bar{\sigma}$ is called the *intrinsic stress*, and the last object, the *hyperstress* tensor $\mathbf{m}$, has components $m_{kji} = m_{kij}$.

- *Natural boundary conditions* (see, e.g., Germain, 1973; Maugin, 1980):

$$n_j t_{ji} + \left(n_j D_p n_p - D_j\right)\left(n_k m_{kji}\right) = T_i^d \quad \text{at} \quad \partial B - \Gamma\uparrow, \tag{4.139a}$$

$$n_k m_{kji} n_j = R_i \quad \text{at} \quad \partial B - \Gamma\uparrow, \tag{4.139b}$$

$$\varepsilon_{ipq}\tau_p\left[n_k m_{kjq} n_j\right] = E_i \quad \text{along} \quad \Gamma\uparrow, \tag{4.139c}$$

where $D_j$ denotes the tangential derivative at the regular parts of $\partial B$, $\Omega = -1/2 D_j n_j$ is the local mean curvature at regular parts of $\partial B$, $\tau$ is the unit tangent along the oriented edge $\Gamma\uparrow$ (if the latter exists), $R_i$ is a so-called *double normal traction*, and $E_i$ is a *lineal force* along the edge. This shows the complexity of prescribing data at the irregular boundary because the *hyperstress* is a complex notion of internal force.

On the one hand, the very expression of $\sigma$ through a *functional derivative* of the Euler–Lagrange type provides the expression in terms of even-order space derivatives (that is, two orders more appear at each step of refinement in the *n*th-order gradient theory). On the other hand, a local experience (real or in thought only) considering a *facet* cut in the material (geometric description at the first order of the cut via its unit normal only) "sees" the Cauchy stress. Only *edges* or the second-order geometric description (tangential derivatives, curvature) can "see" **m** independently (in this regard, see the beautiful work of Dell'Isola and Seppecher [1995] on the generalization of Cauchy's lemma for the representation of stresses). This is bypassed by a weak formulation of the type of the principle of virtual power such as

$$\int_B \rho_0 \dot{u}_i\, v_i^* dv = -\int_B \left(\bar{\sigma}_{ji} v_{i,j}^* + m_{kji} v_{(i,j),k}^*\right) dv + \int_{\partial B} \left(T_i^d v_i^* + M_{ji}^d v_{i,j}^*\right) da$$
$$+ \int_B \rho_0 f_i\, v_i^* dv, \tag{4.140}$$

where $\mathbf{T}^d$ and $\mathbf{M}^d$ are an applied *traction* and an applied so-called *double force* (represented by a symmetric second-order tensor—see Maugin (1980) and Germain (1973)). Other conservation laws and the connection to Lie groups are to be found in Lazar and Maugin (2005).

### 4.3.4 Hamilton's Equations

The formulation using the material momentum **P** in the upper right corner in Figure 3.4—said to be completely material—is the only one among the four formulations that combines simplicity (no convection term, partial derivatives taken with respect to the independent variables **X** and *t*) with the fact that it is expressed in the same framework $K_R$. This endows this formulation with a peculiar nature that does not seem to have been noticed before the papers of Maugin and Trimarco (1992), although the canonical formulation of elasticity—especially in the small-strain approximation—has attracted the attention of some researchers (Holm and Kupershmidt, 1983; Simo et al., 1988). It is in fact a *canonical formulation* from the point of view of *Hamilton's analytical mechanics* of elastic systems. This primarily arises from the fact that the $X^K$'s and the components $\hat{P}_K = \rho C_{KL} V^L$ of the material momentum

per unit volume of $K_t$ are conjugate variables in the sense of Hamilton's mechanics. Indeed, we can define the Hamiltonian density $\hat{H}$ per unit volume in $K_t$ by

$$\hat{H} = J_F^{-1}\left(\mathbf{P}.\mathbf{V} - L\right) = \hat{\mathbf{P}}.\mathbf{V} - \hat{L}, \tag{4.141}$$

so that

$$\hat{\mathbf{P}} = \frac{\partial \hat{L}}{\partial \mathbf{V}}, \quad \mathbf{V} = \left.\frac{\partial \chi^{-1}}{\partial t}\right|_{x\,\text{fixed}} = \frac{\delta \hat{H}}{\delta \hat{\mathbf{P}}}, \tag{4.142}$$

where the Euler–Lagrange functional derivative has been introduced for the sake of generality (but it does reduce to a partial derivative in the case of Equation 4.142). The last of (4.142) is verified by noting that

$$\hat{K} = \frac{1}{2}\rho \mathbf{v}^2 = \frac{1}{2}\rho \mathbf{V}.\mathbf{C}.\mathbf{V} = \frac{1}{2\rho}\hat{\mathbf{P}}.\mathbf{C}^{-1}.\hat{\mathbf{P}}. \tag{4.143}$$

The second of (4.142) is none other than the *first* of Hamilton's canonical equations. The second of these equations should read

$$\left.\frac{\partial \hat{\mathbf{P}}}{\partial t}\right|_{x\,\text{fixed}} = -\frac{\delta \hat{H}}{\delta \mathbf{X}}. \tag{4.144}$$

This, indeed, is none other than the equation of conservation of material momentum. To check this, one has to evaluate

$$\frac{\delta \hat{H}}{\delta \mathbf{X}} = \nabla_R \hat{H} - \nabla.\left(\partial \hat{H}/\partial \mathbf{F}^{-1}\right), \quad \hat{H} = \hat{K} + \hat{W}\left(\mathbf{X}, \mathbf{F}^{-1}\right). \tag{4.145}$$

### 4.3.5 Lie–Poisson Brackets

Consider a materially inhomogeneous elastic body in finite strains but in the absence of body forces. Integrating the balance of material momentum over a regular material region $B_R$ bounded by the regular surface $\partial B_R$, this yields

$$\frac{d}{dt}\int_{B_R} \mathbf{P}\, dV = \int_{\partial B_R} \mathbf{N}.\mathbf{b}\, dA + \int_{B_R} \mathbf{f}^{\text{inh}} dV. \tag{4.146}$$

This is a balance among material forces. But we also note that

$$\int_{B_R} \mathbf{P} dV = \int_B \hat{\mathbf{P}} dv. \tag{4.147}$$

Now define

$$A_B = \int_B A(-)dv, \quad \hat{H}_B = \int_B \hat{H}(-)dv. \tag{4.148}$$

We a priori define the *Lie–Poisson bracket* {.,.} in a global way by

$$\{A, B\} = \int_B \left( \frac{\delta A}{\delta \mathbf{X}} . \frac{\delta B}{\delta \hat{\mathbf{P}}} - \frac{\delta A}{\delta \hat{\mathbf{P}}} . \frac{\delta B}{\delta \mathbf{X}} \right) dv, \tag{4.149}$$

and we propose the following global evolution equation, as is usual in classical field theory, by

$$\dot{A}_B = \left\{ A_B, \hat{H}_B \right\}. \tag{4.150}$$

From this total energy is trivially conserved:

$$\dot{\hat{H}}_B = \left\{ \hat{H}_B, \hat{H}_B \right\} \equiv 0, \tag{4.151}$$

because of the skewsymmetry of the bracket. This holds irrespective of the presence or absence of elastic inhomogeneities—insofar as the system is scleronomic—as inhomogeneity forces are not dissipative per se. Consider now the total material momentum as defined component-wise in (4.147). Applying (4.150) to it and accounting for the definition in (4.149) and the fact that $\hat{\mathbf{P}}$ satisfies the canonical equations (4.142) and (4.144), we obtain that

$$\equiv \frac{d}{dt} \int_B \hat{\mathbf{P}} dV = \int_B \left( \left( \nabla_R \hat{\mathbf{P}} \right) . \mathbf{V} + \left. \frac{\partial \hat{\mathbf{P}}}{\partial t} \right|_x \right) dv \equiv \frac{d}{dt} \int_B \hat{\mathbf{P}} dv, \tag{4.152}$$

on account of (2.40). Thus the right-hand side of (4.152) is zero, hence *total material momentum is conserved* in the sense of the Lie–Poisson brackets, if and only if the global inhomogeneity force vanishes and the boundary conditions on **b** are homogeneous at $\partial B_R$ (no flux at this boundary). This result will be of importance in *soliton theory* (see Chapter 12).

**REMARK 4.3:** Bessel–Hagen extension

Following the remark made after Equation 4.8 the Lagrangian density of interest may be defined up to the divergence of a four-field depending only on the space–time coordinates. For homogeneous bodies, the flux conservation can now be written as

$$\partial_\mu \left( J^\mu + \Omega^\mu \right) = 0. \tag{4.153}$$

This is called the *Bessel-Hagen* (1921) *extension* for a divergence symmetry (cf. Olver, 1986). This may be used for the benefit of the construction of additional conservation equations (see Herrmann and Kienzler [2001] and an application to structural mechanics by Kienzler (1993)).

**REMARK 4.4:** Neutral action

Many physical systems, in particular those exhibiting dissipation, do not possess a Hamiltonian–Lagrangian variational formulation. In other words, their physics is governed by a set of local field equations obtained by substituting appropriate constitutive equations into local balance laws. In principle there is no systematic way to build for those systems a set of conservation laws such as that of material momentum (however, see Chapter 5). Such a system may be stated formally as (for a first-gradient theory)

$$\Delta_\beta\left(\phi^\alpha, \partial_\mu\phi^\alpha, X^\mu\right) = 0, \quad \beta = 1,2,..., \tag{4.154}$$

of which a special case would be Euler–Lagrange equations $E_\beta(L) = 0$. For this special case we have (cf. Equation 4.38) Noether's identity

$$\partial_\mu J^\mu + \sum_\alpha E_\alpha Q^\alpha = 0, \quad \text{hence} \quad \partial_\mu J^\mu = 0, \tag{4.155}$$

where we recall that $Q^\alpha$ are the characteristics of the transformation group. In the case where (4.154) holds, let us look for a set of functions $\bar{Q}^\beta$ such that we could write an expression such as (compare to (4.155))

$$\partial_\mu J^\mu + \sum_\beta \Delta_\beta \bar{Q}^\beta = 0. \tag{4.156}$$

It follows from this that a requirement for the existence of conservation laws associated with (4.154) is that

$$E_\alpha\left(\bar{Q}^\beta \Delta_\beta\right) = 0. \tag{4.157}$$

The reason for this is that, in variational calculus, if a Lagrangian density $L$ is itself a divergence (these are so-called *null* Lagrangians), then $E_\alpha(L) = 0$. Equation 4.157 implies that $\bar{Q}^\beta\Delta_\beta$ is formally a *null* Lagrangian $\tilde{L}$ such that

$$\tilde{A} = \int \tilde{L} d^4X = \int \left(\tilde{Q}^\beta \Delta_\beta\right) d^4X = -\int N_\mu J^\mu d^3S. \tag{4.158}$$

This has vanishing variation for any independent fields. That is, $\delta A = 0$. In other words, this means that to construct conservation laws for any system (whether or not it admits a Lagrangian), such as (4.154), we need to construct the "product" $\bar{Q}^\beta\Delta_\beta$ whose action $\tilde{A}$ is invariant. We can say that *this action*

*behaves neutrally* under its variation. Such a technique, studied by Chien (1992) and referred to as the method of *neutral action*, was illustrated by Chien et al. (1993) in the case of one-dimensional linear viscoelasticity. The remaining problem, with a nonobvious solution in a sufficiently sophisticated case, is to find the functions $\tilde{Q}^{\beta}$.

## 4.4 Conclusive Remarks

What we have developed in this chapter is essentially the variational analytical mechanics of fields with direct application to elasticity. It happens that elasticity is paradigmatic as it appears to be an ideal illustration. The approach chosen has emphasized the role played by material and spatial (Eulerian) variations. This was acknowledged by several authors in special cases (no dynamics, no material inhomogeneities, small strains depending on the case), among them Casal (1978), Rogula (1966, 1977), Edelen (1981), and Golebiewska-Herrmann (1981). But two remarks are essential at this point.

First, the special case of elasticity is indeed more than special in the context of field theory because it leads to some misinterpretation. The reason for this is that in this case the *field* (placement) and the space-parametrization share the same nature: They are *positions* but in different spaces. It is even worse when Lagrangian coordinates are used as space-parametrization because they correspond to a placement occupied in the past! This gives a feeling of strict equivalence by mere pull back or push forward between, or of a strict ontological status of, the balances of linear physical momentum and of material momentum. But the latter, which we can better call *canonical momentum* in view of the general theory of fields, sums up contributions from all fields involved (remember the summation over $\alpha$), whether mechanical or other in nature, and it will include contributions other than those of the actual placement in more complex theories of continua (such as in media with internal degrees of freedom or with coupled fields, which we examine later on in this book). In particular, there are field theories that admit no deformation field, but they still admit the notions of canonical momentum and "Eshelby" stress, a typical example being that of pure electromagnetic fields in a vacuum or in a rigid body. Another example is given in the appendix to this chapter.

Second, the "neutral action" method briefly examined in Section 4.3 offers one possibility to account for some (simple) dissipative processes in low-dimensional systems in order to construct some conservation equations in the absence of starting Lagrangian. But canonical equations for both momentum and energy must exist whatever the precise material behavior of the material. We shall see in the forthcoming chapter how this can be dealt with in a sufficiently general thermodynamic framework for deformable solids.

## Appendix A4.1: Field Theory of the Peach–Koehler Force in Matter with Continuously Distributed Dislocations

Since $\beta_{ij} = u_{j,i}$ for a compatible distortion, if we consider an incompatible distortion $\beta_{ij}$ (not exactly integrable into a displacement gradient) in small strains, we can write

$$\frac{\partial}{\partial t}\beta_{ji} - v_{i,j} = J_{ij} \neq 0, \tag{A4.1}$$

where $J_{ij}$ is called the (material) *dislocation current*. Simultaneously, there holds Equation 3.120 relating to the *dislocation density* $\alpha$ of components $\alpha_{ik}$.

The dislocation current and density are related by

$$J_{ij} = -\varepsilon_{ilk} V_l \, \alpha_{jk}, \tag{A4.2}$$

where $\mathbf{V}$ denotes the dislocation velocity in *material* space. Consider the Lagrangian density $L = \bar{L}(\mathbf{v}, \beta)$. The material force acting on the dislocation density, after variation at fixed actual position, is given by the "inhomogeneity force" present in the balance of material momentum, that is,

$$\mathbf{f}^{\text{disl}} = \frac{\partial \mathbf{P}}{\partial t} - \text{div}_R \mathbf{b} \quad \text{or} \quad f_j^{\text{disl}} = \frac{\partial}{\partial t} P_j - b_{ij,i}, \tag{A4.3}$$

with the canonical definitions

$$P_j = -\frac{\partial \bar{L}}{\partial v_i}\beta_{ji}, \quad b_{ji} = L\delta_{ji} - \beta_{ik}\frac{\partial \bar{L}}{\partial \beta_{jk}}. \tag{A4.4}$$

Effecting now the computation of the right-hand side of Equation A4.3 we obtain

$$f_j^{\text{disl}} = -\varepsilon_{jlk}\left(p_i V_l - b_{li}\right)\alpha_{ik}, \quad p_i = \partial \bar{L}/\partial v_i. \tag{A4.5}$$

But for a single dislocation

$$\alpha_{ik} = \tilde{b}_i \, \tau_k \delta(\xi), \tag{A4.6}$$

where the symbols introduced have the same meaning as in Section 3.7, so that the first of (A4.8) yields

$$f_j^{\text{disl}} = \varepsilon_{jlk}\left(b_{li} - V_l\ p_i\ \right)\tilde{b}_i\ \tau_k\,, \tag{A4.10}$$

a formula due to Rogula (1965), where we recognize in the contribution $\varepsilon_{jlk}V_l p_i \tilde{b}_i \tau_k = (\mathbf{p}.\tilde{\mathbf{b}})(\mathbf{V}\times\tau)_j$ the components of the right-hand side of (3.66.)

# 5

# *Canonical Thermomechanics of Complex Continua*

### Object of the Chapter

Where we discover that canonical conservation laws for continua exhibiting complex dissipative processes can be formulated jointly for energy and canonical momentum, opening up the way to applications to a large spectrum of problems where progress of a material force and dissipation of energy must be considered simultaneously in a compatible manner.

## 5.1 Introduction

Of course, the variational formulation of the foregoing chapter has its limitations, although it does yield canonical conservation laws of energy and material momentum and provides in a direct manner the notions of material stresses and forces. But there is no reason why these should be limited to special classes of physical processes in which the energy density is known from the start, so that, in effect, the material behavior is also specified from the start. Only recently a general canonical formulation of **thermodynamics** was formulated that accommodates large classes of dissipative phenomena and is naturally subjected to the necessary satisfaction of the second law of thermodynamics. To illustrate this general viewpoint, we consider the sufficiently general continuum physics of finitely deformable solids that may conduct heat and exhibit dissipation of different types via the presence of so-called internal variables of state (cf. Chapter 2). The uncontrollability of the internal state variables is reflected in the fact that they have no applied conjugated forces in the bulk and at the surface of the considered body, so that their only virtue, and essence, is to produce a dissipation. Accordingly, the general starting field equations are those of a classical thermodeformable (scleronomic) body.

Working in parallel on the energy equation in a special form and on the associated canonical equation of momentum, we focus attention on the case

of deformable media that are primarily finitely elastic but also admit the existence of thermodynamically irreversible phenomena by means of a diffusive internal variable of state, or alternately an additional degree of freedom, in any case presenting some weak nonlocality (gradient effects). Two descriptions follow thereof, one that can be called standard according to rational thermomechanics (there exists a generalized internal force or thermodynamically conjugated force for a variable and each of its gradients separately, and the entropy flux has its classical definition) and the so-called field-theoretic viewpoint, in which only one generalized force (based on a variational derivative of the energy) is used. In the latter, the entropy flux deviates from its classical definition, but, simultaneously, by virtue of the space–time consistency, the Eshelby stress tensor has to be altered.

Simple examples with diffusion of an internal variable or a true internal degree of freedom illustrate these formulations, which may be valuable in the description of some complex materials. In this respect, we mention that the formulation of a rational theory of continuous media with diffusive effects still presents a challenge in modern continuum thermomechanics. One reason for this is the recurring question whether the field associated with the diffusive process of interest is an *observable* or an *internal* variable of state, whether it constitutes a true additional internal degree of freedom or merely is a parameter compared to the main governing ingredients of the thermomechanical description, that is, the deformation and the temperature fields. These questions have been posed for a long time, including in such classical works as the monograph of de Groot and Mazur (1962) or in more "rational" approaches to fluid mixtures such as in Bowen (1967, 1976). Furthermore, recent developments in the continuum mechanics of complex or microstructured media have led to considering gradients of certain variables, a consideration akin to introducing diffusive effects related to these variables as well as a sort of weak nonlocality concerning these variables (weak and strong nonlocalities were first distinguished in Maugin, 1979). Among cases of particular interest along this line of development we note the case of *liquid crystals* (Leslie, 1968; Kats and Lebedev, 1988; Maugin, 1990, 1999, pp. 160–162), *damage* (Frémond and Nedjar, 1993, 1996; Lorentz and Andrieux, 1999), *second-grade elastic materials* (Forest and Cordona, 2000), and *viscoplasticity* (Forest and Sievert, 2003). One specific point raised in some of these works is whether the entropy flux follows the standard imposed by the Coleman–Noll rational thermodynamics of the 1960s–1970s (cf. Truesdell, 1984) or its definition may be altered by the present diffusive effect (as shown in Maugin, 1990). This alternative, together with the initial question raised, are critically examined in this chapter. A recent work by Ireman and Nguyen Quoc Son (2004) addresses the same problem on the basis of Maugin (1990).

Remember also that a natural ingredient in diffusive theories in fluids is a tensor of *chemical potentials* (cf. Bowen, 1967; Truskinovskii, 1983; Grinfeld, 1991) that was easily related to the Eshelby stress tensor (called the energy-momentum tensor in Eshelby's original works; cf. the synthesis works of Maugin [1993, 1995]). As a matter of fact, this chapter exploits this fruitful

concept and clearly shows that alteration in the definition of the entropy flux goes along with a parallel alteration in the structure of the Eshelby stress tensor. The essential reason for this is the recognition of the complementary roles played by the balance of entropy and the balance of so-called canonical momentum insofar as thermomechanics is concerned. This was already emphasized in Maugin (2000, 2002). The considerations in this chapter, although presented in a somewhat abstract frame, are meant to apply mostly to cases of interest in *geomaterials* (especially for weakly nonlocal damage and plasticity) and *biomaterials* (especially in the theory of growth as formulated—with diffusional effects—in Epstein and Maugin [2000]).

## 5.2 Reminder

For our purposes, we suppose that the following three local balance laws have been deduced from a global statement for sufficiently smooth fields (see Chapter 2). Here we consider the *Piola–Kirchhoff* formulation of the balance of mass, physical (linear) momentum, and energy (no external supply of energy apart from that related to the body force) at any regular material point $\mathbf{X}$ in a continuous body in the presence of a body force $\mathbf{f}_0$ per unit reference volume:

$$\left.\frac{\partial \rho_0}{\partial t}\right|_X = 0, \tag{5.1}$$

$$\left.\frac{\partial(\rho_0 \mathbf{v})}{\partial t}\right|_X - \mathrm{div}_R \mathbf{T} = \mathbf{f}_0\,, \tag{5.2}$$

$$\left.\frac{\partial(K+E)}{\partial t}\right|_X - \nabla_R.(\mathbf{T}.\mathbf{v} - \mathbf{Q}) = \mathbf{f}_0.\mathbf{v}, \tag{5.3}$$

where $\rho_0$ is the mass density, $\mathbf{v} = \partial\bar{\mathbf{x}}/\partial t\big|_X$ is the physical velocity, $\mathbf{T}$ is the first Piola–Kirchhoff stress, $K = \rho_0\mathbf{v}^2/2$ is the kinetic energy, $E$ is the internal energy per unit reference volume, and $\mathbf{Q}$ is the material heat flux. This is complemented by the second law of thermodynamics, written as

$$\Sigma_R := \left.\frac{\partial S}{\partial t}\right|_X + \nabla_R.\mathbf{S} \geq 0, \quad \mathbf{S} = (\mathbf{Q}/\theta) + \mathbf{K}, \tag{5.4}$$

where $S$ is the entropy density, $\theta$ is the absolute temperature ($\theta > 0$, *inf* $\theta = 0$), and $\mathbf{S}$ is the entropy flux. The "extra entropy flux" $\mathbf{K}$ vanishes in most cases.

## 5.3 Canonical Balance Laws of Momentum and Energy

### 5.3.1 A Canonical Form of the Energy Conservation

First, we shall formulate an interesting form of the energy conservation equation. A part of the reasoning is standard. In effect, taking the scalar product of both sides of Equation 5.2 by **v** and performing some elementary manipulations, we obtain the so-called *theorem of the kinetic energy* as

$$\frac{dK}{dt} - \nabla_R.\left(\mathbf{T}.\mathbf{v}\right) + \mathrm{tr}\left(\mathbf{T}.\dot{\mathbf{F}}\right) - \mathbf{f}_0.\mathbf{v} = 0. \tag{5.5}$$

Combining this with the first law of thermodynamics (Equation 5.3) we obtain the so-called *theorem of internal energy*:

$$\frac{dE}{dt} - \mathrm{tr}\left(\mathbf{T}.\dot{\mathbf{F}}\right) + \nabla_R.\mathbf{Q} = 0. \tag{5.6}$$

***Case where*** $\mathbf{K} \equiv \mathbf{0}$

In this case, introducing the Helmholtz free energy function by $W = E - S\theta$, we transform the inequality in $(5.4_1)$ into the celebrated *Clausius–Duhem inequality*:

$$-\left(\frac{dW}{dt} + S\frac{d\theta}{dt}\right) + \mathrm{tr}\left(\mathbf{T}.\dot{\mathbf{F}}\right) - \mathbf{S}.\nabla_R\theta \geq 0. \tag{5.7}$$

As we know (Chapter 2), this is exploited as a constraint in the formulation of thermodynamically admissible constitutive equations, while the "conservation equation" (5.6) is the equation governing heat propagation in a disguise. This can be given several transformed forms. A most interesting form is obtained straightforwardly by noting that $E = W + S\theta$, yielding

$$\frac{d\left(S\theta\right)}{dt} + \nabla_R.\mathbf{Q} = h^{\mathrm{int}}, \quad h^{\mathrm{int}} := \mathrm{tr}\left(\mathbf{T}.\dot{\mathbf{F}}\right) - \left.\frac{\partial W}{\partial t}\right|_X. \tag{5.8}$$

This is of special interest because of the expression in the right-hand side, which a priori appears as an *internal heat source*. Indeed, for a typically thermodynamically reversible behavior such as pure nonlinear elasticity (hyperelasticity), where $W = \bar{W}\left(\mathbf{F}\right)$ depends only on **F,** we have from the exploitation of (5.7)

$$\mathbf{T} = \partial\bar{W}/\partial\mathbf{F} \Rightarrow h^{\mathrm{int}} \equiv 0. \tag{5.9}$$

Note that in the situation where (5.8) holds good, the inequality in (5.7) can also be written in the following enlightening form:

$$S\dot{\theta} + \mathbf{S}.\nabla_R\theta \le h^{\text{int}}. \tag{5.10}$$

We claim that ($5.8_1$) in fact is the most interesting form of the energy conservation equation for our purpose (i.e., establishing canonical equations). This we discover by constructing the canonical equation of momentum as follows.

### 5.3.2 Canonical (Material) Momentum Conservation

Guided by what is valid for pure finite-strain elasticity (Noether's identity; Chapter 4), we apply $\mathbf{F}$ to the right of (5.2) and note that ($T$ = transpose)

$$\left(\frac{\partial(\rho_0\mathbf{v})}{\partial t}\right).\mathbf{F} = -\left.\frac{\partial\mathbf{P}}{\partial \mathrm{t}}\right|_X - \nabla_R\left(\frac{1}{2}\rho_0\mathbf{v}^2\right) + \left(\frac{1}{2}\mathbf{v}^2\right)\left(\nabla_R\rho_0\right) \tag{5.11}$$

(this is nothing but (3.13)), and

$$\left(\text{div}_R\mathbf{T}\right).\mathbf{F} = \text{div}_R\left(\mathbf{T}.\mathbf{F}\right) - \text{tr}\left(\mathbf{T}.\left(\nabla_R\mathbf{F}\right)^T\right), \tag{5.12}$$

where we have set (cf. (3.12))

$$\mathbf{P} := -\rho_0\mathbf{v}.\mathbf{F} \tag{5.13}$$

as the *material* momentum. Introducing now plus and minus the material gradient of an (unspecified) free energy density $W = \bar{W}\left(.,..,..,\mathbf{X}\right)$, we then check that (5.2) yields the following material balance of momentum:

$$\frac{d\mathbf{P}}{dt} - \text{div}_R\mathbf{b} = \mathbf{f}^{\text{int}} + \mathbf{f}^{\text{ext}} + \mathbf{f}^{\text{inh}}, \tag{5.14}$$

in which we have defined the material *Eshelby stress* $\mathbf{b}$, the material *inhomogeneity force* $\mathbf{f}^{\text{inh}}$, the material *external* (or body) force $\mathbf{f}^{\text{ext}}$, and the material *internal* force $\mathbf{f}^{\text{int}}$ by

$$\mathbf{b} = -\left(L_W\mathbf{1}_R + \mathbf{T}.\mathbf{F}\right), \quad L_W := K - W, \tag{5.15}$$

$$\mathbf{f}^{\text{inh}} := \partial L_W/\partial\mathbf{X}\big|_{\text{expl}} \equiv \partial L_W/\partial\mathbf{X}\big|_{\text{fixed fields}} = \left(\mathbf{v}^2/2\right)\nabla_R\rho_0 - \partial\bar{W}/\partial\mathbf{X}\big|_{\text{expl}}, \tag{5.16}$$

$$\mathbf{f}^{\text{ext}} := -\mathbf{f}_0.\mathbf{F}, \quad \mathbf{f}^{\text{int}} := \text{tr}\left(\mathbf{T}.\left(\nabla_R\mathbf{F}\right)^T\right) - \nabla_R W\big|_{\text{impl}}, \tag{5.17}$$

where the subscript notations *expl* and *impl* mean, respectively, the material gradient keeping the fields fixed (and thus extracting the explicit dependence on **X**) and the material gradient taken only through the fields present in the function.

Equation 5.14 is the *canonical* balance of momentum of continuum mechanics *in the absence of specification of constitutive equations.* It is a (mathematically) strict conservation equation only when all source terms in its right-hand side vanish. Here the new notion is that of *material internal force*, which appears in parallel and total analogy with the internal heat source in ($5.8_2$), the action of the material gradient replacing that of the material time derivative. We note that there is no "timelike" scalar equivalent to $\mathbf{f}^{\text{inh}}$ in Equation $5.8_1$ because this inhomogeneity force, which is automatically captured by that equation, has *no* dissipative nature. An explicit dependence of *W* on time (in a rheonomic system) would yield a nonzero term $h^{\text{inh}}$ (see Chapter 4 for rheonomic systems). Similarly, there is no equivalent to the external material force $\mathbf{f}^{\text{ext}}$ in ($5.8_1$) because this equation governs essentially the internal energy. It would be easy to rewrite Equations $5.8_1$ and 5.14 as a single four-dimensional space–time equation (see Maugin, 2000, and the appendix to this chapter), but this serves no special purpose, except for an aesthetic satisfaction, in engineering applications. Still, the *consistency* between the *spacelike* covectorial Equation 5.14 and the *timelike* Equation $5.8_1$ is a fundamental requirement in the thermodynamic study of the progress of singularity sets (e.g., defects) in order that the related dissipation be none other than the power expended by the material force in the material velocity of the defect (cf. Chapters 7 and 8).

Still, in the present approach, to proceed further we need to specify the full functional dependence of *W*. The general expressions ($5.8_1$) and (5.14) are the most general canonical equations for momentum and energy we can write down without a postulate of the full dependency of *W*. However, just like for other equations in continuum mechanics, we could also write the jump relations associated with ($5.8_1$) and (5.14) at a singular surface by using elements of the theory of hyperbolic systems or a more naïve method such as the pill-box method. But since the "conservation laws" ($5.8_1$) and (5.14) already exhibit source terms in the bulk (i.e., they are not conservation laws in a strict mathematical sense), the associated jump relations will also contain surface source terms. The latter, a priori unknown but responsible for the dissipation at the singularity, have to be computed with the help of the standard jump relations associated with Equations 5.1 through 5.3.

***Case where*** $\mathbf{K} \neq \mathbf{0}$

Without reporting the whole algebra, starting with ($5.4_2$), we let the reader check that the thermodynamic inequality in (5.7) is replaced by

$$-\left(\frac{dW}{dt} + S\frac{d\theta}{dt}\right) + \text{tr}\left(\mathbf{T}.\dot{\mathbf{F}}\right) + \nabla_R.\left(\theta\mathbf{K}\right) - \mathbf{S}.\nabla_R\theta \geq 0, \tag{5.18}$$

where **S** is still given by the general expression ($5.4_2$). Equations 5.8 and 5.14 are left unchanged:

$$\frac{d(S\theta)}{dt} + \nabla_R . \mathbf{Q} = h^{\text{int}}, \quad h^{\text{int}} := \text{tr}\left(\mathbf{T}.\dot{\mathbf{F}}\right) - \left.\frac{\partial W}{\partial t}\right|_X , \tag{5.19}$$

$$\frac{d\mathbf{P}}{dt} - \text{div}_R \mathbf{b} = \mathbf{f}^{\text{int}} + \mathbf{f}^{\text{ext}} + \mathbf{f}^{\text{inh}}. \tag{5.20}$$

On account of (5.18), (5.10) is now replaced by

$$S\dot{\theta} + \mathbf{S}.\nabla_R \theta \le h^{\text{int}} + \nabla_R . (\theta \mathbf{K}). \tag{5.21}$$

Now let us illustrate these general equations by specific cases, some of them trivial and others nontrivial.

## 5.4 Examples without Body Force

### 5.4.1 Pure Homogeneous Elasticity

In this case $\rho_0 = \text{const}$ and $W = \bar{W}(\mathbf{F})$ only. We have $h^{\text{int}} \equiv 0$, $\mathbf{f}^{\text{int}} \equiv \mathbf{0}$ since (5.9) holds good, and also $\mathbf{f}^{\text{inh}} = \mathbf{0}$, $\mathbf{Q} \equiv \mathbf{0}$ since the body is homogeneous and nonconducting. Equations 5.8 and 5.14 reduce to the following [in fact Hamiltonian for a (3 + 1)-dimensional canonical momentum ($\mathbf{P}$,$\theta_0 S$)] system ($\theta_0 = \text{const}$):

$$\frac{d\mathbf{P}}{dt} - \text{div}_R \mathbf{b} = \mathbf{0}, \quad \theta_0 \frac{dS}{dt} = 0. \tag{5.22}$$

In four-dimensional form this is the formulation of Kijowski and Magli (1998), in which the second of (5.22) is trivial and 4-momentum is given by $\mathbf{P}_4 = (\mathbf{P}, \theta_0 S)$.

### 5.4.2 Inhomogeneous Thermoelasticity of Conductors

In that case $\rho_0 = \bar{\rho}_0(\mathbf{X})$, and $W = \bar{W}(\mathbf{F},\theta;\mathbf{X})$. We have the constitutive equations:

$$\mathbf{T} = \frac{\partial \bar{W}}{\partial \mathbf{F}}, \quad S = -\frac{\partial \bar{W}}{\partial \theta}, \tag{5.23}$$

which follow from a standard exploitation of the Clausius–Duhem inequality (cf. Chapter 2). Accordingly, we obtain that

$$\mathbf{f}^{\text{int}} \equiv \mathbf{f}^{\text{th}},\ h^{\text{int}} \equiv h^{\text{th}} := S\dot{\theta}, \tag{5.24}$$

where

$$\mathbf{f}^{\text{th}} := S\nabla_R\theta \tag{5.25}$$

is the *material thermal force* first introduced by Bui in small strains (1978)—in fact in a little-known conference paper of 1977—and independently by Epstein and Maugin (1995) in their geometric considerations, so that (5.8) and (5.14) are replaced by the following canonical (*non*-Hamiltonian) system of balance of momentum and energy:

$$\frac{d\mathbf{P}}{dt} - \text{div}_R\mathbf{b} = \mathbf{f}^{\text{inh}} + \mathbf{f}^{\text{th}},\quad \frac{d(S\theta)}{dt} + \nabla_R.\mathbf{Q} = h^{\text{th}}, \tag{5.26}$$

as was first found in Maugin (2000, 2006a).

### 5.4.3 Homogeneous Dissipative Solid Material Described by Means of a Diffusive Internal Variable

Let $\alpha$ be the internal variable of state whose tensorial nature is not specified. This may relate to damage or anelasticity of some sort with a possible diffusion of the said variable so that its material gradient must be taken into account (e.g., in strain-gradient plasticity). This is in the spirit of the thermodynamics developed at length in Maugin (1999a). Then $W$ is specified as the general sufficiently regular function

$$W = \bar{W}(\mathbf{F},\theta,\alpha,\nabla_R\alpha). \tag{5.27}$$

***Case where*** $\mathbf{K} \equiv \mathbf{0}$

First, we assume that $\mathbf{K}$ vanishes. The *equations of state* (in a sense mere definition of the partial derivatives of the free energy) are given by *Gibbs' equation* as

$$\mathbf{T} = \frac{\partial\bar{W}}{\partial\mathbf{F}},\quad S = -\frac{\partial\bar{W}}{\partial\theta},\quad A := -\frac{\partial\bar{W}}{\partial\alpha},\quad \mathbf{B} := -\frac{\partial\bar{W}}{\partial(\nabla_R\alpha)}. \tag{5.28}$$

Accordingly, we find that

$$\mathbf{f}^{\text{int}} = \mathbf{f}^{\text{th}} + \mathbf{f}^{\text{intr}},\quad h^{\text{int}} = h^{\text{th}} + h^{\text{intr}}, \tag{5.29}$$

where the thermal sources have already been defined and the "intrinsic" sources are given by

$$\mathbf{f}^{\text{intr}} := A\left(\nabla_R \alpha\right)^T + \mathbf{B}.\nabla_R\left(\nabla_R \alpha\right)^T, \quad h^{\text{intr}} := A\dot{\alpha} + \mathbf{B}.\left(\nabla_R \dot{\alpha}\right)^T, \tag{5.30}$$

so that we have the following consistent (non-Hamiltonian) system of canonical balance laws:

$$\frac{d\mathbf{P}}{dt} - \text{div}_R \mathbf{b} = \mathbf{f}^{\text{th}} + \mathbf{f}^{\text{intr}}, \quad \frac{d\left(S\theta\right)}{dt} + \nabla_R.\mathbf{Q} = h^{\text{th}} + h^{\text{intr}}, \tag{5.31}$$

while the dissipation reads

$$\Phi = h^{\text{intr}} - \mathbf{S}.\nabla_R \theta \geq 0, \quad \mathbf{K} \equiv \mathbf{0}. \tag{5.32}$$

Here the thermodynamic forces $A$ and $\mathbf{B}$ are purely dissipative by virtue of the "internal" character of the state variable $\alpha$.

This approach with $\mathbf{K} = \mathbf{0}$ favors the *continuum-mechanics* (Coleman–Noll) *standard viewpoint* (cf. Truesdell, 1984) by accepting the classical relationship between heat and entropy flux, and assuming that $\alpha$ and its material gradient are essentially independent. A more *field-theoretic* viewpoint is to envisage the set of (5.18) through (5.21) as holding true and selecting the nonzero $\mathbf{K}$ such that the divergence term in (5.18) is eliminated from this inequality.

*Case where* $\mathbf{K} \neq \mathbf{0}$

To make the divergence term in Equation 5.18 vanish identically, we set

$$\mathbf{K} = -\theta^{-1}\mathbf{B}\dot{\alpha}. \tag{5.33}$$

This follows the scheme originally developed in Maugin (1990) for materials with *diffusive* dissipative processes described by means of internal variables of state.

We let the reader check that Equations 5.31 and 5.32 are then replaced by the following equations:

$$\frac{d\mathbf{P}}{dt} - \text{div}_R \tilde{\mathbf{b}} = \mathbf{f}^{\text{th}} + \tilde{\mathbf{f}}^{\text{intr}}, \quad \frac{d\left(S\theta\right)}{dt} + \nabla_R.\tilde{\mathbf{Q}} = h^{\text{th}} + \tilde{h}^{\text{intr}} \tag{5.34}$$

and

$$\Phi = \tilde{h}^{\text{intr}} - \tilde{\mathbf{S}}.\nabla_R \theta \geq 0, \quad \tilde{h}^{\text{intr}} := \tilde{A}\dot{\alpha}, \tag{5.35}$$

where we have introduced the new definitions

$$\tilde{A} \equiv -\frac{\delta \bar{W}}{\delta \alpha} := -\left( \frac{\partial \bar{W}}{\partial \alpha} - \nabla_R . \frac{\partial \bar{W}}{\partial (\nabla_R \alpha)} \right) = A - \nabla_R . \mathbf{B}, \quad \tilde{\mathbf{S}} := \theta^{-1} \tilde{\mathbf{Q}}, \quad \tilde{\mathbf{Q}} = \mathbf{Q} - \mathbf{B}\dot{\alpha} \tag{5.36}$$

and

$$\tilde{\mathbf{b}} = -\left( L\mathbf{1}_R + \mathbf{T}.\mathbf{F} - \mathbf{B}.(\nabla_R \alpha)^T \right), \quad \tilde{\mathbf{f}}^{\text{intr}} := \tilde{A} \nabla_R \alpha. \tag{5.37}$$

The two thermodynamic approaches just illustrated are to be compared to the constructive comments of Ireman and Nguyen Quoc Son (2004). Here, we additionally show that alteration in the entropy flux definition goes along with a parallel alteration in the expression of the Eshelby stress tensor, thus reinforcing the spacelike complementarity of the equations (5.34). Alteration of the definition of entropy flux is classical in the theory of irreversible processes in the presence of diffusion (cf. de Groot and Mazur, 1962). More on this, with the possible interpretation of $\alpha$ as an additional degree of freedom when it is equipped with its own inertia, can be found in Maugin (2006b; see also next section).

## 5.5 Variable $\alpha$ as an Additional Degree of Freedom

### 5.5.1 General Formulation

Had we considered $\alpha$ as an observable field endowed with an inertia and a flux, where the latter is not necessarily purely dissipative (on the contrary, it could be purely *non*dissipative), we would have started with

- A global statement of the *principle of virtual power* (PVP) following Germain (1973a, 1973b) and Maugin (1980)
- A global statement of the first and second laws of thermodynamics (following Chapter 2)

The first statement (PVP) would read, for a body $B$ occupying the regular region $B_R$ with regular boundary surface $\partial B_R$ (of outward-pointing unit normal $\mathbf{N}$) in its reference configuration $K_R$

$$P_{(\text{inertia})}{}^* = P_{(i)}{}^* + P_{(\text{data})}{}^* \tag{5.38}$$

with

$$P_{(\text{inertia})}{}^{*}=\int_{B_R}\left(\rho_0\mathbf{v}.\mathbf{v}^{*}+\rho_0\left(\mathbf{I}.\dot{\alpha}\right).\left(\dot{\alpha}\right)^{*}\right)dV, \tag{5.39}$$

$$P_{(\text{data})}{}^{*}=\int_{B_R}\left(\hat{\mathbf{f}}.\mathbf{v}^{*}+\hat{A}.\left(\dot{\alpha}\right)^{*}\right)dV_0+\int_{\partial B_R}\left(\hat{\mathbf{T}}_{\mathbf{n}}.\mathbf{v}^{*}+\hat{\mathbf{B}}_{\mathbf{n}}.\left(\dot{\alpha}\right)^{*}\right)dA, \tag{5.40}$$

and

$$P_{(i)}{}^{*}=-\int_{B_R}\left(\text{tr}\left(\mathbf{T}.\left(\nabla_R\mathbf{v}\right)^{*}\right)-A.\left(\dot{\alpha}\right)^{*}-\mathbf{B}.\nabla_R\left(\dot{\alpha}\right)^{*}\right)dA, \tag{5.41}$$

where

$$\hat{\mathbf{f}},\ \hat{A},\ \hat{\mathbf{T}}_{\mathbf{n}},\ \hat{\mathbf{B}}_{\mathbf{n}} \tag{5.42}$$

are prescribed—hence the subscript *data* in the corresponding power—and

$$A,\ \mathbf{T},\ \mathbf{B} \tag{5.43}$$

are *genereralized internal forces* to be given (nondissipative or dissipative or both) *constitutive equations*.

**REMARKS**: In Equations 5.38 through 5.41, an asterisk means that the expression or the field to which it is attached is a virtual field whose choice is at our disposal. Deleting the asterisk means that the expression or the field in question takes its actual value in the initial-value boundary-value problem to be solved. Prescriptions to formulate the various virtual powers, once the basic fields such as the motion of the body and the variable $\alpha$ are chosen, have been clearly enunciated in Maugin (1980). In particular, the virtual power of internal forces $P_{(i)}{}^{*}$ must be written as a linear continuous form on a set of **objective** generalized velocity fields in order that the internal forces introduced by the inherent duality as the set of (5.43) be objective fields (i.e., invariant under superimposed rigid-body motions in the current configuration $K_t$). If $\alpha$ simply is a scalar under such transformations, there are no problems in writing directly the linear form (5.41). For instance, this is done by Frémond and Nedjar (1993, 1996) when $\alpha$ is a scalar damage variable. Then the "inertia" **I** in the expression of the virtual power of inertia force is also a scalar, if it exists at all. The objectivity requirement does not apply to the other virtual powers since neither inertial forces nor externally applied forces are objective. Whenever $\alpha$ is a field of higher tensorial order (e.g., a vector field such as

in the cases of liquid crystals, internally electrically polarized materials—cf. Maugin, 1974b, 1976, or internally magnetized material—cf. Maugin, 1974a), one has to be more thoughtful in writing down $P_{(i)}$; in particular, objective (convected or Jaumann) time derivatives of $\alpha$ and its gradient must be introduced. This remark obviously holds true if $\alpha$ is a tensor of second order (e.g., representative of a rigid or deformable microstructure). The tensorial order of the "inertia" $\mathbf{I}$ is accordingly formulated. The dots between symbols in Equations 5.38 through 5.41 take their full meaning of contractors of indices or inner products in the appropriate space. These technicalities are more or less obvious. The formulation given in Equations 5.38 through 5.41 is of the type of a *first-gradient theory* insofar as both the classical continuum motion *and* the variable $\alpha$ are concerned. Higher-order gradient theories, that is, "stronger nonlocal theories" may be constructed following the same generalized pattern and rules (cf. Maugin, 1980). "First order" is enough to compare with the foregoing "diffusive-internal-variable" theory. Note that there is no obligation that the theory be of the same order for the classical motion and for the additional variable $\alpha$. This choice is at our disposal and depends essentially on our apprehending of the spatial range of interactions.

**REMARK:** Here we call $\alpha$ an observable field. We could as well say "*controllable*" field, meaning by this that, contrary to internal variables of state, their values can be adjusted by a proper action in the bulk and at the surface of the body by the introduced generalized forces present in $P_{(\text{data})}$.

The two laws of thermodynamics are now set forth in the following global form:

**First law of thermodynamics**

$$\frac{d}{dt}\int_{B_R}(K+E)dV = P_{(\text{data})} + \dot{Q}, \quad \dot{Q} = -\int_{\partial B_R}\hat{Q}_{\mathbf{n}}dA \tag{5.44}$$

and

**Second law of thermodynamics**

$$\frac{d}{dt}\int_{B_R} S dV + \int_{\partial B_R}\mathbf{N}.\tilde{\mathbf{S}}dA \geq 0, \quad \tilde{\mathbf{S}} = \theta^{-1}\mathbf{Q} + \mathbf{K}. \tag{5.45}$$

In these two equations, $K$, $E$, and $S$ are the kinetic energy, internal energy, and entropy density per unit **reference** volume. $\dot{Q}$ is the energy rate supply to the body through its boundary. This occurs through heat. We do not introduce any energy supply per unit volume. In writing the second law, we have somewhat anticipated by introducing an entropy flux with the more general relationship to heat and dissipative processes, since, while $\theta$ is the standard

thermodynamic temperature, we have admitted the possible presence of a nonzero extra entropy flux **K**. The kinetic energy here is given by

$$K = \frac{1}{2}\rho_0 \mathbf{v}^2 + \frac{1}{2}\rho_0 \dot{\alpha}.\mathbf{I}.\dot{\alpha}. \tag{5.46}$$

As a first outcome from the application of (5.38) for any virtual fields $(\mathbf{v}^*, (\dot{\alpha})^*)$ in any volume and surface element, we obtain the following balance laws and associated natural boundary conditions:

$$\left.\frac{\partial(\rho_0 \mathbf{v})}{dt}\right|_X - \mathrm{div}_R \mathbf{T} = \hat{\mathbf{f}} \text{ in } B_R, \quad \hat{\mathbf{T}}_\mathbf{n} = \mathbf{N}.\mathbf{T} \text{ at } \partial B_R, \tag{5.47}$$

$$\left.\frac{\partial(\rho_0 \mathbf{I}.\dot{\alpha})}{\partial t}\right|_X = \hat{A} + A - \nabla_R.\mathbf{B} \text{ in } B_R, \quad \hat{\mathbf{B}}_\mathbf{n} = \mathbf{N}.\mathbf{B} \text{ at } \partial B_R. \tag{5.48}$$

A second result is obtained for real virtual velocity fields (no asterisks), on account of (5.46). It is the so-called *equation of kinetic energy* in global form, as

$$\frac{d}{dt}\int_{B_R} K dV = P_{(i)} + P_{(\text{data})}. \tag{5.49}$$

On combining this with the first law (5.44), we obtain the so-called *equation of internal energy* in global form:

$$\frac{d}{dt}\int_{B_R} E dV + P_{(i)} = \dot{Q}, \tag{5.50}$$

the localization of which yields

$$\left.\frac{\partial E}{\partial t}\right|_X = \mathrm{tr}\left(\mathbf{T}.(\nabla_R \mathbf{v})^T\right) - A.\dot{\alpha} - \mathbf{B}.\nabla_R \dot{\alpha} - \nabla_R.\mathbf{Q} \text{ in } B_R, \quad \hat{Q}_\mathbf{n} = \mathbf{N}.\mathbf{Q} \text{ at } \partial B_R. \tag{5.51}$$

Introducing now the Helmholtz free energy $W$ per unit reference volume by

$$W = E - S\theta, \tag{5.52}$$

and combining with the local form of the inequality ($5.45_1$), we arrive at the following *Clausius–Duhem inequality*:

$$-\left(\frac{dW}{dt} + S\frac{d\theta}{dt}\right) + p_{(i)} + \nabla_R.(\theta \mathbf{K}) - \tilde{\mathbf{S}}.\nabla_R \theta \geq 0, \tag{5.53}$$

while evaluating $\theta\, dS/dt$ from Equation $5.51_1$ on account of Equation 5.52 we obtain the "entropy equation," which will ultimately provide the heat-propagation equation, in the form

$$\theta\frac{dS}{dt} = -\left(\frac{dW}{dt} + S\frac{d\theta}{dt}\right) + p_{(i)} - \nabla_R.\mathbf{Q}. \tag{5.54}$$

We have introduced the following notation

$$p_{(i)} := \mathrm{tr}\left(\mathbf{T}.\dot{\mathbf{F}}\right) - A\dot{\alpha} - \mathbf{B}.\nabla_R\dot{\alpha} \tag{5.55}$$

and accounted for the fact that

$$\left(\nabla_R\mathbf{v}\right)^T \equiv \dot{\mathbf{F}}. \tag{5.56}$$

Now we consider three cases of exploitation of the scheme developed in the preceding.

### 5.5.2 The Only Dissipative Process Is Heat Conduction

We have the following obvious reduction:

$$\mathbf{K} \equiv \mathbf{0}, \quad \tilde{\mathbf{S}} \equiv \frac{\mathbf{Q}}{\theta}, \tag{5.57}$$

$$-\left(\frac{dW}{dt} + S\frac{d\theta}{dt}\right) + p_{(i)} = 0, \quad \Phi^{\mathrm{th}} := -\tilde{\mathbf{S}}.\nabla_R\theta \geq 0, \tag{5.58}$$

$$\theta\frac{dS}{dt} + \nabla_R.\mathbf{Q} = 0. \tag{5.59}$$

The last of these can also be written as (since $\theta > 0$ always)

$$\frac{dS}{dt} + \nabla_R.\tilde{\mathbf{S}} = \sigma^{\mathrm{th}}, \quad \sigma^{\mathrm{th}} = \theta^{-1}\Phi^{\mathrm{th}}. \tag{5.60}$$

With a functional dependence $W = \bar{W}\left(\mathbf{F},\theta,\alpha,\nabla_R\alpha\right)$, a classical reasoning applied to the first of (5.58) yields the constitutive equations:

$$S = -\frac{\partial W}{\partial\theta}, \quad \mathbf{T} = \frac{\partial W}{\partial\mathbf{F}}, \quad A = -\frac{\partial W}{\partial\alpha} \quad \mathbf{B} = -\frac{\partial W}{\partial\left(\nabla_R\alpha\right)}. \tag{5.61}$$

It remains to give an expression to the heat flux **Q** to arrive at a fully explicit expression for (5.51).

### 5.5.3 The Coleman–Noll Continuum Thermodynamics Viewpoint

In this case the equations (5.57) are valid a priori independently of any deformation and time-internal evolution of $\alpha$, that is,

$$\mathbf{K} \equiv \mathbf{0} \Rightarrow \tilde{\mathbf{S}} \equiv \frac{\mathbf{Q}}{\theta} \tag{5.62}$$

The generalized internal forces (5.43) are each the sum of a thermodynamically reversible part and a *dissipative* thermodynamically irreversible part, that is,

$$A = A_{\text{rev}} + A_{\text{irrev}}, \quad \mathbf{T} = \mathbf{T}_{\text{rev}} + \mathbf{T}_{\text{irrev}}, \quad \mathbf{B} = \mathbf{B}_{\text{rev}} + \mathbf{B}_{\text{irrev}}. \tag{5.63}$$

The dependent functions $\{W,S,A_{\text{rev}},\mathbf{T}_{\text{rev}},\mathbf{B}_{\text{rev}}\}$ depend all on the same set as

$$W = \bar{W}\left(\mathbf{F},\theta,\alpha,\nabla_R\alpha\right), \tag{5.64}$$

while the remaining dissipative fields $\left\{\tilde{\mathbf{S}},A_{\text{irrev}},\mathbf{T}_{\text{irrev}},\mathbf{B}_{\text{irrev}}\right\}$ depend on the same set *as well as* on the set $\left\{\nabla_R\theta,\dot{\mathbf{F}},\dot{\alpha},\nabla_R\dot{\alpha}\right\}$. Here also a classical reasoning yields constitutive equations similar to those in Equation 5.61 for the nondissipative contributions, that is,

$$\begin{aligned} &\mathbf{T}_{\text{rev}} = \frac{\partial\bar{W}}{\partial\mathbf{F}}, \quad A_{\text{rev}} = -\frac{\partial\bar{W}}{\partial\alpha}, \quad \mathbf{B}_{\text{rev}} = -\frac{\partial\bar{W}}{\partial\left(\nabla_R\alpha\right)}, \\ &S = -\frac{\partial\bar{W}}{\partial\theta}, \quad W = \bar{W}\left(\mathbf{F},\theta,\alpha,\nabla_R\alpha\right) \end{aligned} \tag{5.65}$$

while there remains the following **residual dissipation inequality:**

$$\Phi := \mathbf{T}_{\text{irrev}}.\dot{\mathbf{F}} - A_{\text{irrev}}.\dot{\alpha} - \mathbf{B}_{\text{irrev}}.\nabla_R\dot{\alpha} - \tilde{\mathbf{S}}.\nabla_R\theta \geq 0. \tag{5.66}$$

In exploiting this inequality, one acts as if the gradient of $\dot{\alpha}$ and $\dot{\alpha}$ itself were independent variables. This is a standard method reported and advised in continuum mechanics books. Note that here the entropy flux satisfies the classical formula ($5.62_2$). For instance, this is applied to liquid crystals (where $\alpha$ is a unit "director") by Leslie (1968) or to elastic dielectrics by Maugin (1974b) and elastic ferromagnets in Maugin (1974a)—and also in Maugin (1972), where this was first applied to a sufficiently sophisticated

case. We shall not pursue this exploitation of Equation 5.66 here. It suffices to notice that if the time parity of $\alpha$ as a tensor allows for it, there might be a direct linear coupling between the irreversible effect associated with $\alpha$ and heat conduction. On another occasion such a direct coupling could arise between heat conduction and the dissipative *process* associated with the gradient of $\alpha$.

### 5.5.4 The Field-Theoretic Viewpoint

This is quite different in the sense that a scientist trained in analytical mechanics will not a priori assume that $\dot{\alpha}$ and $\nabla_R\dot{\alpha}$ are independent. He may prefer to keep the general expressions ($5.45_2$) and (5.53) so that (5.66) will be replaced by the following expression in which $\tilde{\mathbf{S}}$ is given by ($5.45_2$) while Equation 5.65 still hold true:

$$\Phi = \mathbf{T}_{\text{irrev}}.\dot{\mathbf{F}} - A_{\text{irrev}}.\dot{\alpha} - \mathbf{B}_{\text{irrev}}.\nabla_R.\dot{\alpha} + \nabla_R.\left(\theta\mathbf{K}\right) - \tilde{\mathbf{S}}.\nabla_R\theta \geq 0. \tag{5.67}$$

But we note that the very form of Equation $5.36_1$ suggests that we consider the grouping

$$\tilde{A} := A - \nabla_R.\mathbf{B}. \tag{5.68}$$

According to Equation 5.68, the reversible part of this is given by

$$\tilde{A}_{\text{rev}} \equiv -\frac{\delta\bar{W}}{\delta\alpha} := -\left(\frac{\partial\bar{W}}{\partial\alpha} - \nabla_R.\frac{\partial\bar{W}}{\partial\left(\nabla_R\,\alpha\right)}\right). \tag{5.69}$$

On the basis of Equation 5.68 we also set

$$\tilde{A}_{\text{irrev}} := A_{\text{irrev}} - \nabla_R.\mathbf{B}_{\text{irrev}}. \tag{5.70}$$

On selecting the extra entropy flux as

$$\mathbf{K} = \theta^{-1}\mathbf{B}_{\text{irrev}}\dot{\alpha}, \tag{5.71}$$

it is easily shown that the inequality (5.67) reduces to the following inequality:

$$\Phi = \mathbf{T}_{\text{irrev}}.\nabla_R\mathbf{v} - \tilde{A}_{\text{irrev}}.\dot{\alpha} - \tilde{\mathbf{S}}.\nabla_R\theta \geq 0, \tag{5.72}$$

where $\tilde{\mathbf{S}}$ is given by Equations $5.45_2$ and 5.71. The exploitation of this inequality would follow the usual formalism of irreversible thermodynamics.

Simultaneously, the heat-propagation equation (5.51) is shown to take on the following form (compare to Equation 5.54):

$$\theta\frac{dS}{dt}+\nabla_R.\tilde{\mathbf{Q}}=\mathbf{T}_{\text{irrev}}:\dot{\mathbf{F}}-\tilde{A}_{\text{irrev}}\dot{\alpha},\quad \tilde{\mathbf{Q}}:=\mathbf{Q}+\mathbf{B}_{\text{irrev}}\dot{\alpha}, \tag{5.73}$$

providing thus a completely coherent theory.

COMMENT: Equation 5.71 is a sufficient condition for the nonexistence of a divergence term in the residual dissipation inequality.

## 5.6 Comparison with the Diffusive Internal-Variable Theory

It is clear that such a comparison must be carried out exactly in the conditions where the internal-variable theory holds good and also while going from the more general to the particular. To that effect, $\alpha$ **not** being an internal degree of freedom, it must have no inertia, so that the left-hand side of Equation $5.48_1$ vanishes identically. Furthermore, accepting Kestin's definition of internal variables of state, as adopted in Maugin (1999), $\alpha$ should **not** be directly controllable by any means, which requires the vanishing of the "data" fields relative to $\alpha$ in the set (5.43). Accordingly, the equations (5.48) reduce to the following "self-equilibrated" form:

$$A-\nabla_R.\mathbf{B}=0 \text{ in } B_R,\quad \mathbf{N}.\mathbf{B}=0 \text{ at } \partial B_R. \tag{5.74}$$

Necessary and sufficient conditions for this to hold at all material points $\mathbf{X}$ are the vanishing of $A$ and $\mathbf{B}$ separately at any point $\mathbf{X}$ in the body. It then follows from Equations 4.26 and 4.28 that the "thermodynamic irreversible" fields $A_{\text{irrev}}$ and $\mathbf{B}_{\text{irrev}}$ are now defined in terms of the energy density $W$ as

$$\begin{aligned} A_{\text{rev}}+A_{\text{irrev}}=0\Rightarrow A_{\text{irrev}}=-A_{\text{rev}}=\frac{\partial\bar{W}}{\partial\alpha},\\ \mathbf{B}_{\text{irrev}}=-\mathbf{B}_{\text{rev}}=\frac{\partial\bar{W}}{\partial(\nabla_R\alpha)} \end{aligned} \tag{5.75}$$

Accordingly,

$$\tilde{A}_{\text{irrev}}=-\tilde{A}_{\text{rev}}\equiv\frac{\delta\bar{W}}{\delta\alpha}:=\left(\frac{\partial\bar{W}}{\partial\alpha}-\nabla_R.\frac{\partial\bar{W}}{\partial(\nabla_R\alpha)}\right) \tag{5.76}$$

and

$$\tilde{\mathbf{S}} = \theta^{-1}\left(\mathbf{Q} + \mathbf{B}_{\text{irrev}}\dot{\alpha}\right) = \theta^{-1}\left(\mathbf{Q} + \frac{\partial \bar{W}}{\partial\left(\nabla_R \alpha\right)}\dot{\alpha}\right). \tag{5.77}$$

On account of these results and in spite of apparent discrepancies in signs, we recover entirely the expressions of the diffusive-internal-variable theory.

**CANONICAL BALANCE EQUATIONS**

Within the framework of the *Coleman–Noll continuum mechanics formulation* we let the reader check that the balances of canonical momentum and energy are given by the following two equations:

$$\left.\frac{\partial \bar{\mathbf{P}}}{\partial t}\right|_X - \operatorname{div}_R \bar{\mathbf{b}} = S\nabla_R\theta + \mathbf{T}_{\text{irrev}} : \left(\nabla_R \mathbf{F}\right)^T - A_{\text{irrev}}\nabla_R\alpha - \mathbf{B}_{\text{irrev}} . \nabla_R\left(\nabla_R\alpha\right) \tag{5.78}$$

and

$$\left.\frac{\partial\left(\theta S\right)}{\partial t}\right|_X + \nabla_R . \mathbf{Q} = S\dot{\theta} + \mathbf{T}_{\text{irrev}} : \dot{\mathbf{F}} - A_{\text{irrev}}\dot{\alpha} - \mathbf{B}_{\text{irrev}} . \nabla_R\dot{\alpha}, \tag{5.79}$$

wherein

$$\bar{\mathbf{P}} = -\rho_0\left(\mathbf{v} . \mathbf{F} + \nabla_R\alpha . \mathbf{I} . \dot{\alpha}\right), \tag{5.80}$$

$$\bar{\mathbf{b}} = -\left(\left(K - W\right)\mathbf{1}_R + \mathbf{T}_{\text{rev}} . \mathbf{F} - \mathbf{B}_{\text{rev}} . \left(\nabla_R\alpha\right)^T\right), \tag{5.81}$$

$$K = \frac{1}{2}\rho_0\left(\mathbf{v}^2 + \dot{\alpha} . \mathbf{I} . \dot{\alpha}\right), \quad W = \bar{W}\left(\mathbf{F}, \alpha, \nabla_R\alpha\right). \tag{5.82}$$

**REMARK:** In the case when $A$ presents no irreversible part, the field $A$ does not appear at all in the reduced forms taken by Equations 5.78 and 5.81. As noticed before, the reason for this is that the reduced form of these equations captures only gradients of fields and $A$ relates to $\alpha$ alone.

**HINT:** Equation 5.78 is obtained by multiplying Equation $5.47_1$ to the right by $\mathbf{F}$ and Equation $5.48_1$ by $\nabla_R\alpha$, adding the two resulting covectorial material expressions and manipulating this on account of the already obtained constitutive equations for the reversible fields. We have assumed that the bulk data $\hat{\mathbf{f}}$ and $\hat{A}$ were nil; otherwise, they jointly add a source term in Equation 5.78 in the form $-\left(\hat{\mathbf{f}} . \mathbf{F} + \hat{A}\nabla_R\alpha\right)$.

If we now consider the *field-theoretic formulation*, it is immediately shown that Equations 5.78 and 5.79 are replaced by

$$\left.\frac{\partial \bar{\mathbf{P}}}{\partial t}\right|_X - \mathrm{div}_R \tilde{\mathbf{b}} = S\nabla_R\theta + \mathbf{T}_{\mathrm{irrev}} : \left(\nabla_R \mathbf{F}\right)^T - \tilde{A}_{\mathrm{irrev}} \nabla_R \alpha \tag{5.83}$$

and

$$\left.\frac{\partial (\theta S)}{\partial t}\right|_X + \nabla_R . \tilde{\mathbf{Q}} = S\dot{\theta} + \mathbf{T}_{\mathrm{irrev}} : \dot{\mathbf{F}} - \tilde{A}_{\mathrm{irrev}} \dot{\alpha}, \tag{5.84}$$

where $\tilde{\mathbf{Q}}$ is given by Equation $5.73_2$ and $\tilde{\mathbf{b}}$ is defined by

$$\tilde{\mathbf{b}} = -\left( (K - W)\mathbf{1}_R + \mathbf{T}_{\mathrm{rev}} . \mathbf{F} - \mathbf{B} . \left(\nabla_R \alpha\right)^T \right). \tag{5.85}$$

The reduction to the case of $\alpha$ being a diffusive internal variable of state, treated in Section 5.6, is straightforward since, then, $\mathbf{T} \equiv \mathbf{T}_{\mathrm{rev}}$ as $\mathbf{T}_{\mathrm{irrev}} \equiv \mathbf{0}$, and the reduction (5.75) and (5.76) applies.

## 5.7 Example: Homogeneous Dissipative Solid Material Described by Means of a Scalar Diffusive Internal Variable

In general, $\alpha$ is an internal variable of state whose tensorial nature is not specified. This may relate to damage or anelasticity of some sort with a possible diffusion of the said variable so that its material gradient must be taken into account (e.g., in strain-gradient plasticity). Then $W$ is specified as the general sufficiently regular function $W = \bar{W}\left(\mathbf{F}, \theta, \alpha, \nabla_R \alpha\right)$. Here we specify that $\alpha$ is a scalar variable $c$ akin to a concentration. We keep the possibility that $\mathbf{K}$ be not zero. The equations of state are given by Gibbs' equation as

$$\begin{aligned} &\mathbf{T} = \frac{\partial \bar{W}}{\partial \mathbf{F}}, \quad S = -\frac{\partial \bar{W}}{\partial \theta}, \\ &\mu := \frac{\partial \bar{W}}{\partial c}, \quad \mathbf{M} := \frac{\partial \bar{W}}{\partial \left(\nabla_R c\right)}. \end{aligned} \tag{5.86}$$

so that $\mu$ is a chemical potential. We find that

$$\mathbf{f}^{\mathrm{int}} = \mathbf{f}^{\mathrm{th}} + \mathbf{f}^{\mathrm{intr}}, \quad h^{\mathrm{int}} = h^{\mathrm{th}} + h^{\mathrm{intr}}, \tag{5.87}$$

where the thermal sources have already been defined and the "intrinsic" sources are given by

$$\mathbf{f}^{\text{intr}} := -\mu\left(\nabla_R c\right)^T - \mathbf{M}.\nabla_R\left(\nabla_R c\right)^T, \quad h^{\text{intr}} := -\mu\,\dot{c} - \mathbf{M}.\left(\nabla_R \dot{c}\right)^T, \tag{5.88}$$

so that we have the following consistent (non-Hamiltonian) system of canonical balance laws:

$$\frac{d\mathbf{P}}{dt} - \text{div}_R\mathbf{b} = \mathbf{f}^{\text{th}} + \mathbf{f}^{\text{intr}}, \quad \frac{d\left(S\theta\right)}{dt} + \nabla_R.\mathbf{Q} = h^{\text{th}} + h^{\text{intr}}, \tag{5.89}$$

while the dissipation reads

$$\Phi = h^{\text{intr}} - \mathbf{S}.\nabla_R\theta \geq 0, \quad \mathbf{K} \equiv \mathbf{0}. \tag{5.90}$$

This approach favors the *continuum mechanics* (Coleman–Noll) *standard viewpoint* by accepting the classical relationship between heat and entropy flux, and assuming that $c$ and its material gradient are essentially independent.

A more *field-theoretic* viewpoint is to envisage a nonzero $\mathbf{K} = \theta^{-1}\mathbf{M}\dot{c}$. We let the reader check that Equations 5.8 and 5.14 are then replaced by the following equations:

$$\frac{d\mathbf{P}}{dt} - \text{div}_R\tilde{\mathbf{b}} = \mathbf{f}^{\text{th}} + \tilde{\mathbf{f}}^{\text{intr}}, \quad \frac{d\left(S\theta\right)}{dt} + \nabla_R.\tilde{\mathbf{Q}} = h^{\text{th}} + \tilde{h}^{\text{intr}} \tag{5.91}$$

and

$$\Phi = \tilde{h}^{\text{intr}} - \tilde{\mathbf{S}}.\nabla_R\theta \geq 0, \quad \tilde{h}^{\text{intr}} = -\tilde{\mu}\,\dot{c}, \tag{5.92}$$

where we have introduced the new definitions

$$\tilde{\mu} \equiv \frac{\delta\bar{W}}{\delta c} := \left(\frac{\partial\bar{W}}{\partial c} - \nabla_R.\frac{\partial\bar{W}}{\partial\left(\nabla_R c\right)}\right) = \mu - \nabla_R.\mathbf{M}, \quad \tilde{\mathbf{S}} := \theta^{-1}\tilde{\mathbf{Q}}, \quad \tilde{\mathbf{Q}} = \mathbf{Q} + \mathbf{M}\dot{c} \tag{5.93}$$

and

$$\tilde{\mathbf{b}} = -\left(L\mathbf{1}_R + \mathbf{T}.\mathbf{F} + \mathbf{M} \otimes \left(\nabla_R c\right)\right), \quad \tilde{\mathbf{f}}^{\text{intr}} := -\tilde{\mu}\nabla_R c. \tag{5.94}$$

This is in the spirit of the approach that we advocated before (Maugin, 1990).

The closure of the thermodynamic system requires the setting of relationships between $(\mu, \mathbf{M})$ and $(\dot{c}, \nabla_R \dot{c})$, on the one hand, or $\tilde{\mu}$ and $\dot{c}$, on the other, and a relationship à la Fourier between $\tilde{\mathbf{S}}$ and $\nabla_R \theta$. We pursue the second line (the field-theoretic one), considering as an example a free energy function $W$ of the type

$$\bar{W}(\mathbf{F}, \theta, c, \nabla_R c) = \frac{1}{2}\gamma(\nabla_R c).(\nabla_R c) + \hat{W}(\mathbf{F}, \theta, c). \tag{5.95}$$

Here the positive scalar coefficient $\gamma$ depends at most on the temperature $\theta$. In agreement with (5.92), we select (sufficient conditions) the evolution equation and heat transport equation as

$$\dot{c} = -\tau^{-1}\tilde{\mu}, \quad \tilde{\mathbf{S}} = -\chi \nabla_R \theta, \tag{5.96}$$

with positive coefficients $\tau$ and $\chi$ (they could be temperature dependent). On account of these and Equations 5.95 and 5.93, we obtain a *nonlinear evolution–diffusion equation* for $c$ in the following form:

$$\tau \dot{c} + f(c; \mathbf{F}, \theta) = \nabla_R.(\gamma \nabla_R c), \tag{5.97}$$

where

$$f(c; \mathbf{F}, \theta) \equiv \frac{\partial \hat{W}}{\partial c} = \mu. \tag{5.98}$$

One could assume that $\hat{W}$ behaves like $c^2$ for small $c$s, but more generally it may be of a higher degree in $c$, or may even be nonconvex in $c$, remaining nonetheless positive. To the same degree of approximation, the nonlinear evolution–diffusion equation for temperature is given by

$$\theta \dot{S} + \left(f - \nabla_R.(\gamma \nabla_R c)\right)\dot{c} + \nabla_R.(\theta \chi \nabla_R \theta) = 0, \tag{5.99}$$

where $S = -\partial W/\partial \theta$ is usually linear in $\theta$ and such that $W$ is *concave* in this variable.

Finally, Equation 5.91, considered with inertia neglected, yields the equation

$$\mathrm{div}_R\left(W\mathbf{1}_R - \mathbf{T}.\mathbf{F} - \lambda(\nabla_R c) \otimes (\nabla_R c)\right) + S\nabla_R \theta + \tilde{\mu}\nabla_R c = 0 \tag{5.100}$$

or, equivalently,

$$\mathrm{div}_R\left(\tilde{G}\mathbf{1}_R - \mathbf{T}.\mathbf{F} - \lambda\left(\nabla_R c\right)\otimes\left(\nabla_R c\right)\right) - \theta\nabla_R S - c\nabla_R\tilde{\mu} = 0, \tag{5.101}$$

where $\tilde{G} = W + S\theta + \tilde{\mu}c = E + \tilde{\mu}\,c$ is Gibbs' energy density.

In the absence of temperature effects and for a nondiffusive variable $c$, this reduces to the simple equation

$$\mathrm{div}_R\left(G\mathbf{1}_R - \mathbf{T}.\mathbf{F}\right) - c\nabla_R\mu = 0, \tag{5.102}$$

where $G = W + \mu c$. In this case (5.97) reduces to a (generally) *nonlinear relaxation equation*:

$$\tau\dot{c} + f\left(c;\mathbf{F}\right) = 0. \tag{5.103}$$

**REMARK:** First, one may think that we have given a peculiar status to the free energy W in expressing the Eshelby stress in terms of W. What is important is that it be the same potential that appears in both canonical equations of energy and momentum. It could have been the internal energy, and then the situation would be more prepared to treat adiabatic situations. This critical dependence of the equations of both energy and material momentum on the same thermodynamic potential was especially noticed by the author (Maugin, 2002) and Abeyaratne and Knowles (2000) when dealing with the jump relations associated with these canonical equations. We return to this in the chapter devoted to discontinuity surfaces.

Second, but nonetheless important, is the fact that the expression for the Eshelby stress contains the gradient of $\alpha$. This means that the conjugate force $\mathbf{B}$ will directly play a role in the evaluation of the critical driving forces if we follow the scheme given in Maugin (2000), while the associated expression of $\tilde{h}^{\mathrm{int}}$ will directly yield an *evolution–diffusion equation* for $\alpha$ in a simple application of the thermodynamics of irreversible processes.

## 5.8 Conclusion and Comments

The preceding developments show that there is no unique thermomechanical description of continuous media exhibiting diffusion of some property. A first choice is that of considering the additional variable required to describe this property either as a true additional degree of freedom (with an inertia and then safely following an application of the PVP) or as an internal variable of state. If the second possibility is selected (essentially when the new

property is fully dissipative), then the main question is whether this variable is diffusive and therefore controllable to some extent via a flux at a material boundary. Finally, it is shown that the field-theoretic viewpoint certainly prevails and is more economical from the point of view of thought even though both notions of entropy and Eshelby's material stress tensor must then be consistently revisited. The resulting formulation offers new perspectives for research in both biomechanics and the mechanics of complex materials exhibiting a microstructure of some kind. These may be inert materials or materials encountered in biological situations. The example of polar materials will be treated in greater detail in a later chapter. This also applies to electromagnetic deformable materials, which will also receive special attention in due place.

### 5.8.1 Two Viewpoints on the Equation of Material Momentum

Here we shall emphasize that there exist two opposite viewpoints concerning the status of the equation of material (or canonical) momentum in continuum mechanics. The viewpoint of the author (Maugin, 1993, 1995) expressed in this chapter is that this equation is never independent of the classical (physical) equation of linear momentum, in Cauchy or Piola–Kirchhoff form, being essentially deduced from the latter by a complete pull back to the reference configuration, even when constitutive equations are not known to start with (i.e., there exists no variational formulation). It is, therefore, an identity at all regular material points—but it is still extremely useful on any singular manifold (see Chapter 7). This viewpoint agrees with the application of Noether's identity when one considers a variational formulation for a nondissipative material, a point of view shared by J.D. Eshelby in his original works (e.g., Eshelby, 1975).

The second viewpoint is that of Gurtin (in several works but particularly Gurtin, 1999), who repeatedly claims that the equation of material momentum (bulk equation for "configurational forces") is an a priori statement independent of the classical balance laws, although in the end it is, for sure (our opinion), always shown to be related to the physical balance of momentum so that Gurtin's statement is somewhat inappropriate. In the preceding, we expanded the view that the balance of canonical or material momentum, albeit following from the balance of physical momentum, can be formulated independently of any constitutive behavior. Moreover, accounting for the fact that this equation is the spacelike equation associated with a particular form of the energy equation, it was shown that the former and the latter can be used in parallel to build a consistent thermomechanics of many behaviors. As a matter of fact, the two canonical equations of momentum and energy must be consistent if, for instance, dissipation due to the irreversible movement of a singularity set is none other than the power expanded by the driving force acting on this set, and this in *all* cases (Maugin, 2000); Gurtin's approach is summarized in Appendix 5.2 of this chapter, while Appendix 5.1 presents a four-dimensional formalism.

## Appendix A5.1: Four-Dimensional Formulation

Equations such as (5.31) and (5.34) hint at a unified four-dimensional (4D) Euclidean formulation (Maugin, 2000). To that purpose it is sufficient to introduce the appropriate notation, for example, to introduce four-dimensional coordinates $X^\alpha$ and a four-dimensional *nabla* operator $\nabla_\alpha$ such that

$$\left\{X^\alpha,\ \alpha=1,2,3,4\right\}=\left\{\mathbf{X}=\left\{X^K,\ K=1,2,3\right\},\quad X^4=t\right\},\tag{A5.1}$$

$$\left\{\nabla_\alpha,\ \alpha=1,2,3,4\right\}=\left\{\nabla_R=\left\{\partial/\partial X^K,\ K=1,2,3\right\},\quad \partial/\partial X^4=\partial/\partial t\right\}.\tag{A5.2}$$

We also set

$$\left\{B^\beta_{.\alpha}\right\}=\begin{pmatrix}B^K_{.L}=-b^K_{.L} & B^K_{.4}=Q^K\\ B^4_{.L}=P_L & B^4_{.4}=S\theta\end{pmatrix},\quad \left\{f_\alpha\right\}=\begin{pmatrix}\mathbf{f}^{\rm th}+\mathbf{f}^{\rm int}\\ h^{\rm th}+h^{\rm intr}\end{pmatrix}.\tag{A5.3}$$

Considering the case of a homogeneous material conducting heat and equipped with an internal variable $\alpha$, we can rewrite (5.31) as the single four-dimensional equation

$$\nabla_\beta B^\beta_{.\alpha}=f_\alpha:=S\nabla_\alpha\theta+A.\nabla_\alpha\alpha.\tag{A5.4}$$

Define a 4-velocity by

$$\left\{V^\alpha,\ \alpha=1,2,3,4\right\}=\left\{V^K,\ K=1,2,3;\ V^4=1\right\}.\tag{A5.5}$$

This corresponds to the "world-invariant" kinematics described by Truesdell and Toupin (1960, Section 152). Then, on account of (A5.4), we have

$$f_\alpha V^\alpha=\left(\mathbf{f}^{\rm th}+\mathbf{f}^{\rm intr}\right).\mathbf{V}+h^{\rm th}+h^{\rm intr}=S\left.\frac{\partial\theta}{\partial t}\right|_x+A.\left.\frac{\partial\alpha}{\partial t}\right|_x,\tag{A5.6}$$

where we implemented the definition of the Eulerian time derivative ($2.40_2$). The result (A5.6) can also be written as

$$f_\alpha V^\alpha=-\left.\frac{\partial\bar{W}}{\partial t}\right|_{x;\,\mathbf{F}\,\text{fixed}},\tag{A5.7}$$

since in the present case the free energy is given by $W=\bar{W}\left(\mathbf{F},\theta,\alpha\right)$. Accordingly, we can say that the four-force and four-velocity are *orthogonal*

when both temperature and internal variable of state do not evolve in the Eulerian framework.

We can integrate (A5.4) over a purely spacelike hypersurface, that is, a 3D material volume $B_R$:

$$\int_{B_R} \nabla_\beta B^\beta_{.\alpha}\, dV = \int_{B_R} f_\alpha\, dV. \tag{A5.8}$$

Notice that the four-dimensional space–time manifold considered here is Euclidean, so that there exists a unique global spacelike section at all of its points, and (A5.8) does make sense.

The formalism introduced obviously resembles a relativistic one, but it is in fact quite neutral geometrically. It only provides a short-hand notation for a (3 + 1)-dimensional formalism. On fixing index $\alpha$, (A5.8) is equivalent to

$$\frac{d}{dt}\int_{B_R} B^4_{.\alpha} dV + \int_{\partial B_R} N_K B^K_\alpha dA = \int_{B_R} f_\alpha\, dV, \tag{A5.9}$$

in the absence of singularities in $B_R$, whence the global balance law of material momentum and energy. Nonnegativeness of energy imposes the condition

$$B^4_{.4} \geq 0. \tag{A5.10}$$

In the same formalism, the global entropy equation reads

$$\int_{B_R} \nabla_\beta S^\beta dV = \int_{B_R} \left(\sigma^{\text{th}} + \sigma^{\text{intr}}\right) dV \tag{A5.11}$$

or

$$\frac{d}{dt}\int_{B_R} S^4 dV + \int_{\partial B_R} N_K S^K dA = \int_{B_R} \left(\sigma^{\text{th}} + \sigma^{\text{intr}}\right) dV, \tag{A5.12}$$

where

$$\left\{S^\alpha,\, \alpha = 1,2,3,4\right\} = \left\{S^K = Q^K/\theta;\, S^4 = S\right\}, \tag{A5.13}$$

and $\sigma^{\text{th}}$ and $\sigma^{\text{intr}}$ are the volume sources of entropy due to thermal processes and intrinsic dissipative processes.

## Appendix A5.2: Another Viewpoint

Here we succinctly present the view of Gurtin (1995, 1999) and some coworkers (e.g., Podio-Guidugli, 2002) on the introduction of the notion of configurational force and, more particularly, the equation governing material momentum or its quasistatic version. This is our interpretation of their standpoint, with our notation, and any misinterpretation, if any, is ours. We consider the case of quasistatics for the sake of simplicity. In this framework and in the Piola–Kirchhoff formalism, the principle of virtual power (2.114) reduces to

$$P_{\text{ext}}{}^{*}\left(B_R, \partial B_R\right) + P_{\text{int}}{}^{*}\left(B_R\right) = 0, \tag{A5.14}$$

wherein

$$P_{\text{ext}}{}^{*}\left(B_R, \partial B_R\right) = \int_{B_R} \rho_0 \mathbf{f}.\mathbf{v}^{*}\, dV + \int_{\partial B_t} \mathbf{T}_R^d.\mathbf{v}^{*}\, dA, \tag{A5.15}$$

and

$$P_{\text{int}}{}^{*}\left(B_R\right) = -\int_{B_R} \text{tr}\left(\mathbf{T}.\dot{\mathbf{F}}\right) dV. \tag{A5.16}$$

Here $B_R$ is a material region bounded by $\partial B_R$ and $\mathbf{N}.\mathbf{T} = \mathbf{T}_R^d$ at the latter. Gurtin et al. consider in the reference configuration $K_R$ a so-called *migration control volume* $M_R$ bounded by $\partial M_R$ with outward-pointing unit normal $\mathbf{N}$. The notion of control volume is frequently used in fluid mechanics, especially to compute global forces or moments acting on bodies placed in a flow. Then introduce a velocity field $\mathbf{U}$, which may be interpreted as the velocity with which some external agency adds material to $M_R$ (the influence of the notion of growth by "accretion" here is visible). At $\partial M_R$, the normal velocity $U_N$ is such that $U_N = \mathbf{U}.\mathbf{N}$. The motion velocity in following $\partial M_R$ will be given by

$$\mathbf{u} = \mathbf{v} + \mathbf{F}\mathbf{U}. \tag{A5.17}$$

That is, the evolution at the actual placement of a point of $\partial M_R$ is made of two terms, the physical velocity $\mathbf{v}$ and the velocity $\mathbf{F}\mathbf{U}$ at which deformed material is transferred to this point. Since $\mathbf{u}$ is in physical space, it is invariant under change of *material* observer, while $\mathbf{U}$ is material and, therefore, invariant under change of spatial observer. Gurtin proposes to introduce a material stress tensor (that we denote by $\mathbf{b}_S$—our notation; it is denoted $\mathbf{C}$ by

Gurtin)—and a material traction $\mathbf{N}.\mathbf{b}_S$ that represents a force that expands power in conjunction with the migration of $\partial M_R$ and has, therefore, conjugate velocity $\mathbf{U}$. Consequently, he proposes, for the region $\partial M_R$, to replace the expression (2.116) or (A5.15) by

$$P_{\text{ext}}\left(M_R, \partial M_R\right) = \int_{M_R} \rho_0 \mathbf{f}.\mathbf{v}\, dV + \int_{\partial M_R} \mathbf{N}.\mathbf{T}.\mathbf{u}\, dA + \int_{\partial M_R} \mathbf{N}.\mathbf{b}_s.\mathbf{U}\, dA. \quad \text{(A5.18)}$$

An argument of invariance under change of material observer (crucial point! see Gurtin, 1999, p. 36) allows one to show that there follows the following local "force balance":

$$\text{div}_R \mathbf{b}_S + \bar{\mathbf{f}}^{\text{int}} + \bar{\mathbf{f}}^{\text{ext}} = \mathbf{0}, \quad \text{(A5.19)}$$

where the two source terms, respectively an *internal* and an *external* "material" body force, could not appear in (A5.18) since they exert no power because their material point of application is fixed in the reference configuration. Furthermore, on using (A5.17), we can rewrite (A5.18) in the form

$$P_{\text{ext}}\left(M_R, \partial M_R\right) = \int_{M_R} \rho_0 \mathbf{f}.\mathbf{v}\, dV + \int_{\partial M_R} \mathbf{N}.\mathbf{T}.\mathbf{v}\, dA + \int_{\partial M_R} \mathbf{N}.\left(\mathbf{b}_s + \mathbf{TF}\right).\mathbf{U}\, dA. \quad \text{(A5.20)}$$

The invariance of this expression under changes of velocity field for which the normal component is unaltered while only the tangential component of $\mathbf{U}$ is changed requires, then, that there holds the result

$$\int_{\partial M_R} \mathbf{N}.\left(\mathbf{b}_S + \mathbf{TF}\right).\mathbf{t}\, dA = 0, \quad \text{(A5.21)}$$

where $\mathbf{t}$ is any tangent vector field at $\partial M_R$. The requirement that the integrand in (A5.21) vanishes for all $\mathbf{N}$ is equivalent to requiring that the tensor quantity within parentheses in (A5.21) be proportional to the unit material tensor. Let $\Pi$ be the coefficient of proportionality, so that

$$\mathbf{b}_S = \Pi \mathbf{1}_R - \mathbf{TF}. \quad \text{(A5.22)}$$

The scalar $\Pi$ may be thought of as a bulk (volume) tension that works to increase the volume of $M_R$ through the addition of material at its boundary (still the idea of "accretion"). Further arguments of invariance under time-dependent changes in reference yield the following expressions for the *external* and *internal* "material" body forces (cf. Gurtin 1999, pp. 38–39):

$$\bar{\mathbf{f}}^{\text{ext}} = -\rho_0 \mathbf{f}.\mathbf{F}, \quad \bar{\mathbf{f}}^{\text{int}} = -\nabla_R \Pi + \mathbf{T}.\left(\nabla_R \mathbf{F}\right)^T, \quad \text{(A5.23)}$$

so that these quantities are not independent of the scalar Π, of the bulk data, and of the description of standard internal forces (Piola–Kirchhoff stress; another crucial point). Finally (very important and crucial point), a thermodynamic study (cf. Gurtin, 1999, pp. 41–43) allows one to identify the scalar pressurelike term as the free energy $W$ per unit reference volume, so that (A5.22) reads

$$\mathbf{b}_s = W\mathbf{1}_R - \mathbf{TF}, \tag{A5.24}$$

in which we recognize the quasistatic *Eshelby material stress*. Extension of the proof to include classical inertia is along the same line of thought, with additional crucial points (cf. Gurtin, 1999, Chapter 7; also Gurtin and Podio-Guidugli, 1996). We do not see any advantage to this approach over the presentation in this chapter (Section 5.3). On the contrary, it contains several dubious ah hoc reasonings, and overemphasized allusion to accretion and surface phenomena clouds the general nature of the balance (conservation or nonconservation) of material momentum as a general (but secondary) law of physics, which, as we know, exists even when there is no mechanics involved.

# 6

# *Local Structural Rearrangements of Matter and Eshelby Stress*

### Object of the Chapter

Where we discover that the notion of Eshelby stress is intimately related to that of local structural rearrangements of matter as happens in many metallurgical and physical processes in inert or living matter, such as in the phenomena of thermal stresses, plasticity, damage, biological growth, initiation of motion of dislocations, phase transformations, fatigue, and so on.

## 6.1 Changes in the Reference Configuration

In the foregoing chapters, when it happens, components of a geometric object or an equation are referred to one reference configuration only, $K$ (no subscript $R$ to simplify the notation), and this is sufficient in most of continuum mechanics. Accordingly, that reference configuration is chosen as the most convenient one for computations depending on the geometry of the deformable body under study. With the consideration of the physics of the problem, this may also be chosen as a stable solution providing a minimum of energy (cf. Lardner, 1974). But we could have been more cautious in noting $\mathbf{F}_K$, $\mathbf{T}_K$, and $\mathbf{S}_K$, the various objects where the relation to the selected reference configuration $K$ is understood, because the question naturally arises of a *possible change of reference configuration*, for example, between configurations $K$ and $K'$. Let $P_{KK'}$ be the transformation between $K$ and $K'$ at a material point $\mathbf{X}$. Given the tensorial nature of $\mathbf{F}$ and $\mathbf{T}$—these are in fact two-point tensor fields, that is, geometric objects having their two feet on different manifolds—we have the following transformations:

$$\mathbf{F}_{K'} = \mathbf{F}_K P_{KK'}, \quad \mathbf{F}_K = \mathbf{F}_{K'} P_{K'K}, \tag{6.1}$$

$$\mathbf{T}_{K'} = J^{-1}_{K'K} P_{K'K} \mathbf{T}_K, \quad \mathbf{T}_K = J^{-1}_{KK'} P_{KK'} \mathbf{T}_{K'}, \tag{6.2}$$

where

$$P_{KK'}P_{K'K} = \mathbf{I}, \quad P_{K'K}P_{KK'} = \mathbf{I}, \tag{6.3}$$

symbol **I** being the identity transformation. Of course, the equations in (6.2) are *Piola transformations*.

Now consider the case of energy-based elasticity for which there exists a potential energy per unit volume of the considered reference configuration, for example, $W_K(\mathbf{F}_K)$, such that

$$\mathbf{T}_K = \partial W_K / \partial \mathbf{F}_K. \tag{6.4}$$

Accordingly, for another reference configuration $K'$, we would have

$$\mathbf{T}_{K'} = \partial W_{K'} / \partial \mathbf{F}_{K'}. \tag{6.4'}$$

Since $W$ is per unit volume, we have

$$W_{K'} = J_{K'K}^{-1} W_K, \quad W_K = J_{KK'}^{-1} W_{K'}. \tag{6.5}$$

By direct computation of (6.4') and use of (6.1) and (6.5), we check that the equations in (6.2) hold identically.

Now let us do something more original by computing the quantity

$$\mathbf{b}_{KK'} = \frac{\partial W_K}{\partial P_{KK'}} = \frac{\partial}{\partial P_{KK'}}\left(J_{KK'}^{-1} W_{K'}\left(\mathbf{F}_K P_{KK'}\right)\right). \tag{6.6}$$

The result is

$$\mathbf{b}_{KK'} = -J_{KK'}^{-1}\left(P_{K'K} W_{K'} - \mathbf{T}_{K'}\mathbf{F}_K\right). \tag{6.7}$$

We call **configurational stress** the geometric object defined in the $K$ configuration by

$$\mathbf{b} = \mathbf{b}_K := -\mathbf{b}_{KK'} P_{KK'}, \tag{6.8}$$

that is, as shown by a simple calculation

$$\mathbf{b} = \mathbf{b}_K = -\frac{\partial W_K}{\partial P_{KK'}} P_{KK'} = W_K \mathbf{I}_K - \mathbf{T}_K \mathbf{F}_K. \tag{6.9}$$

This obviously is the *quasistatic Eshelby material stress* (cf. $(3.5_1)$) but referred explicitly to a specific reference configuration.

Let **P** be the two-point tensor field representing the transformation $P_{K'K}$. Accordingly, (6.1) and (6.9) read ($T$ = transpose):

$$\bar{\mathbf{F}} = \mathbf{FP}, \quad \mathbf{b} = -\frac{\partial \bar{W}}{\partial \mathbf{P}}\mathbf{P}^T = W\mathbf{1}_R - \mathbf{TF}, \tag{6.10}$$

where $\mathbf{1}_R$ is the identity in $K_R = K$, and

$$\bar{W} = J_{\bar{\mathbf{F}}}^{-1} W(\bar{\mathbf{F}}) = \tilde{W}(\mathbf{F},\mathbf{P}). \tag{6.11}$$

This follows Epstein and Maugin (1990a, 1990b), so that

$$\mathbf{T} = \frac{\partial \tilde{W}(\mathbf{F},\mathbf{P})}{\partial \mathbf{F}} = \frac{\partial W(\mathbf{F})}{\partial \mathbf{F}}, \quad \mathbf{b} = -\frac{\partial \tilde{W}(\mathbf{F},\mathbf{P})}{\partial \mathbf{P}}\mathbf{P}^T = W\mathbf{1}_R - \mathbf{TF}. \tag{6.12}$$

This means that **T** measures the elastic energy change in a classical deformation, while **b** measures this change in a change of reference configuration (i.e., purely material mappings). We can also note that

$$\mathbf{TF} = \mathbf{SF}^T\mathbf{F} = \mathbf{S}.\mathbf{C} =: \mathbf{M}, \tag{6.13}$$

where $\mathbf{C} = \mathbf{F}^T\mathbf{F}$ is the Cauchy–Green finite strain on the configuration $K_R$, and **M** is the *Mandel stress tensor* in $K_R$ already introduced in previous chapters (cf. Lubliner, 1990; Maugin, 1992). Therefore, configurational stresses and Mandel stresses are intimately related since they differ only by the presence of an energy isotropic term, that is,

$$\mathbf{b} = W\mathbf{1}_R - \mathbf{M} \quad \text{or} \quad \mathbf{b} + \mathbf{M} = W\mathbf{1}_R. \tag{6.14}$$

This difference reduces to a pure change of sign for an isochoric deformation associated with **b** or **M**.

We have seen before that the symmetry of the Cauchy stress results in the symmetry of **b** with respect to **C**, considered as the deformed metric on the material manifold $M^3$, that is,

$$\mathbf{Cb} = (\mathbf{Cb})^T = \mathbf{b}^T\mathbf{C}, \tag{6.15}$$

as first noticed by Epstein and Maugin (1990a). If, furthermore, the material considered is *isotropic*, then classical symmetry (i.e., with respect to a neutral unit covariant metric) applies because **S** becomes a function of the basic invariants of **C**.

## 6.2 Material Force of Inhomogeneity

If $K_R$ is a global reference configuration over the material body $B$, and $P_{K'K}$ is smooth and *integrable* over the material manifold, then **P** will be the gradient

of a deformation in a classical sense, so that (6.2) is not distinguishable from a standard Piola transformation. The situation may be altogether different in the case when the body is *not* materially homogeneous. Indeed, the case when **T** is a function of **F** and **F** only, where **F** is a true gradient, represents the essence of *pure homogeneous elasticity*—a paradigmatic case as we shall see hereinafter—with

$$\mathbf{T} = \bar{\mathbf{T}}(\mathbf{F}) = \frac{\partial W(\mathbf{F})}{\partial \mathbf{F}}. \tag{6.16}$$

This plays the role of a *standard* with which any other situation in a solid is compared (the case of more complicated functional dependences of $W$). Indeed, as soon as $W$ becomes an explicit function of additional arguments, we are no longer in this ideal framework. This happens whether the additional argument is another field variable such as temperature in thermoelasticity, or electric polarization or magnetization in electro-magneto-elasticity (cf. Maugin, 1988), or else any variables such as so-called internal variables of state supposed to account for the hidden complexity of microscopic processes that have a macroscopic manifestation in the form of thermodynamic irreversibility (i.e., dissipation; cf. Maugin, 1999b). These cases will be examined later on. Another frequent possibility is that the energy $W$ depends explicitly on the material particle **X**, in which case $W = \bar{W}(\mathbf{F};\mathbf{X})$ and the elastic material is said to be *materially inhomogeneous* from the elasticity viewpoint. We have called **material force of inhomogeneity** the material covector defined by

$$\mathbf{f}^{\text{inh}} := -\left.\frac{\partial \bar{W}}{\partial \mathbf{X}}\right|_{\text{expl}}, \tag{6.17}$$

if $\bar{W}$ is a sufficiently smooth function of **X**, and where the subscript *expl* means that the material gradient is taken at fixed field (here **F**). In composite materials where inhomogeneities manifest abruptly by jumps in material properties, (6.17) must be replaced by a distributional (generalized function) definition. The *force* $\mathbf{f}^{\text{inh}}$ belongs in the world of **material forces** (cf. Maugin, 1993, 1995) since it is a covector on the material manifold. It is a directional indicator of the changes of elastic properties as it is oriented opposite to the direct explicit gradient of $W$.

## 6.3 Some Geometric Considerations

Now we can exploit the thought experiment of Epstein and Maugin (1990a, 1990b). To that purpose, imagine that *at each material point* **X** we can give to

the material deformation energy the *appearance* of that of a pure homogeneous elastic body (dependence on one deformation only and nothing else) by applying the appropriate local (at **X**) change of reference configuration here noted **K**, a so-called *uniformity map* in the language of Noll and Wang. We consider this along with the concomitant change of volume (compare to (6.5)) so that

$$W = \bar{W}(\mathbf{F};\mathbf{X}) = J_{\mathbf{K}}^{-1} W(\mathbf{F}\mathbf{K}(\mathbf{X})) = \tilde{W}(\mathbf{F},\mathbf{K}). \tag{6.18}$$

Performing the same operation as in (6.12), we clearly have

$$\mathbf{T} = \frac{\partial \bar{W}(\mathbf{F};\mathbf{X})}{\partial \mathbf{F}}, \quad \mathbf{b} = -\frac{\partial \tilde{W}(\mathbf{F},\mathbf{K})}{\partial \mathbf{K}}\mathbf{K}^T = W\mathbf{1}_R - \mathbf{T}\mathbf{F}. \tag{6.19}$$

Thus there exists a relationship between the notion of material inhomogeneity and that of configurational (or Eshelby) stress. This is made more visible by applying the definition in Equation 6.17:

$$\begin{aligned} \mathbf{f}^{\text{inh}} &= -\frac{\partial \bar{W}(\mathbf{F};\mathbf{X})}{\partial \mathbf{X}}\bigg|_{\text{expl}} = -\frac{\partial \tilde{W}(\mathbf{F},\mathbf{K})}{\partial \mathbf{K}}.\frac{\partial \mathbf{K}}{\partial \mathbf{X}} \\ &= \mathbf{b}.\mathbf{K}^{-T}.\frac{\partial \mathbf{K}}{\partial \mathbf{X}} = \mathbf{b}.\left(\mathbf{K}^{-T}.\left(\nabla_{\mathrm{R}}\mathbf{K}\right)^T\right). \end{aligned} \tag{6.20}$$

On the other hand, if we compute the material divergence of **b** in the case of quasistatics in the absence of body force, for which the equilibrium at **X** is simply given by $\mathrm{div}_R\mathbf{T} = \mathbf{0}$, we have

$$\begin{aligned} \mathrm{div}_R\mathbf{b} &= \nabla_R W - \left(\mathrm{div}_R\mathbf{T}\right).\mathbf{F} - \mathbf{T}.\left(\nabla_R\mathbf{F}\right)^T \\ &= \left(\frac{\partial W}{\partial \mathbf{F}} - \mathbf{T}\right).\left(\nabla_R\mathbf{F}\right)^T + \frac{\partial W}{\partial \mathbf{X}}\bigg|_{\text{expl}}, \end{aligned} \tag{6.21}$$

or, on account of ($6.19_1$) and (6.20),

$$\mathrm{div}_R\mathbf{b} = -\mathbf{f}^{\text{inh}}. \tag{6.22}$$

Here, the material force of inhomogeneity is deduced from (or balanced by) the material divergence of the configurational stress. It is justified to give the

name **configurational forces** to these forces that are deduced through an operation acting on the configurational stress, whether by differentiation or integration (e.g., over a material surface, along a material contour in 2D). If we combine the results of (6.20) and (6.22), we also obtain an equation for **b** that involves the local transformation **K** in a source term, that is,

$$\mathrm{div}_R \mathbf{b} + \mathbf{b}.\Gamma = \mathbf{0}, \tag{6.23}$$

where we have defined a *material connection* $\Gamma(\mathbf{K})$ by

$$\Gamma(\mathbf{K}) = (\nabla_R \mathbf{K}^{-1}).\mathbf{K} = -\mathbf{K}^{-1}.(\nabla_R \mathbf{K})^T. \tag{6.24}$$

The result in (6.23) is due to Epstein and Maugin (1990a, 1990b). If **K** is the same for all points **X**, then $\nabla_R \mathbf{K} = \mathbf{0}$, and (6.23) reduces to the strict conservation law

$$\mathrm{div}_R \mathbf{b} = \mathbf{0}, \tag{6.25}$$

in the case (we remind the reader) of the absence of body force and neglect of inertia (quasistatics). Otherwise, we can write

$$\mathbf{f}^{\mathrm{inh}} = \mathbf{b}.\Gamma(\mathbf{K}), \tag{6.26}$$

Then, the previously reported intellectual construct means that the operation carried out (introduction of **K**) brings the neighborhood of each material point **X** into a *prototypical situation* of the pure elastic type, which allows one to compare the response of different points. Since this is *point-like*, the operation will not result in an overall smooth manifold but instead in a collection of nonfitting neighborhoods or infinitesimal chunks of materials, and **K** will not, accordingly, be itself a gradient. It may at most be a Pfaffian form. Of course, if **K** is not integrable, that is the case of $\bar{\mathbf{F}} = \mathbf{FK}$. With Equations 6.23 and 6.24, we enter the geometrization of continuum mechanics that was started in the mid-1950s by scientists such as Kondo (1952), Kroener (also spelled Kröner; 1958), Noll (1967), and Wang (1967), among others. This was thoroughly reviewed in Maugin (2003a, 2003b). This ambitious program belongs in the Einsteinian tradition of geometrization of physics and to part of David Hilbert's program. Of course, in this line of thought, the writing of (6.23) does not fulfill the whole program because the two sides of (6.23) contain contributions of a different nature, the non-Riemannian geometry being contained only in the right-hand side through the notion of connection based on **K**. However, there is progress here compared to other approaches, in the sense that the whole equation

(6.23) is written on the material manifold, which indeed is the arena of what may happen to the material in its intimacy (e.g., defects). Let us examine the source term in (6.26) more thoroughly and discuss more deeply the geometric connotations.

First of all, in components, (6.23) reads

$$b^J_{I,J} + b^K_{\cdot J}\left(\mathbf{K}^{-1}\right)^K_{\cdot\alpha} K^J_{\cdot\alpha,I} = 0. \tag{6.27}$$

This is a first-order differential equation that is identically satisfied by the tensor **b** associated with a solution of an elastic boundary-value problem. But, generally speaking, the **K** transformation creates a so-called *distant parallelism* (called in the past *absolute parallelism* or *Fernparallelismus*), and thus a (generally nonmetric) *connection* (cf. Choquet-Bruhat, 1968; Lichnerowicz, 1976) as defined by (6.24). In words, following Elie Cartan (probably the main contributor to this field of geometry), distant parallelism in a Riemannian space is materialized by the fact that, if we attach to each point in space a reference frame, and this in some arbitrary manner, then it is sufficient to agree that two vectors of any origin, ***A*** and ***B***, are parallel or equipollent if they have equal projections (components) on the rectangular frames at ***A*** and ***B***. Then the reference frames themselves are parallel to each other in that sense! In this process it is clear that the metric of the relevant space and the parallelism are dependent on one another, but for each given metric there is an infinity of distant parallelisms compatible with that metric, and, conversely, given a distant parallelism there exists an infinity of metrics compatible with it. Of course, in a Riemannian space, the notion of *Riemannian curvature* plays a fundamental role: It is related to the deviation undergone by a vector when the latter is transported in a *parallel* manner around a closed circuit. This notion disappears in the condition of distant parallelism; that is, a Riemannian space with distant parallelism has *no* curvature. Still, something distinguishes it from a Euclidean space, and that is *torsion*. As a consequence all the intrinsic geometric properties that characterize a Riemannian space with distant parallelism derive from its torsion (Elie Cartan, in some uncontrolled enthusiasm, once said that "*if physics can be geometrized at all, then all physical laws must be expressible in terms of partial differential equations governing the torsion of the relevant space*" (Cartan, 1931, my translation). This was very far-sighted insofar as unified gravitational theories are concerned. But in a way it also applies to continuum mechanics on the material manifold, our present concern.

To be more specific, define a *moving crystallographic frame* over the material body *B* by

$$\mathbf{E}_\alpha = K^K_{\cdot\alpha} \frac{\partial}{\partial X^K}. \tag{6.28}$$

Two vectors at different points in the reference configuration are, by definition, **K**-parallel if they have the same components in their respective

crystallographic bases. This leads to the introduction of a covariant derivative (here denoted ";") of a vector **V** of components $V^I$:

$$V^I_{:J}\frac{\partial}{\partial X^I}\otimes dX^J = V^\alpha_{.J}\mathbf{E}_\alpha\otimes dX^J = \left((\mathbf{K}^{-1})^\alpha_{,I}V^I\right)_{,J}K^K_{.\alpha}\frac{\partial}{\partial X^K}\otimes dX^J, \tag{6.29}$$

or

$$V^I_{:J} = V^I_{,J} + \Gamma^I_{KJ}V^K, \tag{6.30}$$

with a connection $\Gamma$ defined by (6.19).

Similarly, for a *one-form* (covector) **W**, working in the dual basis, we classically obtain

$$W_{I;J} = W_{I,J} - \Gamma^K_{IJ}W_K, \tag{6.31}$$

while for a mixed tensor **b**, we will have

$$b^J_{.I;K} = b^J_{.I,K} - \Gamma^L_{IK}b^J_{.L} + \Gamma^J_{LK}b^L_{.I}. \tag{6.32}$$

The connection symbol $\Gamma$ is *not necessarily* symmetric (as is, in contrast, the Christoffell symbol based on a metric). It is the skew part of this connection that defines the *torsion* $\tilde{\mathbf{T}}$ by

$$\tilde{T}^I_{JK} := \Gamma^I_{JK} - \Gamma^I_{KJ}. \tag{6.33}$$

This allows one (Epstein and Maugin, 1990a) to show that (6.27) can be rewritten in the following remarkable form:

$$\bar{b}^J_{.I;J} = \bar{b}^J_{.K}\tilde{T}^K_{JI} + \bar{b}^J_{.I}\tilde{T}^K_{JK}, \quad \bar{\mathbf{b}} \equiv J_K\mathbf{b} \tag{6.34}$$

or

$$\mathrm{div}_{\mathbf{K}}\bar{\mathbf{b}} = B\left(\bar{\mathbf{b}}, \tilde{\mathbf{T}}\right), \tag{6.35}$$

where $\mathrm{div}_{\mathbf{K}}$ denotes the covariant divergence based on **K**, and $B(.,.)$ denotes the specific bilinear form introduced in the first of (6.34). The formula for the divergence of a determinant has been employed in writing this on account of the introduction of the weighted Eshelby stress $\bar{\mathbf{b}}$. Particular cases of (6.35) are easily discussed: (i) If the reference configuration itself is *homogeneous*, then the **K**-parallelism reduces to the Euclidean one and we simply have $\mathrm{div}_R\,\mathbf{b} = \mathbf{0}$. This corresponds to the absence of physical (material) inhomogeneity and of any configurational inhomogeneity (i.e., artificial inhomogeneity due

to the special choice of a reference configuration). (ii) If the body is materially homogeneous but the reference configuration is arbitrary, then we have the *material conservation law* $\mathrm{div}_{\mathbf{K}}\bar{\mathbf{b}} = \mathbf{0}$. We may say that an observer adapted to the crystallographic frame sees no inhomogeneity (somewhat as a geodesic observer does not feel any gravitational field in general relativity, as we need two neighboring observers [notion of *geodesic separation*] to place that field in evidence). (iii) The general case is represented by (6.35), where not even an adapted observer can remove the inhomogeneity as the material is "*intrinsically dislocated*" (see next section). In any case, we say that the so-called *uniformity map* (in the language of Noll (1967) and Wang (1967)) **K** helps us define a local *prototype reference crystal* at each material point **X** on the material manifold.

**REMARK:** In standard treatises on continuum mechanics it is recalled that material symmetry consists in studying the possible isomorphisms of a particle onto itself that leave the response of the material invariant (cf. Noll). This materializes in changes of the reference configuration that belong to a certain group (a *crystallographic group* in general as studied in the appendix of Eringen and Maugin (1990), the group of *orthogonal transformations* in the case of *isotropy*). These transformations have no energetic contents and do not correspond to any dissipative structural rearrangement. For instance, for an elastic body in large strains, we would write the invariance

$$W = \bar{W}(\mathbf{F}) = \bar{W}(\mathbf{FP}), \quad \mathbf{P} \in SO(3), \quad \det \mathbf{P} = +1. \tag{6.36}$$

The first of these looks somewhat like (6.11) but for the determinant factor. What occurs here (Epstein and Maugin, 1990b) is as follows. Although one often concentrates on a discrete symmetry group, here we may consider that the material is a solid with a continuous symmetry group. In a uniform body *B*, the symmetry groups of *W* at different points, although generally different, are all conjugate, via the **K**-mappings, with the symmetry group of the *reference crystal*. Let $\mathbf{G}_{\mathbf{X}}(\lambda)$ be a one-parameter ($\lambda$ real) subgroup of the symmetry group of the energy *W* at **X** with $\mathbf{G}_{\mathbf{X}}(0) = \mathbf{I}$, the identity. From the material symmetry condition we have

$$\bar{W}(\mathbf{F};\mathbf{X}) = \bar{W}(\mathbf{F}\mathbf{G}_{\mathbf{X}}(\lambda),\mathbf{X}), \tag{6.37}$$

which is valid for all real $\lambda$'s and all nonsingular deformation gradients **F**. The remarkable property pointed out by Epstein and Maugin (1990b) is that the Eshelby stress does not produce any work in any small change of reference that belongs, at each material point X, to the *Lie algebra* of the symmetry group, that is,

$$tr\left(\mathbf{b}.\left.\frac{d\mathbf{G}_{\mathbf{X}}(\lambda)}{d\lambda}\right|_{\lambda=0}\right) = 0. \tag{6.38}$$

When applied to the special case of isotropy, this reasoning says that for this case where point-wise symmetry groups are all conjugate via $\mathbf{K}(\mathbf{X})$ with the proper orthogonal group $SO(3)$, the Eshelby stress is symmetric with respect to a Riemannian metric induced by the uniformity map and defined by

$$\mathbf{G}_{\mathbf{K}} := \mathbf{K}^{-T}.\mathbf{K}^{-1}. \tag{6.39}$$

In a stress-free configuration, this reduces to ordinary Euclidean symmetry. This should be contrasted with the **C**-symmetry in (6.15) satisfied by **b** when the Cauchy stress is symmetric. The preceding reasoning involves the theory of so-called **G**-structures admitting $\mathbf{G}_{\mathbf{X}}(\lambda)$ subgroups as discussed by Elzanowski et al. (1990).

## 6.4 Continuous Distributions of Dislocations

Starting with papers by Kroener (1958, 1960) and Bilby (1968), it has been proposed that the *torsion* of the material connection be a measure of the *dislocation density*—a special type of material inhomogeneities—in an elastic continuum presenting a continuous distribution of dislocations. Kroener's original approach considered only small strains, but we can easily reformulate his reasoning in the finite-strain framework. To that effect, we shall note $\alpha^{QK}$, $Q,K = 1,2,3$, the local material components of the dislocation density tensor. The natural way of comparing the defect of closure of a Burgers' circuit given in the material framework is to write the displacement jump in the form (compare to (3.57)):

$$\Delta\mathbf{u} = \oint_C d\mathbf{X} = \oint_C (\mathbf{K}^{-1})^{\alpha}_{.K}\mathbf{E}_{\alpha}dX^K, \tag{6.40}$$

and the relation to dislocation density is written as (cf. (A4.3))

$$\Delta u^Q = \int_S \alpha^{QK}dA_K = \int_S \alpha^{QK}N_K dA, \tag{6.41}$$

where the surface $S$ leans on the contour $C$. On using Stokes' theorem, this yields

$$\Delta\mathbf{u} = \int_S \varepsilon^{KLM}\left(\mathbf{K}^{-1}\right)^{\alpha}_{.K,L}\mathbf{E}_{\alpha}dA_M = \int_S \varepsilon^{KLM}\left(\mathbf{K}^{-1}\right)^{\alpha}_{.K,L}K^J_{.\alpha}\mathbf{G}_J dA_M, \tag{6.42}$$

since $\mathbf{E}_\alpha = K^J_{.\alpha}\mathbf{G}_J$. Here the **G'**s are a local basis on the material manifold**.** On comparing (6.41) and (6.42), we see that the following relation holds:

$$\alpha^{QM} = \varepsilon^{KLM}\Gamma^Q_{KL} = \varepsilon^{KLM}\tilde{T}^Q_{KL}. \tag{6.43}$$

As a result either $\alpha$ or $\tilde{\mathbf{T}}$ can equally characterize the dislocation density. We may conclude this paragraph by noting that the right-hand side of the first of (6.34) can be expanded on account of the definition of the quasistatic Eshelby stress while accounting for the skewsymmetry of the Levi–Civita permutation symbol and the symmetry of $\alpha$ (without loss of generality). We thus obtain the Peach–Koehler force in finite strains as

$$f_I^{(PK)} = J_{\mathbf{K}}F^i_{.Q}T^J_{.i}\varepsilon_{IJM}\alpha^{QM}. \tag{6.44}$$

In small strains this reduces to

$$f_i^{(PK)} = \varepsilon_{ijp}\sigma_{jk}\alpha_{kp}. \tag{6.45}$$

This coincides with the usual Peach–Koehler force in (3.65) for a unique dislocation of Burgers vector $\tilde{\mathbf{b}}$ and unit tangent vector $\tau$ to the dislocation line. Mura (1981) has given a derivation of this type.

## 6.5 Pseudo-Inhomogeneity and Pseudo-Plastic Effects

An example of *internal strains* is provided by thermal strains as given in small strains by (2.139). Corresponding *internal stresses* are obtained by substituting from these into the purely elastic constitutive equations, hence $\sigma_{0ij} = -m\tilde{\theta}\delta_{ij}$ in the case of isotropy according to (2.139). Other examples of internal strains are provided by uniform electric polarization in elastic ferroelectrics and magnetization in elastic ferromagnets via electrostriction and magnetostriction, respectively (see Maugin, 1979). These exist in a uniform state and could happen in the central space in a condenser or in the central space of a coil, causing a practically uniform magnetic field. Kroener (1958) and Indenbom (1965) have dealt in detail with these internal strains in the small-strain framework. In particular, Kroener (1958) created a true geometric theory of these by relating them to the geometry of the material manifold and introducing the notion of *incompatibility* for these strains since these internal strains are not integrable into an elastic displacement. The corresponding Einstein tensor defined in (2.28) does not vanish. The German expression "eigenspannungen" or "eigenstresses" or "proper stresses" has been adopted for them. They were initially introduced to account for

incompatible strains caused by dislocations and ultimately related to a macroscopic manifestation in the form of plasticity. Transformation strains in phase transformations are of the same type. They are additive in small strains. In large strains they naturally become *multiplicative* (see Appendix 6.1 to this chapter). This led us to introduce two qualitative definitions (Maugin, 2003b) as follows:

**DEFINITION 6.1:** We call *pseudo-plastic effects* in continuum mechanics those mechanical effects—due to any physical property—that manifest themselves just like *plasticity*, through the notion of eigenstrains and eigenstresses in the language of Kroener (1958).

**DEFINITION 6.2:** We call *pseudo-inhomogeneity effects* in continuum mechanics those mechanical effects—of any origin—that manifest themselves as so-called material forces in the material (Eshelbian) mechanics of materials (as developed by the author and coworkers since 1990).

These definitions in fact amount to showing that these effects are indeed local structural rearrangements so that the notions of uniformity map such as **K** and Eshelby material stress **b** come naturally into play. This follows from the fact that the reasoning applied in the first two sections of this chapter can also be applied when additional arguments that are true fields (thus depending on **X** in particular) are explicitly present in the energy function *W*. This we show by examining the archetypical examples of thermoelasticity and elastoplasticity in finite strains.

### 6.5.1 Materially Homogeneous Thermoelasticity

In this case we have only one material configuration to start with, but

$$W = \bar{W}(\mathbf{F},\theta), \tag{6.46}$$

where θ is the thermodynamic temperature. We can think of introducing a local map $\mathbf{K}(\theta)$, such that

$$\bar{W}(\mathbf{F},\theta) = J^{-1}_{\mathbf{K}(\theta)} W\left(\bar{\mathbf{F}} = \mathbf{F}\mathbf{K}(\theta)\right) = \tilde{W}(\mathbf{F},\mathbf{K}). \tag{6.47}$$

More classically, we set $\mathbf{K}(\theta) = \mathbf{F}^{-1}_{\text{th}}$, where $\mathbf{F}_{\text{th}}$ is a so-called *finite thermal deformation "gradient."* In this case we can say that

$$\mathbf{F}_e := \bar{\mathbf{F}} = \mathbf{F}\mathbf{F}^{-1}_{\text{th}}, \tag{6.48}$$

is the "elastic" deformation "gradient," such that we have the following **multiplicative** decomposition of the true deformation gradient:

$$\mathbf{F} = \mathbf{F}_e\mathbf{F}_{\text{th}} = \nabla_R \chi. \tag{6.49}$$

Such a decomposition was considered in the 1970s (by Yugoslav researchers such as Naerlovic, Micunovic, etc.). Note that neither $\mathbf{F}_e$ nor $\mathbf{F}_{\text{th}}$ is a true gradient. Using the standard definition of entropy per unit reference volume, a simple computation yields (Epstein and Maugin, 1995a)

$$S = -\frac{\partial \bar{W}}{\partial \theta} = -\mathbf{b}.\mathbf{F}_{\text{th}}.\frac{d\mathbf{F}_{\text{th}}^{-1}}{d\theta}, \tag{6.50}$$

with

$$\mathbf{b} = -\frac{\partial \tilde{W}}{\partial \mathbf{F}_{\text{th}}^{-1}}\mathbf{F}_{\text{th}}^{-T} = W\mathbf{1}_R - \mathbf{T}.\mathbf{F}. \tag{6.51}$$

Consequently, we can write the *material thermal force* of Chapter 5 as

$$\mathbf{f}^{\text{th}} = -\mathbf{b}.\mathbf{F}_{\text{th}}^{-1}.\left(\frac{d\mathbf{F}_{\text{th}}}{d\theta}\right).\left(\nabla_R\theta\right). \tag{6.52}$$

In this example, $\mathbf{F}_{\text{th}}^{-1}$ plays the role of local uniformity map or map of local structural rearrangement, and the results in (6.50) and (6.52) exhibit the relation of entropy density and the material thermal force with the Eshelby stress and this map. Of course, the same formalism will apply whatever the additional variable (such as an internal variable of state) $\alpha$ in the energy $W$.

### 6.5.2 Elastoplasticity in Finite Strains

In this case we identify $\mathbf{K}$ with the inverse of the "anelastic" (or plastic) deformation "gradient" (not a true gradient) as introduced in Chapter 2. That is, we contemplate the multiplicative decomposition of $\mathbf{F}$ as $\mathbf{F} = \mathbf{F}^e.\mathbf{F}^p$. Accordingly,

$$\mathbf{K}^{-1} \equiv \mathbf{F}^p, \quad \mathbf{FK} = \mathbf{F}.\mathbf{F}_p^{-1} \equiv \mathbf{F}^e. \tag{6.53}$$

Remember that in quasistatics for a materially homogeneous body we have a material force $\mathbf{f}^{\text{intr}}$ due to *intrinsic dissipative processes* associated with an internal variable $\alpha$ such that (cf. Chapter 5)

$$\text{div}_R\mathbf{b} + \mathbf{f}^{\text{intr}} = \mathbf{0}, \quad \mathbf{f}^{\text{intr}} = A.\left(\nabla_R\alpha\right)^T, \quad A = -\frac{\partial \bar{W}(\mathbf{F},\alpha)}{\partial \alpha}. \tag{6.54}$$

Then we envisage the following mental operation. Consider that it is possible, by an appropriate change of reference configuration $\mathbf{K}$, to make the material appear as *purely elastic* at point $\mathbf{X}$. This means that the new energy function $W$ will depend only on a finite deformation "gradient" and no other

argument. This is exactly what happens by using the Epstein–Maugin argument (1990a) and writing

$$W = \bar{W}(\mathbf{F},\alpha) = J_K^{-1}\hat{W}(\mathbf{F}\mathbf{K}(\alpha(\mathbf{X},t))) = \tilde{W}(\mathbf{F},\mathbf{K}(\alpha)). \tag{6.55}$$

It follows from this that (compare to (6.50))

$$A = \mathbf{b}.\mathbf{K}^{-T}.\frac{\partial \mathbf{K}^T}{\partial \alpha}. \tag{6.56}$$

Applying this to the case where $\alpha \equiv \mathbf{F}^p$ and (6.53) holds true, we obtain

$$A = -\mathbf{b}.\left(\mathbf{F}^p\right)^{-T} = \left(\mathbf{M} - W\mathbf{1}_R\right).\left(\mathbf{F}^p\right)^{-T}, \tag{6.57}$$

where we introduce the Mandel stress $\mathbf{M} = \mathbf{T}.\mathbf{F} = \mathbf{S}.\mathbf{C}$. Simultaneously, the *intrinsic dissipation* $\Phi^{\text{intr}}$ related to $\alpha$ takes on the following form:

$$\Phi^{\text{intr}} = A\dot{\alpha} = \text{tr}\left(\left(\mathbf{M} - W\mathbf{1}_R\right).\left(\mathbf{F}^p\right)^{-T}.\left(\dot{\mathbf{F}}^p\right)^T\right) = \text{tr}\left(\left(\mathbf{M} - W\mathbf{1}_R\right).\left(\mathbf{L}_R^p\right)^T\right), \tag{6.58}$$

where we introduced the "plastic finite-strain rate in the reference configuration $K_R$" by

$$\mathbf{L}_R^p = \dot{\mathbf{F}}^p.\left(\mathbf{F}^p\right)^{-1}. \tag{6.59}$$

If, as is most often the case, the plastic deformation is assumed to be incompressible, then $\text{tr}\,\mathbf{L}_R^p = 0$, and (6.58) reduces to

$$\Phi^{\text{intr}} = \text{tr}\left(\mathbf{M}.\left(\mathbf{L}_R^p\right)^T\right). \tag{6.60}$$

In plain words this means that *the Mandel stress is the driving force behind plasticity*. The relation (6.60) can be as well expressed with geometric objects pushed forward to the intermediate (elastically released) configuration $K_{\text{relax}}$, a more usual formulation. The first relationship between finite-strain plasticity and the notion of Eshelby stress in an intermediate configuration was established by Maugin (1994). Further works along this line can be found in Epstein and Maugin (1995b) and Cleja-Tigoiu and Maugin (2000).

### 6.5.3 Other Cases

The same can be achieved when the additional argument is electric polarization or magnetization in electro-magneto-elasticity so that electrostriction

and magnetostriction finite deformation "gradients" can be introduced in similar multiplicative decompositions. For example, in deformable magnets (cf. Maugin, 1988), the *local magnetic field* due to the interaction of the magnetization **m** per unit volume of the reference configuration with the crystal lattice is given by

$$\mathbf{H}^L = -\frac{\partial W(\mathbf{F},\mathbf{m})}{\partial \mathbf{m}}. \tag{6.61}$$

Applying the preceding reasoning will yield the local magnetic field and the associated *material magnetic force* in the following form:

$$\mathbf{H}^L = \mathbf{b}.\mathbf{F}_{\text{magn}}^{-1}.\frac{\partial \mathbf{F}_{\text{magn}}}{\partial \mathbf{m}}, \quad \mathbf{f}^{\text{magn}} = \mathbf{b}.\mathbf{F}_{\text{magn}}^{-1}.\frac{\partial \mathbf{F}_{\text{magn}}}{\partial \mathbf{m}}.\left(\nabla_R \mathbf{m}\right)^T, \tag{6.62}$$

where $\mathbf{F}_{\text{magn}}$ is the (nonintegrable) internal magnetization deformation gradient such that $\mathbf{F}$ decomposes multiplicatively as $\mathbf{F} = \mathbf{F}^e.\mathbf{F}_{\text{magn}}$.

If we combine different effects applied in a certain order (decided by the order in the composition), we could have a general decomposition in a thermal magnetized anelastic material (certainly the case in some structural members (plates) used, say, in building electricity transformers). We would have

$$\mathbf{F} = \mathbf{F}^e.\mathbf{F}^{\text{th}}.\mathbf{F}^p.\mathbf{F}_{\text{magn}}, \tag{6.63}$$

where none of the elements present in this composition is a true gradient. In all these cases multiplication reduces to addition in the case of small deformation and fields; that is, instead of (6.63), there will hold the additive relation

$$\left(\nabla \mathbf{u}\right)_S = \boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}^e + \boldsymbol{\varepsilon}^{\text{th}} + \boldsymbol{\varepsilon}^p + \boldsymbol{\varepsilon}_{\text{magn}}. \tag{6.64}$$

All the generalizations given in the preceding deal with a local change of reference configuration in order to formulate an energy in a so-called *elastically released state* (pure homogeneous elasticity). Physically, they all correspond to *local structural rearrangements* (phase transformations also enter this framework with a so-called transformation strain). They all induce the existence of so-called *internal stresses* (stresses in the absence of classical deformation). Because of their similarities both with inhomogeneity effects and plasticity effects, they well deserve to be called pseudo-inhomogeneity or pseudo-plasticity effects (Maugin, 2003a, 2003b). The operation effected by the application of **K** may receive several different names, among which the name *transplant* more vividly appeals to the case of the theory of *material*

*growth* such as in biological tissues since material growth belongs in the same class of phenomena (cf. Epstein and Maugin, 2000). This will be examined in greater detail later on.

## 6.6 A Variational Principle in Nonlinear Dislocation Theory

We return to the line followed in Sections 6.2 through 6.4 by considering a variational formulation in the quasistatics of elastic materials when we account for the constraint imposed by the connection, more precisely the torsion, in terms of **K**. This was done by Kroener (1993) and Maugin (1999a). The total Lagrangian of interest reads:

$$L = \int_{M^3} \left( \tilde{W}(\mathbf{F}, \mathbf{K}, \alpha) - \lambda^{PM}_{\cdot\cdot Q} \left[ \Gamma^{\cdot\cdot Q}_{[PM]} - \left(\mathbf{K}^{-1}\right)^{\alpha}_{\cdot[P,M]} K^{Q}_{\cdot\alpha} \right] \right) dV, \tag{6.65}$$

where $\lambda^{PM}_{\cdot\cdot Q}$ are the components of a Lagrange multiplier tensor and the variation to be taken is the material one $\delta_X$. We note that

$$\delta_X W = \delta_X \left( J_K^{-1} \bar{W}(\mathbf{FK}) \right) = \mathrm{tr}\left(\mathbf{T}.\delta_X \mathbf{F}\right) - \mathrm{tr}\left(\left(\mathbf{K}^{-1}.\mathbf{b}\right).\delta_X \mathbf{K}\right) + \mathrm{tr}\left(\mu.\delta_X \alpha\right), \tag{6.66}$$

wherein

$$\mathbf{b} = W\mathbf{1}_R - \mathbf{T}.\mathbf{F}, \quad \mathbf{T} = \frac{\partial W}{\partial \mathbf{F}}, \quad \mu = \frac{\partial W}{\partial \alpha}. \tag{6.67}$$

With all fields vanishing sufficiently fast at infinity, and on account of (6.66), we deduce from the variation of (6.65) where $\alpha$ is taken as the tensor of dislocation density the following Euler–Lagrange equations:

$$\mathrm{div}_R \mathbf{T} = \mathbf{0} \tag{6.68}$$

and

$$\mathbf{b} - \mathrm{div}_R \lambda - \lambda.\alpha + \lambda^T.\Gamma = \mathbf{0}, \tag{6.69}$$

$$\lambda = \mu; \tag{6.70}$$

By (6.69) we understand the following component equation:

$$b^{K}_{\cdot L} - \partial_M \lambda^{MK}_{\cdot\cdot L} - \lambda^{MN}_{\cdot\cdot L} \alpha^{\cdot\cdot K}_{\cdot MN} + \lambda^{MK}_{\cdot\cdot Q} \Gamma^{\cdot\cdot Q}_{ML} = 0, \tag{6.71}$$

while (6.70) means that the Lagrange multiplier introduced is nothing else than the *hyperstress* associated with the dislocation density. Equation 6.69 relates the Eshelby stress to the flux of this hyperstress via the material divergence of the latter and source terms due to dislocations. This equation is not the balance of material momentum, in which **b** itself is the flux. Now we go one step further in our geometrization scheme. Let

$$\mathbf{G}_{\mathbf{K}}^{-1} = \left(\mathbf{G}_{\mathbf{K}}\right)^{-1} = \mathbf{K}.\mathbf{K}^{T}, \tag{6.72}$$

the reciprocal (material, contravariant) **K**-induced metric. We introduce a covariant derivative on the material manifold $M^3$ with torsion by (here $\partial_J = \partial/\partial X^J$, and $\nabla_K$ denotes the covariant derivative based on $\mathbf{G}_{\mathbf{K}}$)

$$\hat{\nabla}_K = \nabla_K + \alpha_{\cdot KP}^{\cdot P}. \tag{6.73}$$

Then we obtain that **b** and λ jointly satisfy the covariant equation

$$\hat{\nabla}.\hat{\lambda} - \hat{\mathbf{b}} = \mathbf{0}, \tag{6.74}$$

where we have introduced (fully covariant) densities $\hat{\mathbf{b}}$ and $\hat{\lambda}$ by

$$\hat{\mathbf{b}} = J_K^{-1}\,\mathbf{b}.\mathbf{G}_{\mathbf{K}}^{-1}, \quad \hat{\lambda} = J_K^{-1}\lambda.\mathbf{G}_{\mathbf{K}}^{-1}, \quad J_K = \det\mathbf{K} = \left(\det\mathbf{G}_{\mathbf{K}}^{-1}\right)^{1/.2}. \tag{6.75}$$

Then, following Kroener (1993) while accounting for the skewsymmetry of $\hat{\lambda}$ with respect to its first indices, we check that $\hat{\mathbf{b}}$ satisfies the following covariant material balance law:

$$\hat{\nabla}.\hat{\mathbf{b}} - \mathbf{f}_{(\alpha)} = \mathbf{0}, \tag{6.76}$$

where we defined a material force $\mathbf{f}_{(\alpha)}$ due to the distribution of dislocations by

$$\left(\mathbf{f}_{(\alpha)}\right)^{Q} = \alpha_{\cdot ML}^{\cdot P}\nabla_P\hat{\lambda}^{LMQ}. \tag{6.77}$$

This material force, a dislocation-driven one, is very similar to the *Mathisson* (1937) *force* introduced in relativistic spinning media in a gravitational field. Furthermore, (6.74) is tantamount to saying that, on the material manifold, we have the generalized-force structure of a Cosserat continuum, with stress given by the contravariant Eshelby stress and the hyperstress determined by the dislocation density, notwithstanding the fact that our deformable continuum appears rather classical in physical space (cf. Equation 6.68)—for more on Cosserat continua and Eshelby stress, see Chapter 9.

## 6.7 Eshelby Stress as a Resolved Shear Stress

In crystal physics the *activation of slip systems* is governed by Schmid's law (cf. Schmid and Boas, 1935). This is particularly important for single crystals because of its relationship to finite-strain plasticity. Schmid's law in fact is a criterion usually expressed in terms of the local value of the Cauchy stress projected onto the crystal characteristic directions. Only *shear* is involved, and the appropriate projection of the stress is called the *resolved shear-stress.* In finite strains, where plasticity is involved through a multiplicative decomposition of **F**, it would be natural to assume the intervention of the Eshelby stress. This is indeed the case as shown by Le (1999) from whom we borrow the derivation. We assume that slip takes place on families of slip planes equipped with unit normals $\mathbf{m}_0^{(k)}$, regarded as material covectors, and with slip directions described by unit material vectors $\mathbf{s}_0^{(k)}$, such that each pair of these describes one slip system with $\mathbf{m}_0^{(k))}.\mathbf{s}_0^{(k)} = 0$ for $k$ fixed. In single crystals there exists only a finite number $N$ of slip systems. Then the time rate of plastic "gradient" is supposed to satisfy *Taylor's fundamental equation*:

$$\dot{\mathbf{F}}^p = \sum_{k=1}^{N} \left(\dot{\gamma}^{(k)} \mathbf{s}_0^{(k)} \otimes \mathbf{m}_0^{(k)}\right).\mathbf{F}^p, \tag{6.78}$$

where $\gamma^{(k)}$ is the amount of slip for the $k$-slip system. A consequence of (6.78) is that the plastic distortion is *isochoric* (i.e., it preserves the volume). In an elastic deformation $\mathbf{F}^e$, the vectors $\mathbf{s}_0^{(k)}$ and covectors $\mathbf{m}_0^{(k)}$ are transformed according to the transformation rules for vectors and covectors, that is,

$$\mathbf{s}^{(k)} = \mathbf{F}^e \mathbf{s}_0^{(k)}, \quad \mathbf{m}^{(k)} = \left(\mathbf{F}^e\right)^{-T} \mathbf{m}_0^{(k)}, \tag{6.79}$$

while they obviously remain unchanged under slip according to their very definition. The energy per unit of the *reference crystal* configuration (intermediate configuration) is a function of the elastic "gradient" $\mathbf{F}^e$ only (we consider isothermal evolutions). That is,

$$\bar{W}\left(\mathbf{F}^e\right) = \hat{W}\left(\mathbf{C}^e\right); \quad \mathbf{C}^e = \left(\mathbf{F}^e\right)^T \mathbf{F}^e. \tag{6.80}$$

But we note that

$$\mathbf{C}^e = \left(\mathbf{F}^e\right)^T.\mathbf{1}.\mathbf{F}^e = \left(\mathbf{F}^p\right)^{-T} \mathbf{F}^T.\mathbf{F}\left(\mathbf{F}^p\right)^{-1} = \left(\mathbf{F}^p\right)^{-T}.\mathbf{C}.\left(\mathbf{F}^p\right)^{-1}. \tag{6.81}$$

Accordingly, the energy per unit volume of the reference configuration reads

$$W = J^p \hat{W}\left(\mathbf{C}^e\left(\mathbf{C}, \mathbf{F}^p\right)\right) = \tilde{W}\left(\mathbf{F}^p, \mathbf{C}\right). \tag{6.82}$$

The Clausius–Duhem inequality here is reduced to

$$\dot{W} - \frac{1}{2}\mathrm{tr}\left(\mathbf{S}.\dot{\mathbf{C}}\right) \leq 0\,. \tag{6.83}$$

From this, following the classical Coleman–Noll exploitation, we deduce that

$$\mathbf{S} = 2\frac{\partial \hat{W}}{\partial \mathbf{C}}\bigg|_{\mathbf{F}^p} = \frac{\partial \hat{W}}{\partial \mathbf{E}}\bigg|_{\mathbf{F}^p}, \quad \mathrm{tr}\left(\frac{\partial \hat{W}}{\partial \mathbf{F}^p}.\dot{\mathbf{F}}^p\right) \leq 0; \tag{6.84}$$

We set

$$J^{(k)} = \mathrm{tr}\left(\mathbf{J}.\left(\mathbf{s}_0^{(k)} \otimes \mathbf{m}_0^{(k)}\right)\right), \tag{6.85}$$

while we show by differentiation that

$$\mathbf{J} := -\frac{\partial \hat{W}}{\partial \mathbf{F}^p}\bigg|_{\mathbf{C}} \left(\mathbf{F}^p\right)^T = -\left(\mathbf{F}^p\right)^{-T}.\mathbf{b}.\left(\mathbf{F}^p\right)^T, \quad \mathbf{b} = \hat{W}\mathbf{1}_R - \mathbf{S}.\mathbf{C}. \tag{6.86}$$

The remaining dissipation inequality in $(6.84_2)$ reduces to

$$\sum_{k=1}^{N} J^{(k)}\dot{\gamma}^{(k)} \geq 0. \tag{6.87}$$

From this can be deduced a criterion of activation (vanishing or nonvanishing slip) by following general rules of irreversible thermomechanics (Maugin, 1999b; also Chapter 2 in this book). In particular, we can formulate a generalized Schmid law by considering a dissipation function *D, homogeneous of degree one* in the slip rates, such that

$$D = \sum_{k=1}^{N} J_{cr}^{(k)}\left(\gamma^{(1)},\ldots,\gamma^{(N)}\right)\left|\dot{\gamma}^{(k)}\right| \tag{6.88}$$

and

$$J^{(k)} = \frac{\partial D\left(\gamma^{(j)},\dot{\gamma}^{(j)}\right)}{\partial \dot{\gamma}^{(k)}}, \tag{6.89}$$

where the $J_{\mathrm{cr}}^{(k)}$ are critical values, perhaps still functions of the $\gamma$'s. Slip systems of which the shear component of the Eshelby stress reaches its critical

value, leading to a nonzero time evolution of $\gamma^{(k)}$, are said to be *activated*. More precisely, the singular formulation in (6.88) and (6.89) yields

$$\begin{aligned} \left|J^{(k)}\right| < J_{\mathrm{cr}}^{(k)} &\Rightarrow \dot{\gamma}^{(k)} = 0, \\ J^{(k)} = J_{\mathrm{cr}}^{(k))} &\Rightarrow \dot{\gamma}^{(k)} \geq 0, \\ J^{(k)} = -J_{\mathrm{cr}}^{(k)} &\Rightarrow \dot{\gamma}^{(k)} \leq 0, \end{aligned} \tag{6.90}$$

so that activation possibly, but not necessarily, occurs only when the modulus of the corresponding $J^{(k)}$ has reached a critical value. This critical behavior follows from the mathematical homogeneity of degree one of the dissipation function $D$ (see Maugin [1992] for the exploitation of this property in rate-independent plasticity).

The critical role of the Eshelby stress in a criterion has also been recently proposed in the materials mechanics of elastomers, where the question of *fatigue* is crucial (Andriyana, 2006; Andriyana and Verron, 2007). This consideration is based on a remark by Herrmann and Kienzler (2000) that the component $b_{.L}^{K}$ of the Eshelby stress $\mathbf{b}$ is a scalar that represents the negative of energy variation due to a unit material translation of the surface of unit normal $N_K$ in the direction of unit vector $\mathbf{e}_L$. Indeed, if $\delta u$ is the amplitude of the translation in the direction of unit vector $\mathbf{e}_L$, $\delta\Pi$ is the change in energy, $N_K$ is the unit normal to a small element of surface $\Delta S_R$ over which $\mathbf{b}$ is practically uniform, we have (indices $K$ and $L$ fixed)

$$b_{.L}^{K} = -\left(\Delta S_R\right)^{-1} \frac{\delta \Pi}{\delta u}.$$

This serves to define a predictive measure of fatigue in elastomers by considering the smallest of the eigenvalues of $\mathbf{b}$ as initiating the growth of microdefects.

## 6.8 Second-Gradient Theory

Some of the results of previous sections have been generalized to the case of second-gradient elasticity, for which the Lagrangian density may be written as (4.119). We shall focus the attention on the following elastic-potential energy per unit reference volume for an inhomogeneous material:

$$W = \bar{W}\left(\mathbf{F}, \nabla_R \mathbf{F}; \mathbf{X}\right). \tag{6.91}$$

Let us look at this from the point of view of symmetries. Of course, such a material, by its very definition, is sensitive to the first and second-material gradients of the direct motion that yields the placement. When evaluated at a given point **X** at fixed time *t*, the values of these gradients are independent of each other. Therefore, it would appear at first view that insofar as characteristic symmetries at a point are concerned, one should be interested only in the response of two completely independent arguments, a second- and third-order two-point tensor fields. But this cannot be true because material symmetries have to respect *group* properties (Elzanowski and Epstein, 1990). Accordingly, the value taken by the third-order geometric object $\nabla_R\mathbf{F}$ is always the result of evaluating the second gradient of a global deformation, so that special requirements on the law of *composition* of the tensorial objects involved must be envisaged. This law, in turn, will determine what kind of object the symmetry group of the material should be. To that effect, consider the influence of material-particle changes

$$\mathbf{Y} = \bar{\mathbf{Y}}(\mathbf{X}), \tag{6.92}$$

with gradients

$$\nabla_R\bar{\mathbf{Y}} = \left\{H^{\ A}_{.I} = Y^{\ A}_{.,I}\right\}, \quad \nabla_R\nabla_R\bar{\mathbf{Y}} = \left\{H^{\ A}_{.IJ} = Y^{\ A}_{.,IJ} = H^{\ A}_{.JI}\right\}, \tag{6.93}$$

on the material response in (6.91). We immediately have

$$W = \bar{W}\left(J^{\ i}_{.A}H^{\ A}_{.I}, J^{\ i}_{.AB}H^{\ A}_{.I}H^{\ B}_{.J} + J^{\ i}_{.A}H^{\ A}_{.IJ}; X^I\left(Y^A\right)\right) = \hat{W}\left(\mathbf{J}, \nabla_R\mathbf{J}, \mathbf{Y}\right), \tag{6.94}$$

where **J** and $\nabla_R\mathbf{J}$ are the gradients of the direct motion with respect to the second reference. Since a material symmetry is a change of reference configuration that leaves the response function unchanged, we are led to identify all such reference configurations that have the *same* first and second gradients at the point **X** and to group them into an *equivalent class* in which the composition law exhibited in the first of (6.94) applies. Thus, we can say that a material symmetry relative to a given reference at **X** is given by two tensors, **G** and **S**, with the property that

$$W\left(F^{\ i}_{.I}, B^{\ i}_{IJ}; X^I\right) = W\left(F^{\ i}_{.K}G^{\ K}_{.I}, B^{\ i}_{.KL}G^{\ K}_{.I}G^{\ L}_{.J} + F^{\ i}_{.K}S^{\ K}_{.IJ}; \mathbf{Y}\right), \quad S^{\ K}_{.IJ} = S^{\ K}_{.JI}, \quad \det\mathbf{G} > 0, \tag{6.95}$$

for all **F**s and **B**s.

The following properties were enunciated by Elzanowski and Epstein (1990) and proved in a more or less straightforward manner: (i) The symmetries exhibited in (6.95) form a group $H = \{G,S\}$ with typical element $\{\mathbf{G},\mathbf{S}\}$, identity element $\{\mathbf{1},\mathbf{0}\}$, and composition law

$$\left\{\mathbf{G}_3, \mathbf{S}_3\right\} = \left\{\mathbf{G}_1, \mathbf{S}_1\right\} \circ \left\{\mathbf{G}_2, \mathbf{S}_2\right\} = \left\{\mathbf{G}_1\mathbf{G}_2, \left(\mathbf{S}_1\mathbf{G}_2\right)^T\mathbf{G}_2 + \mathbf{G}_1\mathbf{S}_2\right\}. \tag{6.96a}$$

In components, this reads

$$G_{3P}^{.K} = G_{1M}^{.K} G_{2P}^{.M}, \quad S_{3PJ}^{.K} = S_{1MN}^{.K} G_{2P}^{.M} G_{2J}^{.N} + G_{1\mathbf{M}}^{.K} S_{2PJ}^{.M}. \tag{6.96b}$$

(ii) Two symmetry groups, $H$ and $\hat{H}$, at the same point, relative to two different reference configurations, coincide if and only if the values of the first and second gradients of the configuration change are, as a pair $\{H, T\}$, a member of one, and hence of both, of the symmetry groups. Otherwise, the groups are *conjugate* through the constant elements $\{H, T\}$ by the relation

$$\{G,S\} = \{H,T\}^{-1} \circ \{\hat{G},S\} \circ \{H,T\}, \tag{6.97}$$

where inversion and composition have to be understood in the sense of the group operations defined in (6.96). For instance, if $\mathbf{H}^{-1}$ is the ordinary inverse of $\mathbf{H}$, then

$$\left(\mathbf{T}^{-1}\right)_{.JK}^{I} = -T_{.MN}^{L} \left(\mathbf{H}^{-1}\right)_{.L}^{I} \left(\mathbf{H}^{-1}\right)_{.J}^{M} \left(\mathbf{H}^{-1}\right)_{.K}^{N}. \tag{6.98}$$

Now we look for the generalization of the local **K**-transformation of reference introduced in Section 6.3. Accounting for the composition present in (6.95), when a body is materially uniform (there exists a global reference configuration), two mappings $\mathbf{K}(\mathbf{X})$ and $\mathbf{Q}(\mathbf{X})$—and not only $\mathbf{K}$—of a reference crystal on the first *and* second tangent spaces at each point of the global configuration must exist, so that instead of (6.95) we have

$$\bar{W}\left(\mathbf{F}, \nabla_R \mathbf{F}; \mathbf{X}\right) = J_{\mathbf{K}}^{-1} W\left(\mathbf{FK}, \left(\left(\nabla_R \mathbf{F}\right)\mathbf{K}\right)^T .\mathbf{K} + \mathbf{F}.\mathbf{Q}\right) = J_{\mathbf{K}}^{-1} W\left(\bar{\mathbf{F}}, \bar{\mathbf{G}}\right), \tag{6.99}$$

which defines both $\bar{\mathbf{F}}$ and $\bar{\mathbf{G}}$. Applying the chain rule of differentiation and generalizing the computation of Section 6.3, we compute

$$\frac{\partial W}{\partial \left(\bar{\mathbf{F}}\right)_{.\alpha}^{i}} = J_K \left(\mathbf{K}^{-1}\right)_{.J}^{\alpha} \left(\hat{T}_{.i}^{J} - \hat{M}_{.i}^{KL} \left(\mathbf{K}^{-1}\right)_{.K}^{\beta} \left(\mathbf{K}^{-1}\right)_{.L}^{\gamma} Q_{.\beta\gamma}^{J}\right) \tag{6.100}$$

and

$$\frac{\partial W}{\partial \left(\bar{\mathbf{G}}\right)_{.\alpha\beta}^{i}} = J_{\mathbf{K}} \hat{M}_{..i}^{KL} \left(\mathbf{K}^{-1}\right)_{.K}^{\alpha} \left(\mathbf{K}^{-1}\right)_{.L}^{\beta}, \tag{6.101}$$

where $\hat{\mathbf{T}}$ is a first Piola–Kirchhoff stress and $\hat{\mathbf{M}}$ is a *hyperstress* as generically defined by the second of (4.124). From (6.100) and (6.101), one then shows that the derivatives of $\bar{W}$ with respect to $\mathbf{K}$ and $\mathbf{Q}$, that is,

$$\tilde{\mathbf{b}} = -\frac{\partial \bar{W}}{\partial \mathbf{K}}, \quad \tilde{\mathbf{B}} = -\frac{\partial \bar{W}}{\partial \mathbf{Q}}, \tag{6.102}$$

are given in components by

$$\tilde{b}^{\alpha}_{.I} = \left( W\delta^{J}_{I} - \hat{T}^{J}_{.i} F^{i}_{.I} + \hat{M}^{KL}_{..i} F^{i}_{.I} \left(\mathbf{K}^{-1}\right)^{\beta}_{K} \left(\mathbf{K}^{-1}\right)^{\gamma}_{.L} Q^{J}_{.\beta\gamma} - 2F^{i}_{.L,I} \hat{M}^{JL}_{..i} \right) \left(\mathbf{K}^{-1}\right)^{\alpha}_{.J} \tag{6.103}$$

and

$$\tilde{B}^{\alpha\beta}_{.M} = \hat{M}^{KL}_{..i} F^{i}_{.I} \left(\mathbf{K}^{-1}\right)^{\alpha}_{.K} \left(\mathbf{K}^{-1}\right)^{\beta}_{.L}. \tag{6.104}$$

At this point it is natural to isolate those terms that do not depend on the choice of reference crystal in order to define the following *completely material* tensors:

$$b^{N}_{.M} = \tilde{b}^{\alpha}_{.M} K^{N}_{.\alpha} - \tilde{B}^{\rho\sigma}_{.M} Q^{N}_{.\rho\sigma}, \quad B^{NL}_{.M} = \tilde{B}^{\rho\sigma}_{.M} K^{N}_{.\rho} K^{L}_{.\sigma}. \tag{6.105}$$

These are the *material Eshelby stress* and *hyperstress* such that (Maugin and Trimarco, 1992)

$$b^{N}_{.M} = W\delta^{N}_{M} - \hat{T}^{N}_{.i} F^{i}_{.M} - 2\hat{M}^{NL}_{..i} F^{i}_{.M,L}, \quad B^{NL}_{..M} = \hat{M}^{NL}_{..i} F^{i}_{.M}. \tag{6.106}$$

On defining an *effective Eshelby stress* by

$$\mathbf{b}^{\text{eff}} := \mathbf{b} - \text{div}_{R}\mathbf{B} \tag{6.107}$$

and taking the material divergence of this by direct calculation, we obtain the quasistatic version of the balance of material momentum as

$$\text{div}_{R}\mathbf{b}^{\text{eff}} + \mathbf{f}^{\text{inh}} = \mathbf{0}. \tag{6.108}$$

These results (Epstein and Maugin, 1992) may be useful in a geometric description of continuous distributions of *disclinations*.

## 6.9 Continuous Distributions of Disclinations

The most general dislocations need a characterization, not only by a Burgers vector relating to a *translation*, but also by a *rotation* of a finite angle ω around

an axis. This rotation can be manifested by the rotation of a local triad of orthogonal vectors attached at each point of the dislocation line $L$. In the same spirit as the concept of Burgers vector, we may say that this triad, in an unstrained solid, corresponds to a local triad of constant orientation along $L$ in the strained solid. Such rotation dislocations are called *disclinations* (cf. Friedel, 1979). While the geometric concept of torsion seems to capture the concept of translation dislocation characterized by a Burgers vector in a satisfactory manner, the question naturally arises of the geometric characterization of continuous distributions of disclinations in *material* space, the realm of structural defects. Anthony (1970) has advanced the idea that while torsion associated with a certain material connection could relate to translation dislocations, *curvature* should then characterize disclinations. But we already saw that in continuum mechanics all information required to describe smooth distributions of defects is to be found in the material response functional of the body (e.g., $W$, in fact a function), defects being themselves equated with a lack of homogeneity of these functionals. Disclinations cannot be described in the framework of a first-gradient theory (classical elasticity) since the latter gives rise only to a curvature-free material connection. Simultaneously, the structural approach to defective materials suggests the presence of *couple-stresses* in relation with defects in general and disclinations in particular. As a consequence, it seems natural to investigate the possibility that disclinations could be placed under the umbrella of continuum mechanics by considering second-gradient elastic materials, the subject matter of the preceding section. This program has not been completed at the time of writing of this book, but some directions of research can be pointed at (in this respect see also the end of Chapter 9). Of course, the symmetry question, as examined in the foregoing section, is of great importance as, following along the same line as in the curvature-free case, we need to express fundamental identities that derive from the introduction of Eshelby stresses and hyperstresses. Computing directly the inhomogeneity force source in (6.108), that is,

$$\left.\frac{\partial \hat{W}}{\partial X^M}\right|_{\text{exp1}} = \frac{\partial \bar{W}}{\partial K^I_{.\alpha}} K^I_{.\alpha,M} + \frac{\partial \bar{W}}{\partial Q^{\ I}_{.\alpha\beta}} Q^I_{.\alpha\beta,M} = -\left(\tilde{b}^{\ \alpha}_{.I} K^{\ I}_{.\alpha,M} + \tilde{B}^{\alpha\beta}_{..I} Q^I_{.\alpha\beta,M}\right), \quad (6.109)$$

instead of (6.108), we have thus the equation that generalizes (6.23) in the rather frightening form

$$\begin{aligned}\left(\text{div}_R \mathbf{b}^{\text{eff}}\right)_M + \left(b^J_{.I} - B^{KL}_{.I}\left(\mathbf{K}^{-1}\right)^{\rho}_{.K}\left(\mathbf{K}^{-1}\right)^{\sigma}_{.L} Q^J_{.\rho\sigma}\right)\left(\mathbf{K}^{-1}\right)^{\alpha}_{.J} K^{\ I}_{.\alpha,M} \\ + B^{KL}_{..I}\left(\mathbf{K}^{-1}\right)^{\alpha}_{.K}\left(\mathbf{K}^{-1}\right)^{\beta}_{.L} Q^I_{.\alpha\beta,M} = 0.\end{aligned} \quad (6.110)$$

One may wonder how this can possibly be rewritten in terms of covariant material derivatives based on the connection with, this time, *both* torsion and

curvature, so that such a formulation reflects in a purely geometric manner the presence of *both* translation *and* rotation dislocations! There is no unique way to do this. However, the framework of path-independent parallelism on the material manifold (cf. Schouten, 1954), in terms of a non-Euclidean connection in a so-called *Einstein-Cartan space* (cf. Choquet-Bruhat, 1968), with both torsion and curvature, may be an interesting avenue, in which case one would expect a generalization of (6.35) in the self-speaking form

$$\mathrm{div}_{\Gamma}\,\bar{\mathbf{b}}^{\mathrm{eff}} = B\big(\bar{\mathbf{b}},\tilde{\mathbf{T}}\big) + F\big(\bar{\mathbf{B}},\mathbf{R}\big), \tag{6.111}$$

where $\Gamma$ denotes a general nonsymmetric non-Euclidean connection, $\mathrm{div}_{\Gamma}$ denotes the covariant divergence based on this connection, and $B$ and $F$ are bilinear forms on their arguments, $\tilde{\mathbf{T}}$ and $\mathbf{R}$ being the torsion and curvature tensors. Here we enter the domain of speculations, which obviously suggests a close analogy with the geometrization of modern theories of gravitation, including spin effects (cf. Heyde and Hehl, 1977), where the last term in (6.111) again is akin to a Mathisson force. The reader will find in the works of Epstein, Elzanowski, De Leon, and Zubov further advances along the geometric line.

## Appendix A6.1: Unification of Three Lines of Research

In this chapter and previous ones we have uncovered the unification of three of the most productive and creative lines of thought developed in continuum mechanics in the second part of the twentieth century, namely, (i) the *finite-strain line* with the concept of multiplicative decomposition of the deformation gradient, (ii) the *geometric line*, whose purpose, inspired by mathematical physics, was to capture anelastic effects via necessarily involved geometric descriptions of the material manifold, and (iii) the *configurational-force line*, which gave rise to the notion of material force (i.e., a covector on the material manifold) following the pioneering works of Peach and Koehler and Eshelby in the 1950s. Here we go over these three lines in some historical digression; the three great historical figures who emerge thus are J. Mandel (1904–1978), E. Kroener (1919–2000), and J.D. Eshelby (1916–1988). Other characters, although important, remain secondary. Indeed, whether this is an objectively correct view or not being another matter, we like to distinguish three lines of originally independent creative developments in continuum mechanics in the period 1950–2000 (the flowchart in Figure 6.1 was already given in Maugin (2003a, 2003b)) and show how these three lines finally recently united in a grand scheme under the umbrella of thermomechanics and how the viewpoints of the main protagonists (Mandel, Kroener, Noll, Eshelby) find their best combined expression in this powerful unity.

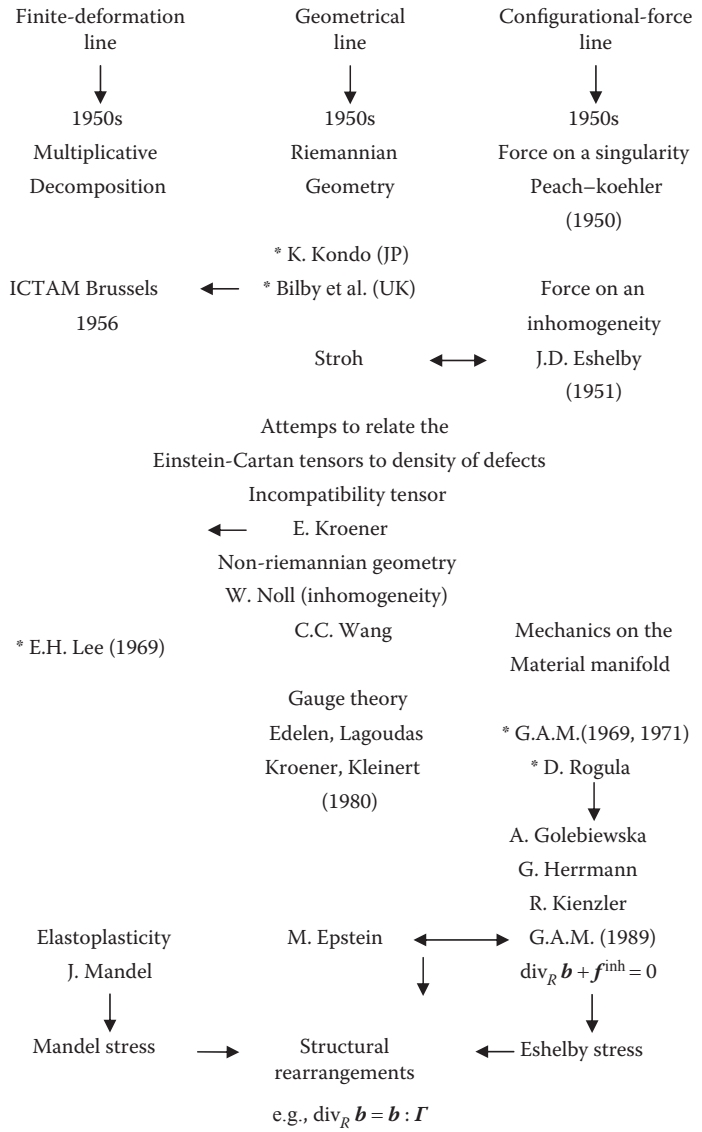


**FIGURE 6.1**
Flowchart showing three converging lines of continuum mechanics. (Adapted from Maugin, G.A., *Zeit. angew. Math. Mech.*, 83: 75–83, 2003a.)

Along the *finite-deformation line* (left column in Figure 6.1), following the natural notion of composition of maps in *analysis*, the main fruitful ingredient was the *multiplicative decomposition* of the deformation gradient into an elastic contribution and an anelastic one (neither of these being integrable into a displacement separately), originally by the U.K. group of Bilby et al. (1957) and

by Kroener and Seeger (1959) and Kroener (1958) in Germany. This may have been anticipated by rheologists (Green and Tobolsky, 1940s) but for exactly integrable members of the decomposition. The geometric line (central column in Figure 6.1) was connected with this initially. But the finite-strain theory of anelasticity stayed dormant until the late 1960s, when this was revived by E.H. Lee (1969) and coworkers, who got most of the credit for it. From our viewpoint, however, definite progress was made by J. Mandel (1971) when the latter showed that what is now referred to as the "Mandel stress" (Lubliner, 1990), expressed in the so-called elastically released or "intermediate" configuration—between the material one and the actual one—is the *driving force* behind anelasticity. The introduction of the "intermediate" configuration is intimately—we should say, *in duality*—related to that of multiplicative decomposition of the finite deformation. Sidoroff (1976) has shown how the richness of the phenomenological description of finite-strain viscoelasticity is enhanced by the decomposition in multiple factors (more than two), introducing thus a series of "intermediate" configurations; so much for this line.

Along the ***geometric line*** (central column in Figure 6.1), we find works by scientists who were greatly influenced by mathematical physics, more particularly the geometric theory of gravitation of A. Einstein, known as the general theory of relativity. Kondo (1952) in Japan was the first to infuse such ideas into continuum mechanics. But the group of Bilby et al. in the United Kingdom, and E. Kroener and A. Seeger in Germany, soon took over this line. In particular, introducing the notion of the *incompatibility tensor* (Kroener, 1955) to describe mathematically the lack of unique determination of the elastic displacement in continuously dislocated bodies, E. Kroener (1958) made a definite step, as he could then relate the density of dislocations (one type of "elastic" defect) and the geometry of the material manifold (nonvanishing curvature). At this point inclusive ideas of T. Levi-Civita and E. Cartan on (geometric) *connections*, *torsion*, and *distant parallelism* entered the scene. This was most forcefully implemented by W. Noll (1967) and C.C. Wang (1967) in landmark papers. But these authors, fruitful and deep as their research was, did not really propose a relationship between a driving force and the geometric background.

The third line (right column in Figure 6.1) is that initially developed by Peach and Koehler (1950) and Eshelby (1951), who established the expression of the *driving force* (*not* a Newtonian force acting per unit of matter) on a singularity line (dislocation line) and a material inhomogeneity, respectively. The celebrated *J*-integral of fracture (force on a crack tip; Rice, 1968) is also such a force. J.D. Eshelby found that this type of "force" is related to the divergence of a peculiar stress tensor, which he identified as the spatial part of what was known as the *energy-momentum tensor* in field theories. This is now referred to as the *Eshelby stress tensor* in honor of this great scientist. However, late in the 1960s, D. Rogula (1977) and G. Maugin (1971)—then relating to studies in general relativistic continuum mechanics—found it convenient to emphasize the duality between projections of the equations of

continuum mechanics, whether in physical space or directly onto the material manifold. It seems that this viewpoint was exported to the United States by A. Golebiewska (1981) in the late 1970s, who initiated a trend followed by G. Herrmann and his coworkers, with efficient applications to the strength of materials of structural members (see the 2000 book by Herrmann and Kienzler). The configurational-force line is also exposed in some detail in Kienzler and Maugin (2001).

Finally, Epstein and Maugin (1990) (also many subsequent papers by these authors, in particular the synthesis works, e.g., Maugin, 1993, 1995), working entirely in material space and exploiting ideas of Noll but pursuing them to a logical end, got the final unifying result: The *Eshelby material stress* is indeed fed by all types of material inhomogeneities and field singularities (defects). This is shown by establishing the material balance law in which the Eshelby stress is the *flux*. This is the fully material balance law missed by Noll and Wang, which represents equilibrium, or dynamics, among all types of inhomogeneities. This establishes the relationship between the geometric and configurational-force lines. Furthermore it happens that the previously mentioned Mandel stress is none other than an easily identified part of the Eshelby stress. All of this they achieved by exploiting the notion of the *uniformity-inhomogeneity map*, or *material transplant* (with a biophysical connotation), or, in yet other words, *local structural rearrangement.*

# 7

# *Discontinuities and Eshelby Stress*

## Object of the Chapter

Where we see how deep was the insight of Gibbs, Duhem, and Hugoniot when they imagined the propagation of large classes of mobile thin zones of rapidly varying fields, and how the Maxwell-Hadamard vision of discontinuity surfaces and Eshelby's ideas of driving force fit in their pioneering views and allow now for a satisfactory approach, analytical and numerical, to the propagation of many physical phenomena involving evolving transition zones, in particular shock waves, phase-transition fronts, and grain boundaries.

## 7.1 Introduction

In many physical situations fields are not as regular as they were supposed to be in the foregoing chapters. In particular, there are often regions of very small extent, that is, thickness (compared to a standard macroscopic length scale such as the overall size of a material body), through which fields suffer very strong gradients, sometimes in relation to a dissipative process (heat conduction, viscosity, plasticity, damage), and this region of mathematically vanishing thickness may be moving under the influence of the environment (differing field solutions on both of its sides). This is what occurs in the observed motion of shock waves and phase-transition fronts, two classes of phenomena related to an increase of entropy because of their irreversible nature. To deal with these we need the set of equations satisfied by the fields at the crossing of these thin zones, or the set of *jump conditions* imposed on these fields when the mathematical idealization of a zero-thickness surface is accepted. An interesting question is the following one. First, if irreversibility is involved, then the jump associated with the entropy equation will of necessity play an important role as it will select the direction in which the singular surface can move in order to respect the second law of thermodynamics. In a different line of thought, the presence of a surface across

which the fields may suffer an irreversible jump to the point that matter on both sides may be considered in two different phases (the case of a phase-transformation front), or altogether so much altered, is an obvious sign of a loss of translational invariance of material properties at the crossing of the discontinuity. Accordingly, the theory of material or configurational forces must also be involved as, in the spirit of dalembertian mechanics, a force of some kind—a *driving force*—must be associated with the motion of the set of points represented by the singular surface, for we see by any means the singular surface move. Although not forbidden, this view is seldom adopted in the classical theory of shock waves, but it comes out naturally in the theory of the propagation of phase-transformation fronts. We shall illustrate this in this chapter, after a general introduction to jump equations in both spatial and material frameworks, and a first approach to the question of the involvement of the Eshelby stress in the simple case of the quasistatics of elasticity.

This goes as follows after Kostrov and Nikitin (1970), Dems and Mroz (1985), and Maugin and Trimarco (1995a). Let the sufficiently regular surface $\Sigma$ separate a nonlinear elastic body of material volume $B_R$ into two regions, $B_R^+$ and $B_R^-$. Let $\mathbf{N}$ be the unit normal to $\Sigma$ oriented from the latter to the former. Let

$$[A] = A^+ - A^- \tag{7.1}$$

denote the finite jump of the quantity $A$, $A^\pm$ being the uniform limits of $A$ in approaching $\Sigma$ along its normal on both sides of $\Sigma$. We consider the material and Eulerian variations already introduced in Chapter 3. These two are related by

$$\delta_X \chi + \mathbf{F}.\delta_x \chi^{-1} = 0 \tag{7.2}$$

at all regular material points. To generate the looked-for equations we consider the following *principle of potential energy* (here we note $B_R$ as $B$ to simplify the notation):

$$\delta\Phi = -\delta_X \int_B W(\mathbf{F}) dV + \int_{\partial B} \overline{\mathbf{T}}^{\mathrm{d}}.\delta_X \chi dA, \tag{7.3}$$

where, indeed (the interface $\Sigma$ is assumed to carry no potential energy of its own),

$$\int_B W(\mathbf{F}) dV = \int_{B^+} W^+(\mathbf{F}) dV + \int_{B^-} W^-(\mathbf{F}) dV, \tag{7.4}$$

where $W+$ and $W^-$ are the elastic energy densities per unit volume of the reference configuration for two essentially different anisotropic but homogeneous elastic materials. Noting $\mathrm{N}_\Sigma = \mathrm{N}^- = -\mathrm{N}+$, a transport theorem yields

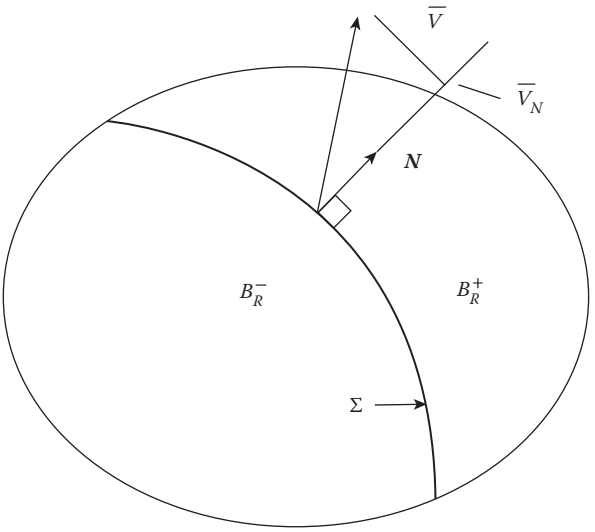


**FIGURE 7.1**
The discontinuity surface Σ in the reference configuration.

$$\delta_X \int_{B^\pm} W^\pm(\mathbf{F}) dV = \int_{B^\pm \text{ fixed}} \delta_X W^\pm dV - \int_{\Sigma^\pm} \left(\mathbf{N}^\pm . \delta_x \mathbf{X}^\pm\right) W^\pm d\Sigma, \tag{7.5}$$

so that

$$\delta_X \int_B W(\mathbf{F}) dV = \int_B \delta_X W(\mathbf{F}) dV + \int_\Sigma \mathbf{N}_\Sigma . \left[W \delta_x \chi^{-1}\right] d\Sigma. \tag{7.6}$$

But in computing the first contribution in the right-hand side of this equation, we obtain

$$\begin{aligned} &\int_B \delta_X W^\pm(\mathbf{F}) dV \\ &= -\int_{B-\Sigma} \left(\text{div}_R \mathbf{T}\right) \cdot \delta_X \chi dV + \int_{\partial B - \Sigma} \left(\mathbf{N} \cdot \mathbf{T}\right) . \delta_X \chi dV + \int_\Sigma \mathbf{N}_\Sigma \cdot \left[\mathbf{T} \cdot \delta_X \chi\right] d\Sigma, \end{aligned} \tag{7.7}$$

where the jump term comes from the application of the divergence theorem in both parts and the gluing back of the two resulting results. From this being valid for any volume and surface element, the classical equilibrium equations read

$$\text{div}_R \mathbf{T}^\pm = \mathbf{0} \quad \text{in} \quad B^\pm, \quad \mathbf{T}^\pm = \partial W^\pm / \mathbf{F}, \tag{7.8}$$

$$\mathbf{N}.\mathbf{T} = \bar{\mathbf{T}}^d \quad \text{at} \quad \partial B - \Sigma, \quad \mathbf{N}.\big[\mathbf{T}\big] = \mathbf{0} \quad \text{across} \quad \Sigma. \tag{7.9}$$

Collecting the remaining contributions we have

$$\delta\Phi = -\int_{\Sigma} \mathbf{N}_{\Sigma}.\big[W\delta_x\chi^{-1} + \mathbf{T}.\delta_X\chi\big]d\Sigma. \tag{7.10}$$

At this point we follow Hill (1986) by selecting the virtual variations in direct and inverse motions in the most realistic way. We cannot control the *direct* motion, which, therefore, can suffer a jump in its first variation. But the situation is different for the inverse motion because, in the absence of defects at $\Sigma$, we have continuity in the displacement, hence we assume continuity of the variation $\delta_x X$. Accordingly, (7.2) renders

$$\big[\delta_X\chi\big] = -\big[\mathbf{F}\big].\delta_x\mathbf{X}. \tag{7.11}$$

On account of the last of (7.9) and of the definition and demonstrable relation,

$$\langle A\rangle := \frac{1}{2}(A^+ + A^-), \tag{7.12}$$

$$[AB] \equiv \langle A\rangle[B] + [A]\langle B\rangle, \tag{7.13}$$

we finally obtain that

$$\delta\Phi = \int_{\Sigma} \mathbf{f}_{\Sigma}.\delta_x\mathbf{X}\,d\Sigma, \tag{7.14}$$

where

$$\mathbf{f}_{\Sigma} := -\mathbf{N}_{\Sigma}.\big[W(\mathbf{F})\mathbf{1}_R - \langle\mathbf{T}\rangle.\mathbf{F}\big]. \tag{7.15}$$

By duality with the inverse-motion variation, this is a *material force* per unit area of $\Sigma$. If potential energy is conserved (no dissipation), then

$$\mathrm{f}_{\Sigma} = 0 \quad \text{at} \quad \Sigma. \tag{7.16}$$

If a potential energy localized at $\Sigma$ exists (e.g., $\Sigma$ constitutes a *third body* of infinitesimal thickness), then a surface energy term must be added in the right-hand side of (7.4). This can be handled with the notion of *surface distribution* (introducing a *delta function* with compact support on $\Sigma$); as a consequence (7.16) will contain a source term akin to *surface tension* for a nonflat interface $\Sigma$.

**REMARK 7.1:** Notice that the quasistatic hypothesis (neglect of inertia) has played a role in the special writing of the expression of $\mathbf{f}_\Sigma$. A more general form is given later on in the fully dynamic case.

## 7.2 General Jump Conditions at a Moving Discontinuity Surface

### 7.2.1 Equations in the Cauchy Format in the Actual Configuration

Two basic theorems are needed for a global approach to the balance laws of a continuum in the presence of a discontinuity surface; one is a generalization of the Green–Gauss theorem and the other is related to transport.

**Generalized Green–Gauss Theorem**

If the field A suffers a finite discontinuity at the discontinuity surface σ, then there holds the following result:

$$\int_B \nabla.\mathbf{A}dv = \int_{\partial B-\sigma} \mathbf{n}.\mathbf{A}da - \int_{\sigma(t))} \mathbf{n}.[\mathbf{A}]d\sigma, \tag{7.17}$$

where $\mathbf{n}$ is the unit oriented normal to the sufficiently regular spatial surface $\sigma(t)$.

The proof consists in considering the two domains on both sides of the surface, applying the regular Green–Gauss theorem to each of these, and gluing back the two parts while noting that the unit normals of the two parts at the discontinuity surface are in opposite directions.

**Generalized Transport (Reynolds) Theorem**

If the field $\phi$ suffers a finite discontinuity at the discontinuity surface $\sigma(t)$ moving with its proper velocity field $v(\mathbf{x}, t)$ in the configuration $K_t$, then there holds the following result:

$$\frac{d}{dt}\int_{B-\sigma} \phi dv = \int_{B-\sigma}\left(\left.\frac{\partial\phi}{\partial t}\right|_x + \nabla.(\mathbf{v}\phi)\right)dv + \int_\Sigma \mathbf{n}.[(\mathbf{v}-v)\phi]d\sigma, \tag{7.18}$$

with the same sign convention as above.

Again the proof is carried out by the same technique of separating the two domains on both sides of σ, applying the "regular" transport theorem to each part, and gluing back the two parts. Of course, the proper velocity v(x, *t*) is continuous, but it generally depends on the point $\mathbf{x}$ of σ.

**Application of these Theorems to the Basic Conservation Laws of Continuum Thermomechanics**

On applying the results in (7.17) and (7.18) to the balance laws (2.64) through (2.68) in the presence of a self-moving spatial discontinuity surface $\sigma(\mathbf{x}, t)$, we obtain the equations at regular points such as (2.80) through (2.85) and, at $\sigma(\mathbf{x}, t)$—not to be mistaken for the Cauchy stress—the following set of jump equations:

$$\mathbf{n}.\left[\rho\left(\mathbf{v}-\nu\right)\right]=0, \tag{7.19}$$

$$\mathbf{n}.\left[\rho\left(\mathbf{v}-\nu\right)\otimes\mathbf{v}-\sigma\right]=\mathbf{0}, \tag{7.20}$$

$$\mathbf{n}.\left[\rho\left(\mathbf{v}-\nu\right)\left(e+\mathbf{v}^2/2\right)-\sigma.\mathbf{v}+\mathbf{q}\right]=0, \tag{7.21}$$

$$\mathbf{n}.\left[\rho\left(\mathbf{v}-\nu\right)\eta-\mathbf{s}\right]=S_\sigma\geq 0, \tag{7.22}$$

where $e$ is the internal energy per unit mass and $S_\sigma$ is the (unknown) non-negative entropy source at $\sigma$. In most cases, $s = q/\theta$. We note the role played by the relative spatial velocity $(\mathbf{v} - \nu)$ and also that of the mass flux

$$m_\sigma := \rho\,\mathbf{n}.\left(\mathbf{v}-\nu\right), \tag{7.23}$$

which is continuous at $\sigma$ according to Equation 7.19: $[m_\sigma] \equiv 0$. Equations 7.19 through 7.22 are sometimes called the *Rankine–Hugoniot–Kotchine equations*. It is of interest, exploiting the continuity of $m\sigma$, to establish the so-called *Hugoniot equation* of shock-wave fame. For that purpose we note that (7.21) reads

$$m_\sigma\left[e+\mathbf{v}^2/2\right]-\left[\mathbf{n}.\sigma.\mathbf{v}-\mathbf{n}.\mathbf{q}\right]=0. \tag{7.24}$$

But on taking the inner product of (7.20) by the mean value $\langle\nu\rangle$ and combining with (7.24) on account of (7.13), we obtain

$$m_\sigma\left[e-m_\sigma^{-1}\left\langle\mathbf{n}.\sigma\right\rangle.\mathbf{v}\right]+\left[\mathbf{n}.\mathbf{q}\right]=0. \tag{7.25}$$

We let the reader show that for a *non-heat-conducting perfect fluid*, this delivers the simple and celebrated *Hugoniot relation*:

$$\left[e+\left\langle p\right\rangle\tau\right]=0, \tag{7.26}$$

where $p$ is the thermodynamic pressure, and $\tau = \rho^{-1}$ is the specific volume.

### 7.2.2 Equations in the Piola–Kirchhoff Format

In that case we start with the statements (2.74) through (2.77) of the basic thermomechanical balance laws but in the presence of a regular discontinuity

surface $\Sigma(\mathbf{X},t)$, image of $\sigma(\mathbf{x},t)$ back in $K_R$. The theorems (7.17) and (7.18) are shown to take on the following form:

$$\int_{B_R} \nabla_R . \mathbf{A} dV = \int_{\partial B_R - \Sigma} \mathbf{N}.\mathbf{A} dS + \int_{\Sigma} \mathbf{N}.[\mathbf{A}] d\Sigma \tag{7.27}$$

and

$$\frac{d}{dt}\int_{B_R-\Sigma} \phi dV = \int_{B_R-\Sigma} \left.\frac{\partial \phi}{\partial t}\right|_X dV - \int_{\Sigma} \bar{V}_N[\phi] d\Sigma, \tag{7.28}$$

where

$$\bar{V}_N \equiv \mathbf{N}.\bar{\mathbf{V}}, \tag{7.29}$$

if $\bar{\mathbf{V}}$ is the material velocity field (a material contravector) of the surface $\Sigma$.

On applying (7.27) and (7.28) to the basic balance laws (2.74) through (2.77), we obtain (2.86) through (2.90) at regular material points and, at $\Sigma$, the following set of jump equations:

$$\bar{V}_N[\rho_0] = 0, \tag{7.30}$$

$$\bar{V}_N[\mathbf{p}_R] + \mathbf{N}.[\mathbf{T}] = \mathbf{0}, \tag{7.31}$$

$$\bar{V}_N[H_R] + \mathbf{N}.[\mathbf{T}.\mathbf{v} - \mathbf{Q}] = 0, \tag{7.32}$$

$$\bar{V}_N[S_R] - \mathbf{N}.[\mathbf{S}] = \sigma_\Sigma \geq 0, \tag{7.33}$$

assuming there are no body forces. We can also remark that, with this hypothesis, Equations 2.86, 2.87, and 2.89 become strict conservation equations in the Piola–Kirchhoff format. Correspondingly, the three associated jump conditions (7.30) through (7.32) are homogeneous (vanishing right-hand side). This is not the case for the entropy condition (7.33), where there remains the possibility of a nonnegative entropy source at $\Sigma$ when the latter is "dissipative." What about the jump condition associated with the canonical equation of momentum and other equations that may be associated with the energy equation? We have shown that in a sufficiently general framework, a consistent system of canonical equations of material momentum and energy reads (in the absence of body force; cf. (5.14) and (5.19))

$$\frac{d\mathbf{P}}{dt} - \mathrm{div}_R \mathbf{b} = \mathbf{f}^{\mathrm{int}} + \mathbf{f}^{\mathrm{inh}}, \quad \frac{d(S\theta)}{dt} + \nabla_R.\mathbf{Q} = h^{\mathrm{int}}, \tag{7.34}$$

at any regular material point **X**. At this point, noting that these two equations are *not* the results of the direct localization of global balance laws (contrary to what is supposed by some for the first equation; see Appendix A5.2) and that (7.30) through (7.33) can also be written down directly from their bulk analogues by using a rule of thumb that consists in replacing formally the operators $\partial/\partial t|_x$ and $\nabla_R$ by the operators $-\bar{V}_N$ and N.[..], respectively (a rule that applies directly to conservative hyperbolic systems), then we could use the same rule for the two parts of (7.35) for their left-hand side and assuming that unknown source terms will appear at the surface. With such a pragmatic rule we obtain the following two jump equations associated with the canonical conservation laws of momentum and energy:

$$\bar{V}_N\left[\mathbf{P}\right]+\mathbf{N}.\left[\mathbf{b}\right]=-\mathbf{f}_\Sigma, \tag{7.35}$$

and

$$\bar{V}_N\left[S\theta\right]-\mathbf{N}.\left[\mathbf{Q}\right]=h_\Sigma, \tag{7.36}$$

where the three quantities $\mathbf{f}\Sigma$, $h_\Sigma$, and $\sigma_\Sigma$ have to be estimated consistently. Of course, in physical reality these correspond to integrated source terms throughout the thickness of a transition zone that is not mathematically of zero thickness (i.e., the discontinuity possesses a structure; such is the case of shock waves that exist only because of dissipation occurring through such a transition region). That is, we could have been less brutal than simply writing (7.35) and (7.36). Indeed, if (7.34) are valid at regular material points, then we can integrate them over a regular material region, yielding thus

$$\frac{d}{dt}\int_{B_R}\mathbf{P}\,dV=\int_{\partial B_R}\mathbf{N}.\mathbf{b}\,dA+\int_{B_R}\left(\mathbf{f}^{\text{int}}+\mathbf{f}^{\text{inh}}\right)dV, \tag{7.37}$$

and

$$\frac{d}{dt}\int_{B_R}\left(S\theta\right)dV=-\int_{\partial B_R}\mathbf{N}.\mathbf{Q}\,dA+\int_{B_R}h^{\text{int}}dV. \tag{7.38}$$

If we apply this to a box (the so-called "pill-box" method) that overlaps a piece of small extent (considered as flat without loss of generality; "the flea sees a flat surface locally") of thickness $\delta$ and plane coordinates $X_2$ and $X_3$, as we squeeze the box to the local surface of $\Sigma$, with nothing occurring at the two lateral ends, (7.37) and (7.38) will provide the following limit conditions per unit area of $\Sigma$:

$$-\bar{V}_N\left[\mathbf{P}\right]=\left[\mathbf{N}.\mathbf{b}\right]+\lim\int_{-\delta/2}^{+\delta/2}\left(\mathbf{f}^{\text{int}}+\mathbf{f}^{\text{inh}}\right)dX_1\quad\text{as}\quad\delta\to 0, \tag{7.39}$$

and

$$-\bar{V}_N\left[S\theta\right] = -\mathbf{N}.\left[\mathbf{Q}\right] - \lim \int_{-\delta/2}^{+\delta/2} h^{\text{int}} dX_1 \quad \text{as} \quad \delta \to 0. \tag{7.40}$$

With singular integrands in the last two expressions in (7.39) and (7.40), we obtain jump relations of the form (7.35) and (7.36). Note that a similar proof holds for the first part of (7.34). Such a reasoning was suggested by Mandel (1966, pp. 268–269) for the entropy inequality, that is, in parallel with (7.39) and (7.40),

$$\bar{V}_N\left[S\right] - \mathbf{N}.\left[\mathbf{Q}/\theta\right] = \lim \int_{-\delta/2}^{+\delta/2} \left(\sigma^{\text{th}} + \sigma^{\text{intr}}\right) dX_1 \geq 0 \quad \text{as} \quad \delta \to 0. \tag{7.41}$$

## 7.3 Thermomechanical Shock Waves

In this case we can keep as large a framework as possible, including the dependence on internal variables of state (cf. Chapter 5) and therefore treat the general case of thermo-anelasticity, since the presence of $\alpha$ (without gradients) does not formally alter the presentation. The jump relations (7.31) through (7.34) constitute the general point of departure. However, if we kept the idea of a transition zone of small but finite thickness from one side of $\Sigma$ to the other, then the source quantities in (7.34), (7.36), and (7.37) would be known in terms of *excess quantities* computed throughout the thickness of the transition zone.

This approach, which can be conceived as a zoom on the front, shows the remarkable role played by thermal and intrinsic entropy sources in the condition of entropy growth at $\Sigma$ and the parallel role of the material forces $\mathbf{f}^{\text{th}}$ and $\mathbf{f}^{\text{int}}$ in writing the jump of the balance of material momentum at $\Sigma$. While equations such as (7.41) are suggested by Mandel (1966) and considered by some authors (Stolz, 1989, 1994), Equations 7.39 and 7.40 are quite recent (Maugin, 1998b, 1998c). The consistency between the source terms in these equations provides the connection between entropy growth at $\Sigma$ and the power expended by the material driving forces, even in the general theory of shock waves where the notion of driving force was heretofore ignored. But we shall consider the purely jumplike description, bearing (7.39) through (7.41) in mind as some "microscopic" justification. We then define the following scalar and vectorial quantities at $\Sigma$ (such quantities are meaningful in themselves only if they are invariant across $\Sigma$; otherwise, they become mathematically meaningful only once an operator such as [.] or $< . >$, attached to

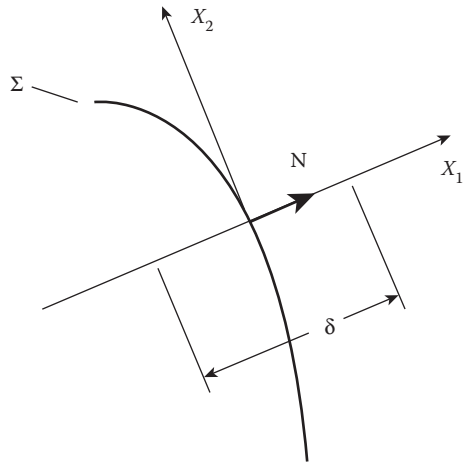


**FIGURE 7.2**
The singular surface Σ as the limit of a transition zone of thickness δ.

Σ, is applied to them. We learned this technique from A. Lichnerowicz [1976] in his studies of shock waves in relativistic fluids.):

$$m_\Sigma := \rho_0 \bar{V}_N, \tag{7.42}$$

$$T_\Sigma := m_\Sigma \mathbf{v} + \mathbf{N}.\mathbf{T}, \tag{7.43}$$

$$m_\Sigma Q_\Sigma := m_\Sigma \bar{H} + \mathbf{N}.\left(\mathbf{T}.\mathbf{v} - \mathbf{Q}\right), \tag{7.44}$$

$$B_\Sigma := m_\Sigma \bar{\mathbf{P}} + \mathbf{N}.\mathbf{b}, \tag{7.45}$$

$$m_\Sigma N_\Sigma := m_\Sigma \bar{S} - \left(\mathbf{N}.\mathbf{Q}/\theta\right), \tag{7.46}$$

where, apart from $\bar{V}_N$, quantities with overbars are per unit mass in the reference configuration $K_R$. On account of these definitions, the jump relations (7.31) through (7.34) and (7.36) now read

$$\left[m_\Sigma\right] = 0, \quad \left[T_\Sigma\right] = \mathbf{0}, \quad m_\Sigma\left[Q_\Sigma\right] = 0 \tag{7.47}$$

and

$$m_\Sigma\left[N_\Sigma\right] = \sigma_\Sigma \geq 0, \quad \left[B_\Sigma\right] + \mathbf{f}_\Sigma = \mathbf{0}. \tag{7.48}$$

This is merely a rewriting, but it allows us to perform some simple manipulations and to express some remarkable results in an attractive manner. Define

$$\bar{L}^{\text{th}} = L^{\text{th}}/\rho_0 = \tilde{L}^{\text{th}}\left(\mathbf{F},\mathbf{v},\theta,\alpha\right). \tag{7.49}$$

Then it is proved that the entropy source at $\Sigma$ is given by the following linear weighted combination (Maugin, 1997):

$$\sigma_\Sigma = m_\Sigma\left[\bar{L}^{\text{th}}/\theta\right] + m_\Sigma Q_\Sigma\left[\theta^{-1}\right] - T_\Sigma.\left[\mathbf{v}/\theta\right] \geq 0. \tag{7.50}$$

The proof of this is carried out by direct computation. Guided by this, we introduce the following *generating* or *Massieu* function $M_\Sigma$ at $\Sigma$ by

$$M_\Sigma := \theta^{-1}\left(m_\Sigma\left(Q_\Sigma + \bar{L}^{\text{th}}\right) - T_\Sigma.\mathbf{v}\right), \tag{7.51}$$

Then we prove the following two results (Maugin, 1997):

$$\sigma_\Sigma = \left[M_\Sigma\right] \geq 0 \tag{7.52}$$

and

$$p_\Sigma := \bar{\mathbf{V}}.\mathbf{f}_\Sigma = \left[\theta M_\Sigma\right]. \tag{7.53}$$

That is, the generating function $M\Sigma$—a notion already used in hydrodynamics and magnetohydrodynamics by Germain (1972) in shock-wave studies—provides *both* the entropy source and the power of the driving force at $\Sigma$, although we do not know yet the explicit form of the latter. From (7.52) and (7.53) there follows the following general relationship between $p_\Sigma$, $\sigma_\Sigma$, and the jump in temperature for a general shock wave relating two regions where adiabaticity is *not* supposed:

$$p_\Sigma = \sigma_\Sigma\langle\theta\rangle + \langle M_\Sigma - \left(m_\Sigma Q_\Sigma/\theta\right)\rangle\left[\theta\right]. \tag{7.54}$$

The proof of results (7.52) through (7.54) is as follows. On the one hand, we compute the power expended by $\mathbf{f}_\Sigma$ by

$$p_\Sigma = \mathbf{f}_\Sigma.\bar{\mathbf{V}} = -\left[m_\Sigma\bar{\mathbf{P}} + \mathbf{N}.\mathbf{b}\right].\bar{\mathbf{V}} = -\left(m_\Sigma\left[\mathbf{v}^2\right] + \left[\mathbf{N}.\mathbf{b}.\mathbf{V}\right]\right) \tag{a}$$

because $\mathbf{V} = \bar{\mathbf{V}}$ at $\Sigma$ and $\bar{\mathbf{P}}.\mathbf{V} = \mathbf{v}^2$ in general. On using the definition of $M_\Sigma$, we can also write this as

$$p_\Sigma = \left[C\theta\right], \quad C := \theta^{-1}\left(m_\Sigma \bar{L}^{\text{th}} - T_\Sigma.\mathbf{v}\right) = M_\Sigma - m_\Sigma Q_\Sigma/\theta. \tag{b}$$

Consequently,

$$p_\Sigma = \left[M_\Sigma\theta\right] - \left[\theta\left(m_\Sigma Q_\Sigma/\theta\right)\right] = \left[\theta M_\Sigma\right] \qquad q.e.d. \tag{c}$$

The result (7.54) follows using the relation (7.50).

**REMARK 7.2:** From the preceding we also obtain that for a discontinuity surface relating *dissipatively* two regions where the working hypothesis of *adiabaticity* holds good (a classical approximation)

$$\sigma_\Sigma = \langle\theta\rangle^{-1}\left\{p_\Sigma + \left\langle \frac{m_\Sigma}{\theta}\left(\frac{1}{2}\mathbf{v}^2 + \bar{W}\right) - \frac{1}{\theta}\mathbf{N}.\mathbf{T}.\mathbf{v}\right\rangle\left[\theta\right]\right\} \geq 0. \tag{d}$$

This follows from the fact that (b) also reads

$$p_\Sigma = \sigma_\Sigma\langle\theta\rangle + \left\langle \frac{m_\Sigma}{\theta}\left(\frac{1}{2}\mathbf{v}^2 - \bar{W}\right) - \frac{1}{\theta}T_\Sigma.\mathbf{v}\right\rangle\left[\theta\right]. \tag{e}$$

But, at $\Sigma$, we check that

$$T_\Sigma.\mathbf{v} = m_\Sigma\mathbf{v}^2 + \mathbf{N}.\mathbf{T}.\mathbf{v}, \quad \left[\mathbf{N}.\mathbf{T}.\mathbf{v}\right] = -\left[m_\Sigma\bar{H}\right], \tag{f}$$

from which (d) follows as a consequence. Here $\bar{W}$ and $\bar{H}$ are the free energy and total (kinetic + internal) energy per unit mass.

Returning to the general case (7.52) and (7.53), for a *homothermal* discontinuity ($[\theta] = 0$ at $\Sigma$), (7.53) provides the reduction

$$p_\Sigma = \theta_\Sigma\left[M_\Sigma\right] = \theta_\Sigma\sigma_\Sigma \geq 0, \tag{7.55}$$

where $\theta_\Sigma$ is the continuous temperature at $\Sigma$. Otherwise, we have at hand a *consistent theory of shock waves* because, contrary to the simple theory in which the shock relates two regions in *adiabatic* situations, we here relate two regions in which dissipation of both thermal and intrinsic origins is taken into account so that we have a justification for the existence of $\sigma_\Sigma$ in which the nonnegativity is not imposed out of the blue. What about the celebrated *Hugoniot* equation of *classical* shock-wave theory (in which there

is neither heat flux nor the variable $\alpha$ present)? This is normally obtained by expanding the following identity on account of other (classical) jump relations:

$$\left[T_\Sigma\right].\langle \mathbf{v}\rangle \equiv 0, \tag{7.56}$$

and combining with the jump of the energy equation (in the absence of heat conduction), resulting in the *Hugoniot equation* for nonlinear elasticity (cf. Duvaut, 1964):

$$\mathrm{Hugo}_{\mathrm{SW}} := \left[E(\mathbf{F},S,\alpha) - \langle \mathbf{N}.\mathbf{T}\rangle.\mathbf{F}.\mathbf{N}\right] \equiv 0 \quad \text{at} \quad \Sigma, \tag{7.57}$$

where it is the *internal energy E* per unit reference volume that is involved.

The proof of (7.57) goes as follows. According to the well-known classification of singular surfaces by Hadamard (cf. Truesdell and Toupin, 1960; Truesdell, 1961), a shock wave in elasticity is a first-order singular surface $\Sigma$ across which the first-order derivatives of the direct motion $\chi(\mathbf{X},t)$, that is, $\mathbf{v}$ and $\mathbf{F}$, suffer a finite discontinuity jump. According to the Maxwell–Hadamard compatibility jump equations, we have thus at $\Sigma$:

$$\left[\mathbf{F}\right] = \mathbf{f} \otimes \mathbf{N}, \quad \mathbf{f} := \left[\mathbf{N}.\nabla_R \chi\right] = \left[\partial \chi / \partial N\right], \tag{7.58}$$

and

$$\left[\mathbf{v}\right] = -\bar{V}_N \mathbf{f}. \tag{7.59}$$

Expanding the identity (7.56), after a short computation, one gets

$$m_\Sigma\left[\mathbf{v}^2/2\right] + \left[\mathbf{N}.\mathbf{T}.\mathbf{v}\right] + \langle \mathbf{N}.\mathbf{T}\rangle\left[\mathbf{F}.\mathbf{N}\right]\bar{V}_N \equiv 0. \tag{7.60}$$

On combining this with the last of (7.47) and assuming that the wave front indeed propagates (i.e., $\bar{V}_N \neq 0$) we obtain (7.57). Simultaneously, $\mathbf{N}.\mathbf{Q}$ no longer appears in (7.46) so that the first part of (7.48) reduces to

$$m_\Sigma\left[\bar{S}\right] \geq 0, \tag{7.61}$$

Thus *adiabaticity* in the regular material regions on both sides of $\Sigma$ is not translated into *isentropy* across $\Sigma$: The entropy density, if it changes at all, necessarily grows. This, legitimately, leads to comparison of the thermodynamic transition through the shock with an isentropic one (see Maugin et al., 1992, pp. 171–173). This is achieved by introducing the Hugoniot function.

The scalar quantity $\text{Hugo}_{\text{SW}}$ defined in (7.57) is in fact a *functional* since it depends on values at two limit points. It may be considered a thermodynamic force (having the physical dimension of a surface traction or a volume energy) for all practical purposes. The thermodynamic constraint (7.57) relates the two states on both sides of the shock and is subjected to the additional constraint (7.61). We still have the validity of the general relation in (7.52). The present framework shows that the following force power vanishes identically:

$$p\left(\text{Hugo}_{\text{SW}}\right) = \text{Hugo}_{\text{SW}}.\bar{V}_N = 0. \tag{7.62}$$

If $\text{Hugo}_{\text{SW}}$ is interpreted as the driving force of the shock, then this force has the property to be identically zero, and a fortiori, to expend no power by the very definition of the shock wave contemplated here. However, the evolution of the shock front may be accompanied by an entropy growth in spite of this! There is here some kind of apparent logical contradiction that stems from the neglect of intrinsic and thermal dissipations through the shock structure. Indeed, imagine now that these dissipations are no longer neglected and we logically account for the fact that gradients of temperature and internal variables of state take place through the finite thickness $\delta$ of the zone front. These gradients take infinite values when $\delta$ tends toward zero, so that $\Sigma$ is indeed singular from the point of view of both dissipation and the balance of material momentum. The general approach given in the preceding does account for this.

## 7.4 Thermal Conditions at Interfaces in Thermoelastic Composites

Now we can revisit the problem of interfaces in composites—mentioned in Section 3.6—but with thermal effects taken into account (cf. Maugin et al., 1999). As there already exists a nonzero *thermal material force* at all regular material points in the bulk of a thermoelastic material, it is quite normal that such a notion a fortiori exists at the crossing of an interface between two composite components having different thermoelastic properties. We shall again call such a *surface material thermal force* $\mathbf{f}_\Sigma$ when it exists at the junction of two thermoelastic conductors. From the viewpoint of mechanics we assume *perfect* matching between the two components so that we have

$$\left[\mathbf{X}\right] = \mathbf{0}, \quad \left[\mathbf{V}\right] = \mathbf{0} \quad \text{at} \quad \Sigma. \tag{7.63}$$

This supposes that we have neither dislocations nor delamination present at Σ. A variety of interface thermal conditions can be applied at Σ. We may have *perfect thermal contact*,

$$\left[\theta\right] = 0 \quad \text{at} \quad \Sigma, \tag{7.64}$$

or we can impose a heat source per unit area, $q\Sigma$, for instance, via Joule heating of a very thin layer of electric conductor sandwiched between the two components, or further, we may consider a kind of mixed *adiabatic–isentropic* conditions:

$$\mathbf{N}.\mathbf{Q}^{\pm} = 0 \Rightarrow \mathbf{N}.\left[\mathbf{Q}\right] \equiv 0, \quad \left[S\right] = 0 \quad \text{at} \quad \Sigma. \tag{7.65}$$

A temperature difference

$$\vartheta = \left[\theta\right] \tag{7.66}$$

could be imposed by some kind of *thermocouple.* In any case we assume that there generally exist a heat source $q_\Sigma$ and an entropy source $\sigma\Sigma$ in such a way that the jump relations for energy and entropy at Σ read (quasistatics is sufficient for our purpose)

$$\mathbf{N}.\left[E\bar{\mathbf{V}} + \mathbf{T}.\mathbf{v} - \mathbf{Q}\right] + q_\Sigma = 0 \tag{7.67}$$

and

$$\mathbf{N}.\left[S\bar{\mathbf{V}} - \left(\mathbf{Q}/\theta\right)\right] = \sigma_\Sigma \geq 0. \tag{7.68}$$

The corresponding jump of the (quasistatic) balance of material momentum then yields

$$\mathbf{N}.\left[\mathbf{b}\right] + \mathbf{f}_\Sigma = \mathbf{0}, \tag{7.69}$$

while (7.37) reads

$$\mathbf{N}.\left[S\theta\bar{\mathbf{V}} - \mathbf{Q}\right] = h_\Sigma, \tag{7.70}$$

where we emphasize that we do *not* know the expression of $\mathbf{f}_\Sigma$. The *inhomogeneous* Equations 7.69 and 7.70 must be consistent with the statements (7.67) and (7.68). If the perfect thermal matching prevails (7.64), then θ factorizes

out in (7.68) and (7.70), and compatibility between the resulting equations and (7.68) and (7.70) imposes that the internal heat source at $\Sigma$ be necessarily hot (or zero), since then

$$h_\Sigma = \theta_\Sigma \sigma_\Sigma \geq 0. \tag{7.71}$$

But Equation 7.69 must also be consistent. This is implemented by computing the power expended by the "force" $\mathbf{f}_\Sigma$ in a motion of material velocity $\bar{\mathbf{V}}$ such as in an oscillatory motion (at low frequency to respect the quasistatics hypothesis, or else a virtual velocity field). On account of the reduced mechanical matching condition $\mathbf{N}.[\mathbf{T}] = \mathbf{0}$, we obtain thus

$$p_\Sigma = \mathbf{f}_\Sigma . \bar{\mathbf{V}} = -\mathbf{N}.[\mathbf{b}].\bar{\mathbf{V}} = \theta_\Sigma [S] \bar{V}_N + q_\Sigma . \tag{7.72}$$

From this we obtain $\left(\bar{V}_N \neq 0, \quad q_\Sigma = 0\right)$

$$\mathbf{f}_\Sigma = \theta [S] \mathbf{N}. \tag{7.73}$$

In that case we see that the purely normal but *fictitious* thermal surface force is determined by the entropy source and is directed in the direction of entropy growth.

In the case where conditions such as those in (7.65) prevail, then a similar computation yields the dual formula compatible with (7.37):

$$p_\Sigma \equiv h_\Sigma = \mathbf{f}_\Sigma . \bar{\mathbf{V}} = S[\theta] \bar{V}_N , \tag{7.74}$$

so that the thermal driving force at the interface is given by

$$\mathbf{f}_\Sigma = \mathbf{f}_\Sigma^{\text{th}} := S[\theta] \mathbf{N}. \tag{7.75}$$

This "force" is purely normal and directed *from the colder to the warmer face of the interface*. Clearly, this is a limit case of the expression of the bulk thermal material force exhibited in Chapter 5 (cf. (5.25)). To see this, one could sum the total thermal force (5.25) across a unit area of a layer of infinitesimally small thickness across which $S$ is practically constant and then one flattens the layer to the zero-thickness interface. This is in fact what is done in a different context when trying to justify the existence of $\mathbf{f}\Sigma$ across singular surfaces (compare (7.39)). In the present case the temperature jump present in (7.75) could be imposed just the same as in (7.66).

## 7.5 Propagation of Phase-Transformation Fronts

### 7.5.1 Definition

Phase transitions are physicochemical phenomena that normally take place over some time and space intervals. The word *transition* expresses the passing over from one state to another one, so-called phases, of the same material. For an outsider these phases may be viewed as two different materials. But some theoretically distinguishable phases may be of equal energy, differing only in their arrangement of basic elements such as atoms in a lattice. Thus two energetically equal phases of martensite differ only by a sign of their shear in two dimensions. The passing from one of these to the other may be realized mechanically by a shearing process that brings one phase back in exact superposition with the other. We then say that the transition is stress induced. But the progress of phase-transition fronts that separate phases and are clearly observable in some thermoelastic solids is essentially controlled by *temperature.* For instance, the existence of several minimizers of the elastic potential depends on temperature in the Landau vision of the phenomenon. Consequently, thermal effects cannot be left out of the picture, and they are essential in the following developments. We consider here the possible irreversible progress of a phase into another one, the separation between the two phases being idealized as a sharp discontinuity surface $\Sigma$ across which most of the fields suffer finite discontinuity jumps. Only if we look at a smaller scale do we observe the structure of the necessarily nonzero-thickness interface between the two phases (cf. Maugin and Inoue, 1998; Maugin, 2000b). The thermodynamically irreversible processes occurring within that relatively "thick" interface are responsible for the irreversible motion of the idealized mathematical discontinuity (just as in the shock-wave theory examined in the foregoing sections). We consider the classical theory of thermoelastic conductors with the possible presence of internal variables of state, that is, with free energy per unit of reference configuration,

$$W = \bar{W}(\mathbf{F}, \theta, \alpha), \tag{7.76}$$

and acknowledge from the start that a phase transition consists in a local *material rearrangement* of the material. Accordingly, a nonintegrable transformation strain could be introduced (e.g., a shear between two martensitic phases), but the physically characteristic parameter of a phase transition in a solid (*order parameter* in Landau's theory) may be more complex than that, such as a definite combination of components of an infinitesimal strain. Therefore, a "material" description based on the exploitation of the Eshelby stress imposes itself. The presence of $\Sigma$ breaks the material symmetry of the material body as a whole and manifests a *material inhomogeneity*.

Consequently, the critical equation for the description of the phenomenon is not only that relating to dissipation but also the equation associated with the *lack* of conservation of material momentum across Σ, that is, the associated *jump relation* that is generated by a change of "particle" on the material manifold: The driving force acting on the transition front will, therefore, be a "material" or *configurational* force.

### 7.5.2 Driving Force and Kinetic Relation

The main problem here consists in writing down a consistent set of thermomechanical jump relations across the front Σ. Let $[A] = A^+ - A^-$ the jump of a discontinuous field $A$ across Σ, the unit normal $\mathbf{N}$ to Σ being oriented from the minus to the plus side. Let $\bar{\mathbf{V}}$ be the material velocity of the geometric point of Σ. The phase-transition fronts considered are *homothermal* (no jump in temperature; the two phases coexist at the same temperature at which the transition occurs) and *coherent* (they present no defects such as dislocations). The first condition requires continuity of temperature, while the second requires the continuity of the displacement or, in dynamics on the material manifold, that of the material velocity. Consequently, we have the following continuity conditions:

$$\left[\theta\right] = 0, \quad \left[\mathbf{V}\right] = \mathbf{0} \quad \text{at} \quad \Sigma. \tag{7.77}$$

Jump relations associated with strict conservation laws in the bulk are formulated according to the theory of *weak solutions* of hyperbolic systems. That is, following previous developments, we merely replace the operators $\partial/\partial t|_{\mathrm{x}}$ and $\nabla_{\mathrm{R}}$ by the jump operators $-\left(\bar{\mathbf{V}}.\mathbf{N}\right)\left[.\right]$ and $\mathbf{N}.[.]$, respectively. Thus the jump equations associated with the bulk equations that are strict conservation laws read

$$\bar{V}_N\left[\rho_0\right] = 0, \tag{7.78}$$

$$\bar{V}_N\left[\mathbf{p}\right] + \mathbf{N}.\left[\mathbf{T}\right] = \mathbf{0}, \tag{7.79}$$

$$\bar{V}_N\left[H\right] + \mathbf{N}.\left[\mathbf{T}.\mathbf{v} - \mathbf{Q}\right] = 0, \tag{7.80}$$

where $\bar{V}_N = \bar{\mathbf{V}}.\mathbf{N}$ is the normal speed of the points of Σ. The same pragmatic rule can be applied to the bulk equations of entropy and material momentum—which are *not* strict conservation laws—if we formally add *unknown* source terms; that is, we a priori write the following two jump equations:

$$\bar{V}_N\left[S\right] - \mathbf{N}.\left[\mathbf{Q}/\theta\right] = \sigma_\Sigma \tag{7.81}$$

and

$$\bar{V}_N[\mathbf{P}] + \mathbf{N}.[\mathbf{b}] + \mathbf{f}_\Sigma = \mathbf{0}. \tag{7.82}$$

The second law of thermodynamics at Σ reads

$$\sigma_\Sigma \geq 0. \tag{7.83}$$

The problem consists in finding the expressions of $\sigma_\Sigma$ and $f_\Sigma$ that are compatible. We know the formal expression of both **P** and **b**. The only manipulation we can do on Equation 6.6 is to compute the power expended by $\mathbf{f}_\Sigma$ in the irreversible motion of Σ. To that purpose, we compute

$$p_\Sigma = \bar{\mathbf{V}}.\mathbf{f}_\Sigma \tag{7.84}$$

on account of the remaining jump Equations 7.77 through 7.80. The proof then goes as follows. First we have

$$\mathbf{f}_\Sigma.\bar{\mathbf{V}} = -[\bar{V}_N \mathbf{P}.\mathbf{V}] - \mathbf{N}.[\mathbf{b}.\mathbf{V}]; \tag{a}$$

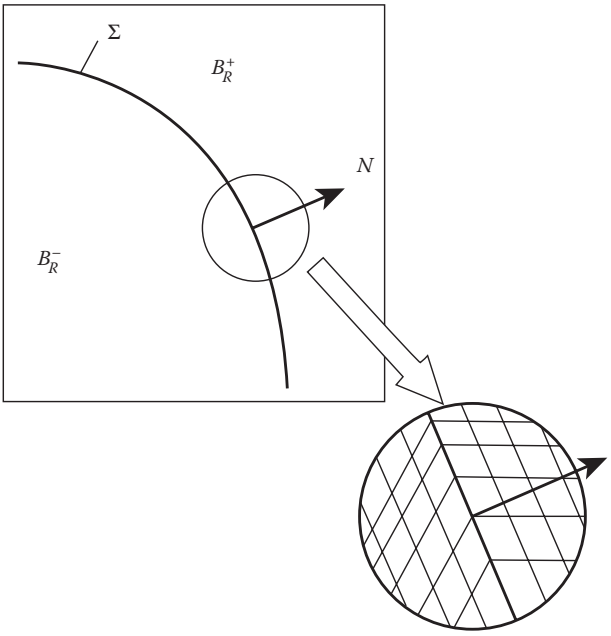


**FIGURE 7.3**
A phase-transition front without structural defects.

but on the one hand,

$$\mathbf{P}.\mathbf{V} = -\rho_0 \mathbf{v}.\mathbf{F}.\mathbf{V} = \rho_0 \mathbf{v}^2 \tag{b}$$

and ($\mathbf{F}.\mathbf{V} = -\mathbf{v}$)

$$\mathbf{b}.\mathbf{V} = -\left(\frac{1}{2}\rho_0 \mathbf{v}^2 - W\right)\mathbf{V} + \mathbf{T}.\mathbf{v}. \tag{c}$$

Substituting from these into (a) we have then

$$\mathbf{f}_\Sigma.\bar{\mathbf{V}} = -\left[\bar{V}_N \rho_0 \mathbf{v}^2\right] + \left\lfloor \mathbf{N}.\left(\frac{1}{2}\rho_0 \mathbf{v}^2 - W\right)\mathbf{V} - \mathbf{N}.\mathbf{T}.\mathbf{v} \right\rfloor, \tag{d}$$

or

$$p_\Sigma = \bar{\mathbf{V}}.\mathbf{f}_\Sigma = -\left\lfloor \bar{V}_N\left(\frac{1}{2}\rho_0 \mathbf{v}^2 + W\right) + \mathbf{N}.\mathbf{T}.\mathbf{v} \right\rfloor. \tag{e}$$

But from the energy jump equation we extract

$$\mathbf{N}.[\mathbf{Q}] = \bar{V}_N [H] + [\mathbf{N}.\mathbf{T}.\mathbf{v}]. \tag{f}$$

It is here that the working hypothesis of homothermality ($7.76_1$) enters, because the entropy jump relation then yields (compare to (7.70))

$$\mathbf{N}.[\mathbf{Q}] = \bar{V}_N [\theta S] - \theta_\Sigma \sigma_\Sigma. \tag{g}$$

On combining (f) and (g) and accounting for the relation $W = E - S\theta$, we have thus $p_\Sigma = \theta_\Sigma \sigma_\Sigma$. But we also have

$$[\mathbf{N}.\mathbf{T}.\mathbf{v}] = [\mathbf{N}.\mathbf{T}].\langle \mathbf{v} \rangle + \langle \mathbf{N}.\mathbf{T} \rangle.[\mathbf{v}], \tag{h}$$

$$[\mathbf{N}.\mathbf{T}].\langle \mathbf{v} \rangle = -\bar{V}_N [\rho_0 \mathbf{v}].\langle \mathbf{v} \rangle = -\bar{V}_N [\rho_0 \mathbf{v}^2 / 2], \tag{i}$$

$$[\mathbf{N}.\mathbf{T}.\mathbf{v}] = -\bar{V}_N [\rho_0 \mathbf{v}^2/2] - \langle \mathbf{N}.\mathbf{T} \rangle.[\mathbf{F}.\mathbf{N}]\bar{V}_N. \tag{j}$$

The Maxwell–Hadamard lemma here yields

$$\left[\mathbf{v}\right] = -\left[\mathbf{F}.\mathbf{N}\right]\bar{V}_N. \tag{k}$$

On collecting the intermediate results (f) through (k) in (e), we finally obtain

$$p_\Sigma = f_\Sigma \bar{V}_N = \theta_\Sigma \sigma_\Sigma \geq 0, \tag{7.85}$$

together with the fact that

$$q_\Sigma = p_\Sigma = \theta_\Sigma \sigma_\Sigma \geq 0 \tag{7.86}$$

is a *hot* heat source localized at Σ. In these equations $\theta_\Sigma$ is the uniquely defined temperature at Σ (a characteristic parameter of the phase transition), $f_\Sigma$ is the scalar driving force for which we need a *kinetic equation*, and we have at Σ the following *balance of "material" forces*:

$$f_\Sigma + \mathrm{Hugo}_{\mathrm{PT}} = 0, \tag{7.87}$$

wherein we have defined the scalar *material* force as

$$Hugo_{PT} := \left[W - \langle \mathbf{N}.\mathbf{T} \rangle . \mathbf{F}.\mathbf{N}\right], \tag{7.88a}$$

with the symbolism < .. > indicating the mean value at Σ.

When inertia is fully disregarded from the start, then $\mathbf{N}.[\mathbf{T}] = \mathbf{0}$ across Σ. We then let the readers show for themselves with the help of the Maxwell-Hadamard condition for **F** that (7.88a) can also be written as

$$\mathrm{Hugo}_{\mathrm{PT}}(\text{quasistatics}) = \left[W - \mathrm{tr}\left(\langle \mathbf{T} \rangle . \mathbf{F}\right)\right]. \tag{7.88b}$$

The surface "balance" Equation 7.87 is written down just to emphasize the different roles of $\mathrm{Hugo}_{\mathrm{PT}}$—a field quantity that is known once we know the field solution by any means on both sides of Σ—and the driving force $f_\Sigma$ that is the thermodynamic conjugate of the normal speed $\bar{V}_N$. The expression of $\bar{V}_N$ in terms of $f_\Sigma$ is the *kinetic law* for normal progress, examples of which based on a more microscopic approach can be found in Truskinowsky (1994). In the absence of microscopic justification, one simply applies the thermodynamic constraint (7.87) to formulate a priori an admissible kinetic law. A linear relation between the two terms in the left-hand side of (7.87) is most of the time unrealistic, as the dynamic kinetic relation is extremely

nonlinear as we shall see later in some examples. A typical kinetic law would read formally

$$\bar{V}_N = \tilde{V}\left(f_\Sigma ; \theta_\Sigma\right), \tag{7.89}$$

a relation that emphasizes the *normal growth behavior* (of one phase in the other). This may be of the threshold type (i.e., $\bar{V}_N = 0$ if $|f_\Sigma|$ has not reached a critical value $f_{cr}$, or $\bar{V}_N$ possibly, but not necessarily, nonzero when this critical value is reached). More sophisticated criteria that satisfy the constraint (7.86) can be imagined. The engineering approach, however, consists in computing $\text{Hugo}_{\text{PT}}$ by any means at each point of $\Sigma$ and applying the criterion $f_\Sigma = -\left(\text{Hugo}_{\text{PT}}\right)_{\text{Comput}}$, and this decides whether there is further progress at that point and in what direction, and then incrementing the problem by incrementing the data (this is the strategy in related problems such as elastoplasticity and fracture; see Maugin [1992]). For a physicist, however, while (7.86) must hold, the relationship (7.89) must be supported by a local analysis of the transition phenomenon at a smaller scale, involving the structure of the front. We shall examine this in a later chapter.

The thermomechanical approach given in the preceding finds its roots in a paper by Truskinowskii (1987), but the present formalism, including the consideration of the material-momentum jump relation in material space is due to Maugin and Trimarco (1995a, 1995b, 1995c). Much work along these lines was done independently by Abeyaratne et al. (1990–2003).

But a phase-transition front is a particular case of the general framework developed in Sections 7.2 and 7.4, for which the special conditions (7.82) hold good. The result obtained in the preceding can therefore be deduced from general equations. In particular, from the results (7.52) and (7.53), we directly have

$$\sigma_\Sigma = \frac{q_\Sigma}{\theta_\Sigma} = \frac{1}{\theta_\Sigma}\mathbf{f}_\Sigma.\bar{\mathbf{V}} = -\frac{1}{\theta_\Sigma}\text{Hugo}_{\text{PT}}\bar{V}_N = \left[M_\Sigma\right] \geq 0. \tag{7.90}$$

### 7.5.3 Nondissipative Phase Transition—Maxwell Rule

What must be remarked concerning the preceding construct is that the normal "material force" $\text{Hugo}_{\text{PT}}$ is practically never zero since it must satisfy the inequality (7.86). However, one may artificially impose a vanishing $\text{Hugo}_{\text{PT}}$ for a progressing front (nonzero $\bar{V}_N$). This means a nondissipative phase transition although we relate through $\Sigma$ the phases that are in nonadiabatic evolution ($\mathbf{Q} \neq \mathbf{0}$), that is, in the condition

$$\text{Hugo}_{\text{PT}} = 0 \quad \text{at} \quad \Sigma, \tag{7.91}$$

although $\bar{V}_N \neq 0$. It is readily realized that this "condition" of nondissipativity is the three-dimensional version of the rule of the Maxwell line (rule of equal areas) in phase-transition theory relating to a scalar order parameter (so-called Landau's theory). To see this, it is sufficient to use the definition of $Hugo_{PT}$ and the elastic constitutive equation to rewrite (7.76) as

$$\int_{\text{phase}-}^{\text{phase}+} \text{tr}\left(\mathbf{T}.d\mathbf{F}\right)\Big|_{\text{fixed }\theta,\alpha} = \langle \mathbf{N}.\mathbf{T} \rangle.\left[\mathbf{F}.\mathbf{N}\right]. \tag{7.92}$$

In one dimension, all quantities becoming scalars, this gives

$$\int_{\text{phase}-}^{\text{phase}+} TdF\Big|_{\text{fixed }\theta,\alpha} = \frac{1}{2}\left(T^+ + T^-\right)\left(F^+ - F^-\right). \tag{7.93}$$

This is indeed Maxwell's rule of equal areas in a graph (elastic constitutive equation) *T*-versus-*F* on which one phase is on one stable branch, and the other is on the other stable branch of an *S*-shaped curve. The same manipulation cannot be achieved for the shock condition of (7.57) because *E* depends on *F* and *S*, and the latter, entropy, is not fixed in passing from one side to the other side of the shock.

In the same conditions as (7.91) holds true, (7.79) yields

$$\bar{V}_N^2 = \frac{\left(T^+ - T^-\right)}{\rho_0\left(F^+ - F^-\right)}, \tag{7.94}$$

but this would provide the normal wave speed $\bar{V}_N$ only if the jump solution were known, which is not the case beforehand.

The statements (7.57) and (7.91) exhibit the singularity of the "unstructured" shock wave and "nondissipative" phase-transition front. The fact that *internal energy* is involved in the first case, while *free energy* appears in the second case, deserves comments that are given in a later section. Generalizations to more complex cases than thermoelasticity are given in other chapters.

For a fluid, the condition (7.91) in fact materializes in the continuity of the *chemical potential*. The relationship of chemical potential and the Eshelby stress (sometimes called the chemical potential tensor) was noticed by Grinfeld (1991). However, there is something more in the preceding results: No quasistatic hypothesis was used, although it is exactly *shown* that no kinetic energy can enter the final expression (7.88). This agrees with the perspicacious view of Gibbs and Duhem, who indeed foresaw that only the *free enthalpy* must govern the local matter rearrangement represented by a

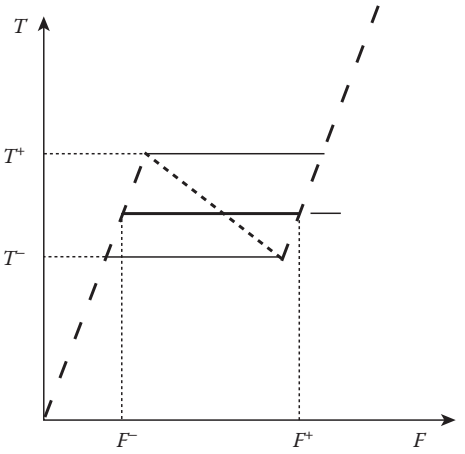


**FIGURE 7.4**
The Maxwell-line construction.

phase transition. Thus only the quasistatic part of the Eshelby stress finally contributes to the Hugoniot–Gibbs functional $\text{Hugo}_{\text{PT}}$—in agreement with their vision.

The result obtained in the preceding can be generalized to more complex material bodies such as electromagnetic ones (e.g., Fomethe and Maugin, 1997) or polar thermoelasticity (Maugin, 1998a), as well as thermoanelastic materials. Furthermore, nothing is fundamentally changed in this argument in the presence of anelastic behaviors described by means of internal variables of state (cf. Maugin, 1998c). These generalizations to more complex cases than thermoelasticity are reported in other sections or chapters.

## 7.6 On Internal and Free Energies

It is classically remarked that *internal energy* is most important in treating problems involving a condition of adiabaticity, while *free energy* is the relevant thermodynamic potential to deal with isothermal situations. This was introduced in the preceding by the classical theory of shock waves and that of phase-transition fronts, respectively. We have based our initial approach to the notion of Eshelby stress in thermomechanics on the use of the free energy. A question that naturally arises, then, is whether this is a prejudice or not. That is, ignoring external body forces and any true material inhomogeneity, at each regular material point $\mathbf{X}$, we had

the Eshelby stress and the material momentum equation in the form (cf. Chapter 5):

$$\mathbf{b} = -\left(L1_R + \mathbf{T}.\mathbf{F}\right), \quad \mathbf{T} = \left(\frac{\partial W}{\partial \mathbf{F}}\right)_\theta, \quad S = -\left(\frac{\partial W}{\partial \theta}\right)_\mathbf{F}, \quad L = K - W, \tag{7.95}$$

and

$$\left.\frac{\partial \mathbf{P}}{\partial t}\right|_X - \mathrm{div}_R \mathbf{b} = \mathbf{f}^{\mathrm{th}}, \quad \mathbf{f}^{\mathrm{th}} = S\nabla_R \theta. \tag{7.96}$$

We should have been more careful in the notation, emphasizing by some means the fact that it is the *free energy* that appears in *L*. Thus following Maugin (2002) we rewrite some of these equations in an obvious notation:

$$\left.\frac{\partial \mathbf{P}}{\partial t}\right|_X - \mathrm{div}_R \mathbf{b}_W = \mathbf{f}_W^{\mathrm{th}}, \quad \mathbf{f}_W^{\mathrm{th}} = S\nabla_R \theta, \quad L_W = K - W,$$
$$\mathbf{T}_W = \left(\frac{\partial W}{\partial \mathbf{F}}\right)_\theta, \quad \mathbf{b}_W = -\left(L_W \mathbf{1}_R + \mathbf{T}_W.\mathbf{F}\right). \tag{7.97}$$

This is well adapted to the treatment of some isothermal situations. For prevailing adiabatic conditions, it would be better to consider the internal energy density *E* per unit reference volume, such that

$$E = W + S\theta, \quad \theta = \left(\frac{\partial E}{\partial S}\right)_\mathbf{F} > 0. \tag{7.98}$$

Here $E = \bar{E}$ ($S$, $\mathbf{F}$ fixed) must be a monotonically increasing function of entropy *S*. But we immediately check that

$$\mathbf{T}_W = \left(\frac{\partial W}{\partial \mathbf{F}}\right)_\theta = \left(\frac{\partial E}{\partial \mathbf{F}}\right)_\theta + \theta\left(\frac{\partial S}{\partial \mathbf{F}}\right)_\theta = \left(\frac{\partial E}{\partial \mathbf{F}}\right)_S = \mathbf{T}_E = \mathbf{T}. \tag{7.99}$$

Accordingly,

$$\mathbf{b}_W = \mathbf{b}_E - (\theta S)\mathbf{1}_R, \quad \mathbf{b}_E \equiv -\left(L_E \mathbf{1}_R + \mathbf{T}_E.\mathbf{F}\right), \quad L_E \equiv K - E. \tag{7.100}$$

Then we can write instead of the first of (7.97)

$$\left.\frac{\partial \mathbf{P}}{\partial t}\right|_X - \mathrm{div}_R \mathbf{b}_E = \mathbf{f}_E^{\mathrm{th}}, \quad \mathbf{f}_E^{\mathrm{th}} \equiv -\theta \nabla_R S, \tag{7.101}$$

with the relationship

$$\mathbf{f}_W^{\mathrm{th}} = \mathbf{f}_E^{\mathrm{th}} + \nabla_R . \left(\theta S \mathbf{1}_R\right). \tag{7.102}$$

Equation 7.101 should be the equation of material momentum to be considered preferably if we have to deal with adiabatic conditions since $\mathbf{f}_E^{\mathrm{th}}$ will vanish with spatially uniform entropy.

**Consequences for Jump Relations**

In previous paragraphs we have considered (using now the new, more accurate notation) the jump of material momentum as

$$\bar{V}_N \left[\mathbf{P}\right] + \mathbf{N}.\left[\mathbf{b}_W\right] = -\mathbf{f}_{\Sigma,W}, \tag{7.103}$$

where the material force on the right-hand side is an unknown quantity. We could have as well considered the a priori jump equation

$$\bar{V}_N \left[\mathbf{P}\right] + \mathbf{N}.\left[\mathbf{b}_E\right] = -\mathbf{f}_{\Sigma,E}, \tag{7.104}$$

where the right-hand side force is equally unknown. But accounting for the first of (7.100), we deduced the necessary relation

$$\mathbf{f}_{\Sigma,E} = \mathbf{f}_{\Sigma,W} - \mathbf{N}\left[S\theta\right], \tag{7.105}$$

an expression which is in harmony with (7.102). This leads us to look at *another approach* to the driving force problem (Abeyaratne and Knowles, 2000). First, remember equations (e) and (g) in the proof of (7.85) earlier. The entropy jump condition (7.76) can also be written as

$$\bar{V}_N \left[S\right] - \mathbf{N}.\left[\mathbf{Q}\right]\left\langle\frac{1}{\theta}\right\rangle - \mathbf{N}.\left\langle\mathbf{Q}\right\rangle\left[\frac{1}{\theta}\right] = \sigma_\Sigma. \tag{7.106}$$

But Abeyaratne and Knowles (2000) astutely note that both adiabatic and nonadiabatic conditions can be gathered in a single product equation

$$\mathbf{Q}\left[\theta\right] = 0, \tag{7.107}$$

an equation that has no more physical meaning than telling that either temperature is continuous or the material heat flux vanishes. Therefore, necessarily,

$$\mathbf{N}.[\mathbf{Q}]\left(\left\langle\frac{1}{\theta}\right\rangle-\frac{1}{\langle\theta\rangle}\right)=0 \quad \text{and} \quad \mathbf{N}.\langle\mathbf{Q}\rangle\left[\frac{1}{\theta}\right]=0. \tag{7.108}$$

Accounting for the conditions (7.107) and (7.108) in the previously mentioned equations (e) and (g), we obtain

$$\bar{V}_N\langle\theta\rangle[S]-\bar{V}_N[H]-\mathbf{N}.[\mathbf{T}.\mathbf{v}]=\langle\theta\rangle\sigma_\Sigma. \tag{7.109}$$

And remembering the definition of the free energy, this becomes

$$\bar{V}_N\langle\theta\rangle[S]-\left[\bar{V}_N\left(\left(\rho_0\mathbf{v}^2/2\right)+W\right)+\mathbf{N}.\mathbf{T}.\mathbf{v}\right]=\langle\theta\rangle\sigma_\Sigma. \tag{7.110}$$

Comparing with (e), we conclude that

$$\mathbf{f}_{\Sigma,W}.\bar{\mathbf{V}}-\bar{V}_N\langle S\rangle[\theta]=\langle\theta\rangle\sigma_\Sigma. \tag{7.111}$$

This can be written as

$$\left(\mathbf{f}_{\Sigma,W}-\mathbf{N}\langle S\rangle[\theta]\right).\bar{\mathbf{V}}=\langle\theta\rangle\sigma_\Sigma. \tag{7.112}$$

The expression within parentheses on the left-hand side of the last equation is considered as the driving force by Abeyaratne and Knowles (2000). It obviously coincides with $\mathbf{f}_{\Sigma,W}$ in isothermal processes for which $[\theta] = 0$, while in *adiabatic processes* we have

$$\mathbf{f}_{\Sigma,W}-\mathbf{N}\langle S\rangle[\theta]=\mathbf{N}\langle\theta\rangle[S], \tag{7.113}$$

and this yields

$$\mathbf{f}_{\Sigma,W}=\mathbf{N}[S\theta], \tag{7.114}$$

a result in full accord with (7.105), since then $\mathbf{f}_{\Sigma,W} = 0$, and also with (7.76).

## 7.7 The Case of Complex Media

To prepare applications to more complex bodies than thermo-anelastic bodies governed by a free energy such as (7.76), we consider the case of media described by an additional variable $\alpha$ with its gradients such as in Chapter 5, and more particularly Sections 5.3 and 5.4. In particular, at any regular material point we should have the following set of equations, no balance (case of an additional internal degree of freedom) or evolution (case of an internal variable of state) equation being specified for the variable (field) $\alpha(\mathbf{X}, t)$, but with energy density:

$$W = \bar{W}\left(\mathbf{F}, \alpha, \nabla_R \alpha, \theta; \mathbf{X}\right) \tag{7.115}$$

- Balance of mass:

$$\left.\frac{\partial}{\partial t}\rho_0\right|_X = 0 \tag{7.116}$$

- Balance of physical momentum:

$$\left.\frac{\partial}{\partial t}\mathbf{p}\right|_X - \mathrm{div}_R \mathbf{T} = \mathbf{0} \tag{7.117}$$

- Balance of material momentum:

$$\left.\frac{\partial}{\partial t}\mathbf{P}\right|_X - \mathrm{div}_R \mathbf{b} = \mathbf{f}^{\mathrm{inh}} + \mathbf{f}^{\mathrm{th}} + \mathbf{f}^{\mathrm{intr}} \tag{7.118}$$

- Balance of energy:

$$\left.\frac{\partial}{\partial t}H\right|_X - \nabla_R.\left(\mathbf{T}.\mathbf{v} + \mathbf{M}\dot{\alpha} - \mathbf{Q}\right) = 0 \tag{7.119}$$

- Heat-propagation equation:

$$\theta\left.\frac{\partial}{\partial t}S\right|_X + \nabla_R.\mathbf{Q} = A\dot{\alpha} \tag{7.120}$$

- Balance of entropy:

$$\left.\frac{\partial}{\partial t}S\right|_X + \nabla_R.\mathbf{S} = \sigma_B \geq 0 \tag{7.121}$$

The dependence on $\nabla_R\alpha$ indicates a *weak nonlocality* in the $\alpha$ variable. No *inertia* of a classical type is here granted to $\alpha$. We set

$$\mathbf{T} = \partial\bar{W}/\partial\mathbf{F}, \quad S = -\partial\bar{W}/\partial\theta,$$
$$A = \bar{A} + \nabla_R.\mathbf{M} = -\delta\bar{W}/\delta\alpha,$$
$$\bar{A} = -\partial\bar{W}/\partial\alpha, \quad \mathbf{M} = \partial\bar{W}/\partial(\nabla_R\alpha),$$

where $\delta/\delta\alpha$ indicates the Euler–Lagrange functional derivative with respect to $\alpha$. Furthermore,

$$\mathbf{P} = -\mathbf{F}^T.\mathbf{p}, \tag{7.122}$$

$$\mathbf{b} = -\left(\mathbf{L}^{\text{th}}\mathbf{1}_R + \mathbf{T}.\mathbf{F} + \mathbf{M}.(\nabla_R\alpha)^T\right), \tag{7.123}$$

$$\mathbf{f}^{\text{inh}} = \left(\frac{\partial L^{\text{th}}}{\partial\mathbf{X}}\right)_{\text{expl}}, \quad L^{\text{th}} := \frac{1}{2}\rho_0(X)\mathbf{v}^2 - \bar{W}, \tag{7.124}$$

$$\mathbf{f}^{\text{th}} := S\nabla_R\theta, \quad \mathbf{f}^{\text{intr}} := A\nabla_R\alpha \tag{7.125}$$

are, respectively, the *canonical* (material) *momentum*, the *Eshelby* material stress, the "material" force of the *true* material inhomogeneities, an effective Lagrangian density, the "material" thermal force, and a "material" force due to spatial disuniformities in the $\alpha$ variable. The latter, just like $\mathbf{f}^{\text{th}}$, may be referred to as a material force of *quasi*-inhomogeneitiy, that is, manifesting itself just like $\mathbf{f}^{\text{inh}}$ in the balance equation (7.118). Notice that the definition of $\mathbf{P}$ is left unchanged because the variable $\alpha$ does not carry inertia.

Concerning the assumed functional dependence (7.115), once the variable $\alpha$ is specified, the *rotational invariance* of the scalar-valued function $\bar{W}$ (not a functional of time) in *physical* space imposes a condition of the following general type (cf. Maugin, 1980; Capriz, 1989):

$$skew\left(\frac{\partial\bar{W}}{\partial\mathbf{F}}\mathbf{F}^T\right) + SO\left(\frac{\delta\bar{W}}{\delta\alpha}\right) = 0, \tag{7.126}$$

where the second contribution means the action of members of the proper orthogonal group $SO(3)$ on $W$ considered as a function of the tensorial object

$\alpha$ and its first material gradient. For instance, if $\alpha$ is a vector field $\mathbf{n}(\mathbf{X}, t)$ in $K_t$, then (7.126) reads, in components,

$$skew_{[ij]}\left(\frac{\partial \bar{W}}{\partial F^i_{.K}} F^k_{.K}\delta_{kj} + \frac{\partial \bar{W}}{\partial n^i} n^k \delta_{kj} + \frac{\partial \bar{W}}{\partial n^i_{.K}} n^k_{.K}\delta_{kj}\right) = 0. \tag{7.127}$$

This potentially contains the local balance of moment of (physical) momentum. Equation 7.127 applies to the case of liquid crystals (cf. Appendix 9.1 of Chapter 9).

Applying now the formalisms of weak solutions, corresponding to (7.116), (7.117), and (7.119), we have the following homogeneous jump conditions at the singular surface $\Sigma$:

$$\bar{V}_N\left[\rho_0\right] = 0, \tag{7.128}$$

$$\mathbf{N}.\left[\bar{\mathbf{V}} \otimes \mathbf{p} + \mathbf{T}\right] = \mathbf{0}, \tag{7.129}$$

$$\mathbf{N}.\left[H\bar{\mathbf{V}} + \mathbf{T}.\mathbf{v} + \mathbf{M}\dot{\alpha} - \mathbf{Q}\right] = 0. \tag{7.130}$$

Proceeding as in previous sections, for the jump conditions corresponding to (7.118), (7.119), and (7.121), we a priori write

$$\mathbf{N}.\left[\bar{\mathbf{V}} \otimes \mathbf{P} + \mathbf{b}\right] + \mathbf{f}_\Sigma = 0, \tag{7.131}$$

$$\mathbf{N}.\left[\bar{\mathbf{V}} S\theta - \mathbf{Q}\right] - q_\Sigma = 0, \tag{7.132}$$

$$\mathbf{N}.\left[\bar{\mathbf{V}} S - \mathbf{S}\right] = \sigma_\Sigma \geq 0, \tag{7.133}$$

where the expressions of the surface heat source $q_\Sigma$, the surface entropy source $\sigma_\Sigma$, and the surface material force of inhomogeneity $\mathbf{f}_\Sigma$ are to be found or related to one another from some analysis on account of the expression of all other quantities involved in the jump relations (7.128) through (7.130), with the inequality in (7.132) imposing a direction of evolution. We are particularly interested in finding the expression of this surface entropy source. Of course, on considering (7.128) we see that $\rho_0$ must be continuous across $\Sigma$ for a really moving surface $\Sigma$, while a nonzero jump in $\rho_0$ would require that surface to be frozen in the material. Second, compatibility between (7.130) and (7.131) for a *homothermal* front (no jump in temperature) yields

$$\sigma_\Sigma = \theta_\Sigma^{-1} q_\Sigma \geq 0, \tag{7.134}$$

so that $q_\Sigma$ is necessarily a hot source.

Now, as in previous sections, we contemplate the computation of the power $p_\Sigma = \mathbf{f}_\Sigma . \bar{\mathbf{V}}$. This will be much complicated by the presence of $\alpha$, but the result is *canonical* being independent of the precise physical meaning of this variable. First, we note the following partial results, already established in simpler cases:

$$[\mathbf{v}] = -[\mathbf{F}.\mathbf{V}] = -\mathbf{f}\bar{V}_N, \quad \mathbf{f} := [\mathbf{F}].\mathbf{N}, \quad [\mathbf{F}] = \mathbf{f} \otimes \mathbf{N}, \tag{7.135}$$

$$\mathbf{N}.\mathbf{V} = \mathbf{N}.\bar{\mathbf{V}} = \bar{V}_N = V_N^+ = V_N^- \quad \text{at} \quad \Sigma, \tag{7.136}$$

$$[\mathbf{N}.\mathbf{T}] = -\rho_0 [\mathbf{v}] \bar{V}_N, \tag{7.137}$$

$$[\mathbf{N}.\mathbf{T}].\langle \mathbf{v} \rangle = -\bar{V}_N [K], \quad K = \rho_0 \mathbf{v}^2/2, \tag{7.138}$$

$$[\mathbf{N}.\mathbf{T}.\mathbf{v}] = -\bar{V}_N ([H] + \langle \mathbf{N}.\mathbf{T} \rangle .[\mathbf{v}]). \tag{7.139}$$

Also, we note that

$$\left.\frac{\partial \alpha}{\partial t}\right|_X = \left.\frac{\partial \alpha}{\partial t}\right|_x + \mathbf{v}.\nabla \alpha = \left.\frac{\partial \alpha}{\partial t}\right|_x - \mathbf{V}.\nabla_R \alpha, \tag{7.140}$$

and thus

$$[\mathbf{N}.\mathbf{M}\dot{\alpha}] = \left[\mathbf{N}.\mathbf{M}\left.\frac{\partial \alpha}{\partial t}\right|_x\right] - [\mathbf{N}.\mathbf{M}(\mathbf{V}.\nabla_R \alpha)], \tag{7.141}$$

and

$$\left[\mathbf{N}.\mathbf{M}\left(\nabla_R \alpha\right)^T\right].\mathbf{V} = [\mathbf{N}.\mathbf{M}(\mathbf{V}.\nabla_R \alpha)]. \tag{7.142}$$

If $\alpha$ itself is continuous at $\Sigma$, an application of the Maxwell–Hadamard lemma (see (7.135)) yields

$$[\nabla_R \alpha] = \mathbf{N} \otimes \bar{\alpha}, \quad \bar{\alpha} := [\mathbf{N}.\nabla_R \alpha], \tag{7.143}$$

so that

$$[(\mathbf{V}.\nabla_R \alpha)] = \bar{V}_N \left[\frac{\partial \alpha}{\partial N}\right]. \tag{7.144}$$

Consequently, after a short calculation, (7.142) yields

$$\left[\mathbf{N}.\mathbf{M}\left(\nabla_R\alpha\right)^T\right].\mathbf{V} = \bar{V}_N\left\langle\mathbf{N}.\mathbf{M}\right\rangle\left[\frac{\partial\alpha}{\partial N}\right] + \left[\mathbf{N}.\mathbf{M}\right]\left\langle\left.\frac{\partial\alpha}{\partial t}\right|_x - \left.\frac{\partial\alpha}{\partial t}\right|_X\right\rangle. \tag{7.145}$$

But

$$p_\Sigma = \mathbf{f}_\Sigma.\bar{\mathbf{V}} = -\left[\mathbf{N}.\mathbf{b}.\mathbf{V} + \bar{V}_N\left(\mathbf{P}.\mathbf{V}\right)\right], \tag{7.146}$$

transforms to

$$p_\Sigma = \left[L^{\text{th}}\bar{V}_N + \mathbf{N}.\mathbf{T}.\mathbf{F}.\mathbf{v} + \mathbf{N}.\mathbf{M}\left(\mathbf{V}.\nabla_R\alpha\right) - 2K\bar{V}_N\right], \tag{7.147}$$

or

$$p_\Sigma = -\left[\left(K+W\right)\bar{V}_N + \mathbf{N}.\mathbf{T}.\mathbf{v} - N.\mathbf{M}\left(\mathbf{V}.\nabla_R\alpha\right)\right]. \tag{7.148}$$

On the other hand, we can extract [**N**.**Q**] from (7.130) to obtain

$$\mathbf{N}.\left[\mathbf{Q}\right] = \left[\left(E+K\right)\bar{V}_N + \mathbf{N}.\mathbf{T}.\mathbf{v} + \mathbf{N}.\mathbf{M}\dot{\alpha}\right]. \tag{7.149}$$

Accounting now for (7.132) and (7.141) and comparing the result with (7.148), we obtain the sought relationship as

$$q_\Sigma = p_\Sigma - \left[\left.\mathbf{N}.\mathbf{M}\frac{\partial\alpha}{\partial t}\right|_x\right], \tag{7.150}$$

where, we emphasize, the time derivative of $\alpha$ is taken at fixed **x**.

It remains to find the precise expression of $p_\Sigma$, and thus $q_\Sigma$. For this we start from (7.148) and note that $p_\Sigma$ reads

$$p_\Sigma = -\text{Hugo}_{\text{PT}}\bar{V}_N + \left[\mathbf{N}.\mathbf{M}\right]\left\langle\left.\frac{\partial\alpha}{\partial t}\right|_x - \left.\frac{\partial\alpha}{\partial t}\right|_X\right\rangle \tag{7.151}$$

on account of (7.139), (7.145), and the following definition:

$$\text{Hugo}_{\text{PT}} := \left[W - \left\langle\mathbf{N}.\mathbf{T}\right\rangle.\frac{\partial\chi}{\partial N} - \left\langle\mathbf{N}.\mathbf{M}\right\rangle.\frac{\partial\alpha}{\partial N}\right]. \tag{7.152}$$

We let the reader finish the proof by establishing that the second law at Σ reads (Maugin, 1998c)

$$q_\Sigma = -\mathrm{Hugo}_{\mathrm{PT}}\bar{V}_N - \left( [\mathbf{N}.\mathbf{M}] \left\langle \left. \frac{\partial \alpha}{\partial t} \right|_X \right\rangle + \langle \mathbf{N}.\mathbf{M} \rangle \left[ \left. \frac{\partial \alpha}{\partial t} \right|_x \right] \right) \geq 0, \tag{7.153}$$

a result that is general enough so as not to involve any particular condition on the evolution equation satisfied by the variable α, and where we point out the coexistence of two different types of time derivative. But we must realize that in most, if not all, cases of interest, the quantity within large parentheses in (7.153) vanishes identically. The reason for this is as follows. First, if, as implicitly assumed, the additional variable α is of the internal variable type, then the natural boundary (jump) condition associated with the continuity of the normal flux associated with α reads

$$\mathbf{N}.[\mathbf{M}] = 0 \quad \text{at} \quad \Sigma. \tag{7.154}$$

In addition, if the front Σ is *coherent* as regards the property related to the variable α, then by analogy with the condition

$$[\mathbf{V}] = \left[ \left. \partial \chi^{-1}(\mathbf{x}, t)/\partial t \right|_x \right] = \mathbf{0}, \tag{7.155}$$

we will have to satisfy the following constraint at Σ:

$$\left[ \left. \partial \alpha(\mathbf{x}, t)/\partial t \right|_x \right] = 0. \tag{7.156}$$

The conditions (7.154) and (7.156) together entail the vanishing of the second contribution in (7.153), so that we can now write

$$\theta_\Sigma \sigma_\Sigma = q_\Sigma = f_\Sigma \bar{V}_N \geq 0, \tag{7.157}$$

with the auxiliary equilibrium condition

$$f_\Sigma + \mathrm{Hugo}_{\mathrm{PT}} = 0,$$

just like in the classical case, but with a more general expression for the material force (7.152).

We have given the proof of the preceding result in some detail because of its quite general validity. In effect, if Σ is still of the coherent type with

respect to both the inverse classical motion (see (7.155)) and $\alpha$ (see (7.156)), but $\alpha$ in fact is an additional degree of freedom carrying its own inertia, then (7.154) will be replaced by an equation such as

$$\mathbf{N}.\left[\mathbf{M}+\bar{\mathbf{V}}\otimes\mathbf{p}_{\alpha}\right]=\mathbf{0}, \tag{7.158}$$

where the $\alpha$-momentum is such that the kinetic energy associated with $\alpha$ be homogeneous of degree two in $\dot{\alpha}$, hence itself homogeneous of degree one in $\dot{\alpha}$, and so

$$\left[K_{\alpha}\right]=\left[\mathbf{p}_{\alpha}\right].\left\langle \partial\alpha\left(\mathbf{X},t\right)/\partial t\big|_{\mathrm{X}}\right\rangle. \tag{7.159}$$

Then it can be shown (Maugin, 1998c) on account of (7.158) and (7.159) that the first contribution within large parentheses in (7.153) will compensate an inertial term that would have naturally appeared in the Eshelby stress in the derivation, had we considered (7.158) to start with. Therefore, with the coherence condition (7.156) still valid, this case also reduces the heat surface source to the form (7.157), which exhibits only *normal growth*, as only the normal component of $\bar{\mathbf{V}}$ is involved and the driving force $f_{\Sigma}$ acting on $\Sigma$ is a mere scalar.

## 7.8 Applications to Problems of Materials Science (Metallurgy)

### 7.8.1 Equilibrium Shape of Precipitates

There is a great deal of interest in the morphology of heterogeneous materials. In particular, it is observed that some initially nearly spherical particles or precipitates in a matrix evolve to cuboidal ones with rounded corners during growth. These cuboidal shapes may have concave or convex interfaces, depending on the specific alloy considered and the volume fraction of the precipitated phase. This problem of stable or unstable equilibrium morphology has been especially examined by various groups of authors, including the group of D. Gross in Darmstadt (in particular, Schmidt and Gross, 1997; Mueller and Gross, 1997) with convincing numerical simulations of the variety of equilibrium shapes. This problem is examined in quasistatics in pure elasticity in small strains with an interface energy between the two solid phases, the matrix and the precipitate. The total energy in question reaches a minimum for a stable equilibrium morphology. Two effects are combined here, the difference in elasticities between the precipitate and the matrix,

and the presence of the interfacial energy. Mathematically we have thus to minimize the total energy

$$\Phi = \int_V W dV + \int_\Sigma \gamma dA, \tag{7.160}$$

where $W = (1/2)\mathrm{tr}\left(\sigma.\varepsilon^e\right)$ is the strain energy per unit volume with different elasticity coefficients $C^{in}$ and $C^{out}$ in the precipitate and the matrix, respectively; $\gamma$ is the interfacial energy per unit area of the interface $\Sigma$ bounding the misfit particle $B$; and $V$ is the volume of the whole system. The local equations, outside $\Sigma$, are those of pure quasistatics, possibly anisotropic, linear elasticity, that is,

$$\mathrm{div}\,\sigma = \mathbf{0} \quad \text{in} \quad V, \tag{7.161}$$

$$\sigma = \mathbf{C}^{\text{in}} : \varepsilon^e = \mathbf{C}^{\text{in}} : \left(\varepsilon - \varepsilon^0\right) \quad \text{in} \quad B, \tag{7.162}$$

$$\sigma = \mathbf{C}^{\text{out}} : \varepsilon \quad \text{outside} \quad B, \tag{7.163}$$

$$\lim \sigma = \mathbf{0} \quad \text{as} \quad |\mathbf{x}| \to \infty. \tag{7.164}$$

where $\sigma$ is Cauchy's stress, $\varepsilon = (\nabla \mathbf{u})_S$ is the standard infinitesimal strain, and $\varepsilon^0$ is the so-called nonelastic *transformation* or *eigenstrain*, which is a measure of the mismatch between the crystalline lattices of the two elastic phases. It is a spatially constant geometric quantity. We assume that in the process of deformation the inhomogeneity $B$ keeps its volume. Accordingly, we have to satisfy the following constraint:

$$\int_B dV = V_0 . \tag{7.165}$$

Introducing a Lagrange multiplier $\lambda$ to account for this, we will have to minimize the global expression

$$\Phi_\lambda = \int_V W dV + \int_\Sigma \gamma d\Sigma - \lambda\left(\int_B dV - V_0\right). \tag{7.166}$$

The first variation of this will yield necessary conditions for equilibrium, while the positiveness of the second variation will yield a sufficient condition for stable equilibrium. The variation considered is one of the interface positions along its normal, say by an amount $\delta w$. For the variation of

the first term in (7.166), we can use the method and result of Section 7.1, for example, (7.14) and (7.15)—caution: change of sign—with $\delta_x \mathbf{X} = \mathbf{N}\delta w$, hence

$$\delta \int_V W dV = \int_\Sigma \mathbf{N}.\left[\mathbf{b}_S\right].\mathbf{N}\delta w d\Sigma, \tag{7.167}$$

where

$$\mathbf{b}_S = W\mathbf{1}_R - \mathbf{T}.\mathbf{F} = W\mathbf{1} - \sigma.\left(\nabla \mathbf{u}\right)^T, \tag{7.168}$$

the last of these being the reduction to small strain of the quasistatic Eshelby stress. For the second term in (7.166), we have

$$\delta \int_\Sigma \gamma d\Sigma = \delta \int_\Sigma \left(\gamma \mathbf{N}\right).\mathbf{N} d\Sigma = \int_\Sigma \gamma \Omega \mathbf{N}.\delta_x \mathbf{X} d\Sigma = \int_\Sigma \gamma \Omega \delta w d\Sigma, \tag{7.169}$$

where $\Omega = (\nabla.\mathbf{N})/2$ is the mean curvature of $\Sigma$. The third term in (7.166) will simply yield (by use of the divergence theorem applied to the integrand equal to unity):

$$V_B = \int_B dV = \frac{1}{3}\int_\Sigma \mathbf{x}.\mathbf{N} d\Sigma = V_0,$$

a term proportional to $\lambda$. Gathering these intermediary results we find that the vanishing first variation of (7.166) leads to the following necessary condition of equilibrium of the precipitate:

$$\tau_N = 0 \quad \text{at} \quad \Sigma, \quad \tau_N := \mathbf{N}.\left[\mathbf{b}_S\right].\mathbf{N} - \gamma\Omega + \lambda, \tag{7.170}$$

along with the side condition (7.165). Equation 7.170 means that this condition results from a balance between various scalar configurational forces representing the difference of elasticities (i.e., the *inhomogeneity* effect per se) on both sides of $\Sigma$, the surface tension via $\gamma$ and a *material* force $\lambda$ to keep the volume unchanged. This $\lambda$ may be sought as the difference between the free energies of the matrix and the particle phase. This result is quite general (cf. Leo and Sekerka, 1989; Schmidt and Gross, 1997), but it does not account for any "inertia." It can be specialized to the case of a misfit inhomogeneous inclusion. This is based on other successful works of Eshelby (the so-called

inclusion problem). Indeed, it can be shown, on account of the classical jump conditions at $\Sigma$ (continuity of displacement and traction)

$$[\mathbf{u}] = \mathbf{0}, \quad \mathbf{N}.[\sigma] = \mathbf{0} \quad \text{at} \quad \Sigma, \tag{7.171}$$

that the jump of all the field quantities can be expressed in terms of the total strain $\varepsilon$ adjacent to the interface inside the inclusion (see Appendix B in Schmidt and Gross, 1997). Numerical simulations of a variety of equilibrium shapes are reported by Schmidt and Gross (1997) and Mueller and Gross (1997), accounting for size and concentration effects.

Insofar as the stability of the shape satisfying (7.170) is concerned, one should check the sign of the second variation of (7.166). Such a second variation has been established for general problems by Petryk and Mroz (1986). In the present case this condition reduces to the condition

$$\delta^2\Phi = -\int_{\Sigma} \delta\tau_N \delta w d\Sigma > 0, \quad \forall \delta w. \tag{7.172}$$

Here $\delta\tau_N$ is the variation of the configurational force $\tau_N$ with respect to a small variation $\delta w$ of the interface along its own normal. Graphical results on this morphological stability are reported by Mueller and Gross (1997).

### 7.8.2 Inelastic Discontinuities and Martensitic Phase Transitions

In some processes inelastic strains result from physical discrete mechanisms where, for instance, the existence of a given eigenstrain (Burger's vector, transformation strain) is manifest, and the deformation progresses by nucleation of new domains or the growth of preexisting ones, with the formation of a strain-induced microstructure at the intergranular scale (for example, pile-up of dislocations at a grain boundary). In such physical situations there occurs a discontinuity in anelastic strain, and this can be either fixed or stress-dependent along one or several moving boundaries of the line or wall type. Looking at this problem in a relatively "cheap" phenomenological way, one needs to derive the *driving force* acting on such a moving boundary. It is no surprise here that the Eshelby stress will be involved and that intrinsic dissipation due to the anelastic nature of deformation will combine with dissipation due to morphological changes. This problem can be approached with simplifying assumptions concerning the latter phenomenon, such as ellipsoidal growth (cf. Cherkaoui and Berveiller, 2000). This problem is relevant to martensitic phase transitions and the overall behavior of polycrystalline transformation-induced plasticity (TRIP) steels and is considered first in the framework of micromechanics, with a homogenization procedure in a second step. Of course, only small strains are involved, and the starting reasoning applies at the scale of a so-called

representative volume element (RVE) much smaller than any macroscopic scale. In the spirit of this book, only the first step (construction of the driving force) is illustrated here.

The energy description of this problem is quite different from the one in Section 7.8.1. One reason for this is that the surface energy due to the presence of interfaces between different phases is here disregarded, being thought much weaker than other contributions; these other contributions are chemical free energy directly coupled with temperature and a stress-dependent energy due to elasticity. That is, only mechanisms where the change in mechanical properties with temperature is low compared to the change in chemical energy with temperature are considered. Let $V$ be the volume of the RVE. Averages of chemical and stress energy are defined by

$$\bar{\varphi} = \frac{1}{V}\int_V \varphi(\mathbf{r})dV, \quad \bar{w} = \frac{1}{V}\int_V w(\mathbf{r})dV, \tag{7.173}$$

where the spatial dependence of $\varphi$ and $w$ is emphasized within the RVE. In small strains the elastic energy $w(\mathbf{r})$ is given by

$$w(\mathbf{r}) = \frac{1}{2}tr\left(\sigma(\mathbf{r})\varepsilon^e(\mathbf{r})\right) = \frac{1}{2}\sigma_{ij}(\mathbf{r})\varepsilon^e_{ij}(\mathbf{r}), \quad \varepsilon^e = \varepsilon - \varepsilon^a, \tag{7.174}$$

where $\varepsilon^a$ is the anelastic strain. Only $\varepsilon$ is exactly integrable into a displacement as $\varepsilon = (\nabla\mathbf{u})_S$.

The total free energy per unit volume of RVE is the sum of the two energies in (7.173), that is,

$$\bar{\psi} = \bar{\varphi} + \bar{w}. \tag{7.175}$$

Changes in this energy will result from the evolution of anelastic strains in each phase and also from the moving boundaries in the specimen at the scale of the RVE. Thus, jumps in both $\varphi$ and $w$ take place at discontinuities moving with local velocity $\nu$ and equipped with unit oriented normal $\mathbf{n}$ so that the normal speed is noted $\nu_n = \nu.\mathbf{n}$. Applying the transport theorem (7.29) to the time derivative of (7.175), we obtain

$$\frac{d}{dt}\bar{\psi} = \frac{1}{V}\int_V \left\{\dot{w}(\mathbf{r}) + \dot{\varphi}(\mathbf{r})\right\}dV - \frac{1}{V}\int_S \left\{\left[w(\mathbf{r})\right] + \left[\varphi(\mathbf{r})\right]\right\}\nu_n dS. \tag{7.176}$$

Following Cherkaoui and Berveiller (2000) we consider that $\varphi$ remains constant during the anelastic deformation in different phases at the current

configuration of the RVE. Thus we set $\dot{\varphi}(\mathbf{r}) = 0$ in (7.176). On the two sides (+) and (–) of the moving boundary $S$, we have Hooke's law:

$$\sigma^{\pm} = \mathbf{C}^{\pm} : \varepsilon^{e\pm}, \quad \varepsilon^{e} = \varepsilon - \varepsilon^{a}, \tag{7.177}$$

with elasticity tensors **C** and, if needed, compliance tensors **S**. On computing the jump of $w(\mathbf{r})$ from (7.174) and accounting for the usual symmetries of the **C**s, we obtain

$$[w(\mathbf{r})] = \langle\sigma\rangle : [\varepsilon - \varepsilon^{a}] + \frac{1}{2}(\varepsilon^{e})^{+} : [\mathbf{C}] : (\varepsilon^{e})^{-}, \tag{7.178}$$

or, equivalently, introducing the compliance tensors,

$$[w(\mathbf{r})] = \langle\sigma\rangle : [\varepsilon - \varepsilon^{a}] - \frac{1}{2}\sigma^{+} : [\mathbf{S}] : \sigma^{-}. \tag{7.179}$$

As a result (7.176) reads

$$\frac{d}{dt}\bar{\psi} = \frac{1}{V}\int_{V} \sigma : \dot{\varepsilon}^{e} dV - \frac{1}{V}\int_{S}\left(\langle\sigma\rangle : [\varepsilon^{e}] - \frac{1}{2}\sigma^{+} : [\mathbf{S}] : \sigma^{-} + [\varphi]\right)\nu_{n} dS. \tag{7.180}$$

We must also evaluate the power expended by external forces (tractions) on the external boundary $\partial V$ of the RVE. We have thus

$$p^{\text{ext}} = \frac{1}{V}\int_{\partial V} \mathbf{T}.\dot{\mathbf{u}} dS = \frac{1}{V}\int_{V} \operatorname{div}(\sigma.\mathbf{v}) dV + \frac{1}{V}\int_{S} [\mathbf{n}.\sigma.\mathbf{v}] dS, \tag{7.181}$$

where use has been made of the generalized Green–Gauss theorem. The evaluation of the integrand in the second contribution in (7.181) by use of the Maxwell–Hadamard lemma applied to [**v**] and [∇**u**] on account of the continuity conditions [**u**] = 0 and [**n**.σ] = **0** at $S$ yields

$$[\mathbf{n}.\sigma.\mathbf{v}] = -\langle\sigma\rangle : [\varepsilon]\nu_{n}. \tag{7.182}$$

Collecting terms, we have from (7.181)

$$p^{\text{ext}} = \frac{1}{V}\int_{V} \sigma(\mathbf{r}) : \dot{\varepsilon}(\mathbf{r}) dV - \frac{1}{V}\int_{S} \langle\sigma\rangle : [\varepsilon]\nu_{n} dS, \tag{7.183}$$

where we note that the *total strain* is involved here whereas the elastic strain is involved in (7.180).

The dissipation $d$ attached to the RVE is given by the difference between the power input in the system, $p^{\text{ext}}$, and the time change in free energy. Thus,

$$d = p^{\text{ext}} - \frac{d}{dt}\bar{\psi}. \tag{7.184}$$

This is straightforward on account of (7.183) and (7.180) and the remark just made about various strains. The result is

$$d = \frac{1}{V}\int_V \sigma : \dot{\varepsilon}^a dV + \frac{1}{V}\int_S f_S \, v_n dS, \tag{7.185}$$

in which we have defined the driving force $f_S$ acting on $S$ by

$$f_S := \left[ \varphi - \langle \sigma \rangle : \varepsilon^a - \frac{1}{2}\sigma^+ : \mathbf{S} : \sigma^- \right]. \tag{7.186}$$

This is consistent with the normal component of an Eshelby stress modified by the term involving stresses and the compliance tensor. The first contribution in (7.185) has the standard form of an intrinsic bulk dissipation (compare to (2.173)).

To complete the solution of the present problem, one would first have to evaluate the surface dissipation contribution in (7.185) and then implement a homogenization technique to pass from the RVE to the macroscopic behavior useful to engineers. This is outside the scope of the present book. Suffice it to notice that in many situations (e.g., dislocation loops, twinning, and formation of martensitic plates), the evolving boundaries summarized by the single symbolism $S$ may be considered as ellipsoid inclusions. This allows one to exploit another of Eshelby's powerful results about such inclusions; see Berveiller and Fischer (1997). In the case of martensitic transformations, the jump in chemical free energy is commonly approximated by the expression

$$[\varphi(\mathbf{r})] = -B(\theta - \theta_0), \tag{7.187}$$

where $\theta_0$ is the temperature at which the free energies of the two phases are equal (zero jump) and $B$ is a positive material constant. The final expression of the thermodynamic force deduced from (7.186) for nucleation and growth of martensitic microdomains belonging to different martensitic variants (there may be 24 such possible variants) in an austenitic single crystal is obtained

by Cherkaoui and Berveiller (2000, Equation 55 and applications thereof). Other related works are by Fischer and Reisner (1998) and Cherkaoui et al. (1998).

### 7.8.3 Remark on a Mechano-Biological Problem

Some physiological problems involving mechanics may look like problems dealing with phase-transition fronts. This is the case of the growth of long bones under the influence of mechanical factors. Here the main phenomenon is the growth at the so-called growth plate $\Gamma$ that connects the metaphyseal bone and the epiphyseal bone (cf. Sharipova et al., 2008). This transition zone, which may be called the "chondro-osseous junction" (from bone to cartilage), has a very slow stationary motion that occurs with a competition between proliferation and hypertrophy of chondrocytes and ossification process. In spite of the complexity and multiplicity of processes involved in the activation of the different behaviors of the chondrocytes, the growth plate, considered as a singular surface of vanishingly small thickness, has a steady motion (during the lengthening of the bone that takes years) that is governed by a kinetic law such as

$$V_\Gamma = K\tau_N, \quad K > 0, \tag{7.188}$$

where (compare to (7.170))

$$\tau_N = -\mathbf{N}.\left[\mathbf{b}_S\right].\mathbf{N} = -\left(\mu_{\text{bone}} - \mu_{\text{cart}}\right), \quad \mathbf{b}_S = W\mathbf{1}_R - \mathbf{T}.\mathbf{F}, \tag{7.189}$$

so that the local dissipation inequality $V_\Gamma f_\Gamma \geq 0, f_\Gamma + \tau_N = 0$, is satisfied. Bone and cartilage have different elastic potentials. $\mathbf{N}$ is the unit normal to the growth plate, and both displacement and traction are continuous at $\Gamma$. The stability of the motion (7.188) can be studied. It is found that compression decreases the interface rate while traction favors the lengthening of the bone (increase in $V_\Gamma$), as experimentally observed (cf. Sharipova et al., 2008).

# 8

# *Singularities and Eshelby Stress*

## Object of the Chapter

Where Irwin, Griffith, Eshelby, Cherepanov, Rice, Budiansky, Sobolev and Schwartz, and many others join efforts to show that material-configurational forces provide the basic formulation of the theory of fracture, whether brittle or ductile, where topological changes take over and cause an irreversible thermodynamic evolution, yielding a global dissipation, where the total energy of a system is shown to consist of elastic energy and the appropriately defined energy of defects and, finally, where it is shown to the anxious reader how to devise evolution criteria for engineering purposes while good mathematics are at work in the background.

## 8.1 The Notion of Singularity Set

Considering the purely elastic case of Section 3.1, it may happen that the elastic solution of a boundary-value problem based on integrating (3.4) or (3.13) and the associated boundary conditions over a material body presents a singular behavior over a certain manifold. Working in three-dimensional physical space, these manifolds may only be of certain integer dimensions if we make abstraction of the appearance of fractals. Typically, one will observe the singularity of the strain and stress field at a *point*, along a *line* (in the case of dislocations, macroscopic cracks), or across a *two-dimensional surface* (in the case of a shock wave or a phase-transition front). The last case was in fact considered at length in the preceding chapter where the singularity amounted to a finite discontinuity in the basic fields (strains, velocities). Following Dascalu and Maugin (1994)—also Maugin (1998)—one must clearly distinguish between what may thus be considered an *elastic defect*, $D$, and what is the *set of extension points*, $ED$, of the said elastic defect. For example, in the crack problem, the defect $D$ is really two-dimensional (the crack itself, flat or not, with its two faces), while the set $ED$ is the line representing the

front or tip of the crack. This line itself can be obtained by a limiting process involving a family of open notches (see Section 8.2). In two dimensions, the crack is seen as a line (or a curve) in a plane and the crack tip as an *ED* point. The situation is similar for dislocations, where *D* in fact is the missing half plane of atoms, while *ED* is the dislocation line. For shock waves and phase-transition fronts—see Chapter 7—the material on one side of the singular surface across which fields suffer finite discontinuities governed by the second law of thermodynamics sees the other side as the *invading* or *progressing* defect, which is therefore three-dimensional (a volume), *ED* being really the singular surface itself. The same holds true for the growth of a cavity where *D* is the cavity itself (therefore three-dimensional; an open set of $R^3$) and *ED* is the surface of the cavity.

In other problems such as the appearance of *damage*, *plasticity*, and *growth*, *ED* is potentially the whole body. This is particularly evident in the case of *volumetric growth* (cf. Epstein and Maugin, 1999, 2000) or elastoplasticity. This does not mean that there does not exist a surface separating the already damaged, plasticized, or grown 3-D region from the rest of the body, and we can speak of the damage boundary, plastic boundary, and so on, which is obviously 2-D and is an *unknown* in the evolution problem (free-boundary problem) resulting from the time evolution of physical (Newtonian) loads. However, in all cases the driving force causing the growth of the considered defect *D* is acting on the set of extension points *ED*, which is therefore one-, two-, and three-dimensional for dislocations and cracks, shock waves, and phase-transition fronts (and also walls between domains in ferroelectrics and ferromagnets), and damage, plasticity, and growth, respectively. In Chapter 7 where the *ED* set was a surface, we simply mentioned that the basic fields were discontinuous at the *ED* set. This allows one to exploit the Maxwell–Hadamard jump conditions on derivatives of these fields. In the present chapter, the situation is, as we shall see, more involved, because we need to know the degree of singularity of fields to proceed with their thermomechanical behavior. We illustrate this first with the case of *brittle fracture*. But the preceding discussion hints at introducing the *energy* of an elastic defect as a quantity defined over *D* (Dascalu and Maugin, 1994), and this contradicts a classical vision; for instance, the energy of a defect such as a cavity is a bulk energy and *not* a surface energy. Before working in the general framework, let us recall what the basic problem of fracture is.

## 8.2 The Basic Problem of Fracture and Its Singularity

The fundamental problem that we have to face is shown in a schematic way in Figure 8.1. The two "lips" $\Sigma^{\pm}$ of a straight crack $\Sigma$, a semiplane of infinite extent in the direction perpendicular to the figure, under the effect of some traction

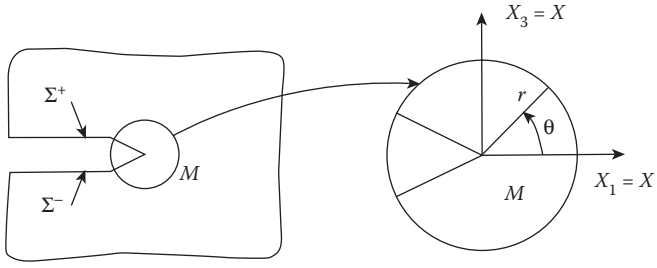


**FIGURE 8.1**
Straight-through crack (frame moving with the tip). (Adapted from, Maugin, G.A., *The thermomechanics of plasticity and fracture*. p. 13, Cambridge: Cambridge University Press. 1992.)

applied at the boundary of an elastic body, are separated, and, although under the effect of new forces they might come back in contact, we admit that this contact cannot solder back the lips of the crack. Accordingly, along Σ, there is absence of cohesion and, therefore, incapacity of the material to further transmit across Σ a stress whose normal component is a traction. Although *elasticity* is the mechanical behavior considered in so-called *brittle fracture*, globally the phenomenon of fracture is *thermodynamically irreversible*. By crack *front* we mean the neighborhood of the end point $M$ of the crack and the *tip* of the crack at this end point. The fundamental problem of fracture is whether, starting with a given length $l$ of the crack, this length will grow or remain constant under the influence of external stimuli (applied tractions). Of course, whether the crack continues in its direction or curves or branches is also a most relevant question, but that comes next. An astute way to approach the solution from the engineering viewpoint is to introduce a *growth or extension criterion* for cracks. For example, the purely *elastic* solution of an elastic problem involving a straight crack in a body of finite extent exhibits a singularity in stresses at the tip of the crack. Roughly speaking, the elastic displacement of the solution in the neighborhood of the tip is of the type (various techniques can be used to prove this, including the complex-function representation of two-dimensional elasticity problems; see Maugin, 1992, Appendix 4):

$$\mathbf{u} = \sqrt{r}\, K\mathbf{f}(\theta), \tag{8.1}$$

where $\mathbf{f}(\theta)$ is a vector-valued function depending only on the polar angle θ in Figure 8.1, $r$ is the radius vector from the tip of the crack, and $K$ is a numerical factor called the *stress-intensity factor* (see the following) with physical dimension (pressure) $\times\sqrt{m}$, which depends on the considered boundary-value problem. As the elastic stress in linear elasticity behaves like $\nabla\mathbf{u}$, we have the following behavior as $r$ goes to zero at $M$:

$$\sigma \cong \frac{1}{\sqrt{r}} Kg(\theta), \tag{8.2}$$

where $g(\theta)$ is an angular distribution function. Then Irwin and Kries (1951), in a celebrated paper, proposed the following *growth criterion for fracture*:

1. If $K < K_c$, there is no propagation, symbolically $\dot{l} = 0$.
2. If $K = K_c$, then propagation is *possible*, that is, symbolically $\dot{l} \neq 0$, but we do not know whether it will actually happen or not, so that $\dot{l} = 0$ is not excluded.

Here $K_c$ is a characteristic material parameter called the *fracture toughness* or *tenacity* (expressed in $(Pascal) \times \sqrt{m}$). The previously stated criterion conveys the simple idea that we must "pull rather strongly" to obtain some crack propagation. But a global reasoning involving a possible extension of the crack and acknowledging the irreversible nature of the global phenomenon is certainly more satisfactory. We present such an analysis in quasistatics for small strains.

## 8.3 Global Dissipation Analysis of Brittle Fracture

Consider Figure 8.1 and a system of tractions $\mathbf{T}^d$ acting on the boundary $\partial V$ of the body except along the traction-free lips of the crack. We neglect body forces if any. Then the *global dissipation* is the difference between the power expended by external forces (here tractions) and the time-rate of change of the stored (potential) elastic energy. We already exploited such a reasoning in Section 7.8.2 for a RVE instead of a whole body. That is, we write

$$D(V) = \int_V \mathbf{T}^d . \dot{\mathbf{u}} \, dV - \frac{d}{dt} \int_V W(\boldsymbol{\varepsilon}) dV, \tag{8.3}$$

with $\mathbf{T}^d = \mathbf{n}.\boldsymbol{\sigma}$ at $\partial V$ and $\boldsymbol{\varepsilon} = (\nabla \mathbf{u})_S$.

We must evaluate the right-hand side of (8.3) *when the crack is propagating*, that is, when the domain of integration is evolving in time. Of course, if the crack is not propagating and $\mathbf{T}^d$ is a so-called dead loading, then (8.3) reduces to

$$D(V) = -\frac{d}{dt} E_{\text{potential}}(V), \tag{8.4}$$

that is, $D$ is the opposite of the time-rate of change of the total elastic potential energy. But this is zero in the absence of crack propagation as the global potential energy has reached a minimum, and this is left unchanged thereafter. But returning to the case of possible propagation, we must pay more

attention and be more cautious in the computation of the time derivative involved in (8.3). We must, in a sense, isolate the singularity occurring at the crack tip and write that derivative as

$$\frac{d}{dt}\int_V W(\varepsilon)dV = \frac{d}{dt}\int_{V_\Gamma} W(\varepsilon)dV + \frac{d}{dt}\int_{V-V_\Gamma} W(\varepsilon)dV, \tag{8.5}$$

where $V_\Gamma$ is the material volume enclosed in the contour surface $\Gamma$ around the crack tip. Let $(X,Y)$ be a frame attached to that tip in the two-dimensional representation in Figure 8.1. In computing $\dot{\varepsilon}$ we must use the composition rule for time derivatives between two frames, a fixed one, and one accompanying the $(X,Y)$ frame. Thus we can write

$$\dot{\varepsilon} = \dot{\varepsilon}_t(X,Y) - \varepsilon_{t,1}(X,Y)\dot{l}, \tag{8.6}$$

because $X = x - l(t)$, and the symbolism ",1" means the derivative with respect to $X$. As $\Gamma$ is fixed in the $(X,Y)$ frame, we have

$$\frac{d}{dt}\int_{V_\Gamma} W(\varepsilon)dV = \int_{V_\Gamma} \sigma : \dot{\varepsilon}_t(X,Y)dV, (X,Y) \text{ fixed}. \tag{8.7}$$

For the second contribution to (8.5), we must use Reynolds transport theorem for the material time derivative of a nonmaterial volume integral (here extended to $V - V_\Gamma$). With the present change of frame, which is just a time-dependent translation along the $x_1$-axis, this yields

$$\frac{d}{dt}\int_{V-V_\Gamma} W(\varepsilon)dV = \int_{V-V_\Gamma} \sigma : \dot{\varepsilon}dV - \int_\Gamma W(\varepsilon)\dot{l}n_1 d\Gamma, \tag{8.8}$$

where we have set $n_1 = \mathbf{n}.\mathbf{e}_1$, if $\mathbf{e}_1$ is the unit vector along the $x$- or $X$-axis. Noting, then, that $\mathbf{n}(\Gamma) = -\mathbf{n}(\partial(V - V_\Gamma))$ at $\Gamma$, we obtain

$$\int_V \sigma : \dot{\varepsilon}dV = \int_{\partial V-(-\Gamma)} \mathbf{T}^d.\dot{\mathbf{u}}dA - \int_\Gamma (\mathbf{n}.\sigma.\dot{\mathbf{u}})d\Gamma. \tag{8.9}$$

Collecting now the various contributions, we obtain the expression

$$D(V) = \int_{V_\Gamma} \sigma : \dot{\varepsilon}dV + \int_\Gamma \{W\dot{l}n_1 + (\mathbf{n}.\sigma).\dot{\mathbf{u}}\}d\Gamma. \tag{8.10}$$

The integrand in the first contribution is integrable (on account of the singularity order mentioned in Section 8.2). Hence the first contribution in (8.10) yields zero as we shrink $\Gamma$ to the tip of the crack. We are thus left with

$$D(V) = \lim \int_{\Gamma} \left( W \dot{l} n_1 + \mathbf{n}.\boldsymbol{\sigma}.\dot{\mathbf{u}} \right) d\Gamma \quad \text{as} \quad \Gamma \to 0. \tag{8.11}$$

But we can remark that for any physical quantity $f$ attached to the tip of the crack, $\dot{f}$ has the same singularity as $\left(-f_{,1}\dot{l}\right)$—compare Gurtin (1979a). This applies to $\dot{\mathbf{u}}$ in (8.11). Accordingly, factorizing out the extension speed $\dot{l}$, we can rewrite (8.11) in the following illuminating form:

$$D(V) = F(C)\dot{l}, \tag{8.12}$$

a typical bilinear dissipation form involving a "force" and a "velocity," where the *configurational* force $F(C)$ has been defined by

$$F(C) = \lim \int_{\Gamma} \left( W n_1 - \mathbf{n}.\boldsymbol{\sigma}.\mathbf{u}_{,1} \right) d\Gamma \quad \text{as} \quad \Gamma \to 0. \tag{8.13}$$

Two remarks are in order. First, in the limit, $F(C)$ is a quantity pertaining to the crack tip $C$. It is possible to show that $F(C)$ is also given by (cf. Maugin, 1992, pp. 149–151)

$$F = -\frac{\partial}{\partial l} W_{\text{potential}}(l). \tag{8.14}$$

Second, the "force" $F(C)$ is in fact *path-independent* as shown by a simple calculation involving two different contours of integration $\Gamma_1$ and $\Gamma_2$ (under the condition that the crack lips are indeed traction free and there are no body forces). Thus $F(C)$ is none other than the celebrated path-independent integral usually noted $J$, that is,

$$J = J_{\Gamma} = \int_{\Gamma} \left( W n_1 - \mathbf{n}.\boldsymbol{\sigma}.\mathbf{u}_{,1} \right) d\Gamma,$$

which may be referred to as a the *Eshelby–Cherepanov–Rice integral* in honor of the most prominent contributors to it (in chronological order, in particular, Cherepanov, 1967; Rice, 1968). The path-independence is a valuable property that allows one to select the integration contour in a manner that yields the simplest and least expensive computation.

## 8.4 The Analytical Theory of Brittle Fracture

Now we can look at the same problem but in *finite strains* and *full dynamics* in a much more powerful framework, that of material-configurational forces. To that purpose, we consider general anisotropic finite-strain elasticity in *materially homogeneous* bodies. Outside singularity sets (at all regular material points $\mathbf{X}$ in $B$) we have locally the following reduced forms of the momentum equation in spatial Piola–Kirchhoff and completely Eshelbian formats (cf. Chapter 3):

$$\frac{\partial \mathbf{p}}{\partial t} - \mathrm{div}_R \mathbf{T} = \mathbf{0}, \quad \frac{\partial \mathbf{P}}{\partial t} - \mathrm{div}_R \mathbf{b} = \mathbf{0}, \tag{8.15}$$

with

$$\begin{aligned} &\mathbf{p} = \rho_0 \mathbf{v}, \quad \mathbf{P} = -\mathbf{p}.\mathbf{F}, \quad \mathbf{b} = -\big((K - W)\mathbf{1}_R + \mathbf{T}.\mathbf{F}\big), \\ &\mathbf{T} = \partial \bar{W}(\mathbf{F})/\partial \mathbf{F}, \quad W = \bar{W}(\mathbf{F}). \end{aligned} \tag{8.16}$$

On account of the assumed smoothness of all fields (in particular, $\mathbf{F}$ and $\mathbf{v}$), the two equations (8.15) are entirely equivalent—redundant—according to the Noether–Ericksen identity. Each of these can be integrated over an extended *regular* material region $B = B_R$, where the Green-divergence and Reynolds' transport theorems can be used without specific precaution. We have commutation rules for space integration and time differentiation since $(\mathbf{X},t)$ is a good set of independent space–time parameters from that viewpoint. We obtain thus

$$\frac{\partial}{\partial t}\int_B \mathbf{p}\, dV = \int_{\partial B} \mathbf{N}.\mathbf{T}\, dA, \tag{8.17}$$

$$\frac{\partial}{\partial t}\int_B \mathbf{P} dV = \int_{\partial B} \mathbf{N}.\mathbf{b}\, dA. \tag{8.18}$$

Reasoning in the same way on the energy equation, in the absence of sources and heat conduction, we have

$$\frac{\partial}{\partial t}\int_B H dV = \int_{\partial B} \mathbf{N}.\mathbf{T}.\mathbf{v}\, dA. \tag{8.19}$$

Note that (8.17) and (8.18) are no longer in direct correspondence since convection is lost in the space integration. Equations 8.17 and 8.18 are meaningful component-wise only.

Now if the fields **v** and **T**, which are time and space derivatives of the basic field (motion), present a certain order of singularity over some subset of $M^3$, quantities like **P**, $H$, and **b** that are at least quadratic in these fields will even be *more* singular. Thus, if the stress **T** is *not* a good indicator of the presence of field singularities (see Maugin, 1995, Section 5), **b** may be a good indicator. This is exactly what happens in brittle fracture, where the integration of $(8.15_2)$ and the local energy equation over a subset of $M^3$ containing a field singularity *captures this singularity* by making additional nonvanishing terms, characteristic of the singularity, appear in global equations of the type of (8.18) and (8.19). These terms are, respectively, the *material driving force* acting on the singularity and the so-called *energy-release rate* associated with the energy consumed in the irreversible progress of the defect, that is, the evolution of *ED*; the two must be related through the notion of power expended by the driving force. We follow Dascalu and Maugin (1994) in this illustration of fracture. Note that the present case already illustrates the different roles played *at singular manifolds* by Equations $8.15_{1-2}$.

Following Rice (1968), a sharp-ended straight-through crack $C$ is viewed as the uniform limit of a family of end-rounded notches (cf. Figures 8.2 and 8.3). The flat faces of a notch and the rounded cylindrical end are assumed to be free of traction. We consider the body $B$ of limiting surface $\partial B$ excluding the notch, and the notch's end $\Gamma_\delta$, which is assumed to propagate inside the body with uniform material velocity $\bar{\mathbf{V}}$ parallel to the flat faces and to the axis $\mathbf{E}_1$. This region is regular but geometrically evolving in time (configurational change!) due to the extension of the notch. In integrating $(8.15_2)$ and the energy equation over $B$, we simply have to use generalized Green's and Reynolds' theorems. These yield (compare to (8.18) and (8.19))

$$\frac{\partial}{\partial t}\int_B \mathbf{P}dV + \mathbf{F}^{\text{notch}}(\delta) = \int_{\partial B} \mathbf{N}.\mathbf{b}\,dA, \tag{8.20}$$

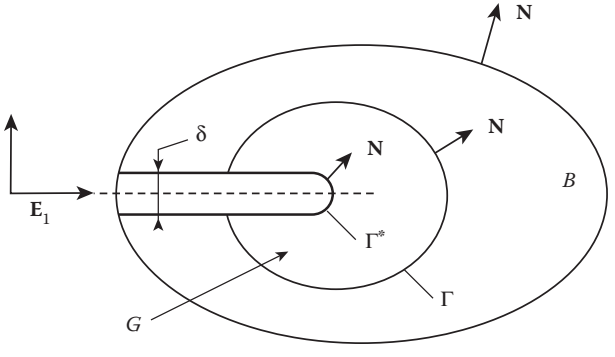


**FIGURE 8.2**
The notch problem. (Adapted from Dascalu, C. and Maugin, G.A., *C.R. Acad. Sci. Paris, Ser. II* 317, 1135–40, 1993.)

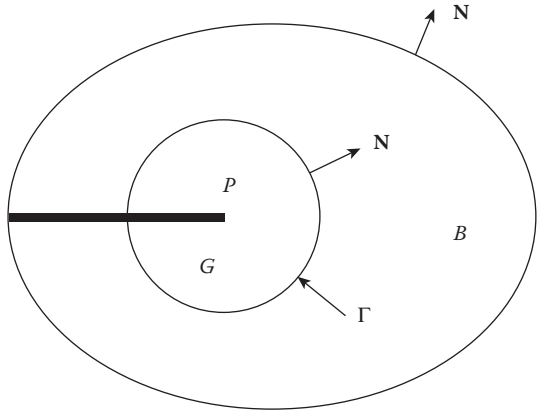


**FIGURE 8.3**
The limit straight-through crack problem. (Adapted from Dascalu, C. and Maugin, G.A., *C.R. Acad. Sci. Paris, Ser. II* 317, 1135–40, 1993.)

and

$$\frac{\partial}{\partial t}\int_B HdV + G^{\text{notch}}(\delta) = \int_{\partial B} \mathbf{N}.\mathbf{T}.\mathbf{v}\,dA, \tag{8.21}$$

where we have defined a material force $\mathbf{F}^{\text{notch}}(\delta)$ and an *energy-release rate* $G^{\text{notch}}(\delta)$ by

$$\mathbf{F}^{\text{notch}}(\delta) = \mathbf{E}_1 \int_{\Gamma_\delta} \left(P_1\left(\bar{\mathbf{V}}.\mathbf{N}\right) - LN_1\right)dA, \tag{8.22}$$

and

$$G^{\text{notch}}(\delta) = \int_{\Gamma_\delta} H\left(\bar{\mathbf{V}}.\mathbf{N}\right)dA. \tag{8.23}$$

Assuming the convergence of the family of notches indexed δ toward the sharp crack and that the limit of the solutions of the corresponding sequence of elasticity problems converges toward the solution for the sharp crack and the first term in each of (8.20) and (8.21) converges to zero in this limit (this follows from the singularity of elasticity solutions and the fact that $\mathbf{v} + \mathbf{F}.\mathbf{V} = 0$), we obtain for the driving force on the crack and the corresponding energy-release rate the following illuminating formulas:

$$\mathbf{F}^{\text{crack}} = -\lim_{\delta\to 0} \mathbf{E}_1 \int_{\Gamma_\delta} \left(LN_1 - P_1\left(\bar{\mathbf{V}}.\mathbf{N}\right)\right)dA, \tag{8.24}$$

$$G^{\text{crack}} = \lim_{\delta \to 0} \int_{\Gamma_\delta} H\left(\bar{\mathbf{V}}.\mathbf{N}\right) dA. \tag{8.25}$$

We have referred to these two basic formulas as those of the *analytical theory of brittle fracture*, because they involve the elasticity Lagrangian and Hamiltonian densities. The meaning of (8.25) is clear: It represents the energy consumed ("swallowed") per unit time by the inward crack motion. The tip of the crack acts as an *energy sink*.

But we can equally well integrate ($8.15_2$) and the energy equation over the regular material region of volume extension $G$ of external (cylindrical) boundary $\Gamma$ equipped with unit outward normal $\mathbf{N}$ and the notch as indicated in Figure 8.2, and moving inward with uniform material velocity $\bar{\mathbf{V}}$. Combining, then, the resulting expression with (8.24) and (8.25), we obtain more classical (but less elegant) formulas for the quantities in (8.24) and (8.25):

$$F_1^{\text{crack}} = \int_\Gamma \left( \left(\mathbf{N}.\mathbf{b}\right)_1 + P_1 \left(\bar{\mathbf{V}}.\mathbf{N}\right) \right) dA - \frac{\partial}{\partial t} \int_G P_1 \, dV \tag{8.26}$$

and

$$G^{\text{crack}} = \int_\Gamma \left( H\left(\bar{\mathbf{V}}.\mathbf{N}\right) + \mathbf{N}.\mathbf{T}.\mathbf{v} \right) dA - \frac{\partial}{\partial t} \int_G H dV. \tag{8.27}$$

It is readily checked that (8.26) reduces to the celebrated path-independent $J$-integral of brittle fracture in quasistatics and small strains. Indeed, in these conditions, the material momentum and kinetic-energy contributions are discarded, and

$$\mathbf{F} = \mathbf{1} + \left(\nabla_R \mathbf{u}\right)^T, \tag{8.28}$$

where $\mathbf{u}(\mathbf{X}, t)$ is the elastic displacement. On expanding the expression of $\mathbf{T}.\mathbf{F}$, we find that the first contribution in the stress contributes nothing because of its order of singularity, and there remains the well-known expression

$$F^{\text{crack}} = J = \int_\Gamma \left( WN_1 - \mathbf{t}.\frac{\partial \mathbf{u}}{\partial X_1} \right) dL \tag{8.29}$$

per unit thickness of the body, where $\mathbf{t}$ is the traction at $\Gamma$.

More remarkably, a relationship can be established between (8.25) and (8.24) in the fully dynamic and finite-strain case. Following Gurtin (1979)

and Nguyen Quoc Son (1980), let $P$ be a point of $\Gamma_\delta$ for the notch $\delta$ and $\mathbf{r}$ the vectorial position of any point with respect to $P$. We can write

$$\chi(\mathbf{X},t) = \chi(\mathbf{X}_P + \mathbf{r},t), \tag{8.30}$$

and through differentiation

$$\mathbf{v} = -\mathbf{F}.\bar{\mathbf{V}} + \frac{\partial\bar{\chi}}{\partial t}, \quad \bar{\mathbf{V}} := \frac{\partial \mathbf{X}_P}{\partial t}. \tag{8.31}$$

On multiplication by $\mathbf{F}^{-1}$ to the left of $(8.31_1)$, we get

$$\mathbf{V} = \bar{\mathbf{V}} - \mathbf{F}^{-1}.\frac{\partial\bar{\chi}}{\partial t}, \quad \bar{\mathbf{V}} // \mathbf{E}_1. \tag{8.32}$$

Let all the points of $\Gamma_\delta$ be in uniform motion; then we can reasonably assume that the deformation is the same at all points of $\Gamma_\delta$ and set $\partial\bar{\chi}/\partial t = \mathbf{0}$. Since the only nonzero component of $\bar{\mathbf{V}}$ is along $\mathbf{E}_1$, multiplying the one-component of (8.22) by $\bar{V}_1$, and accounting for the simplified form of (8.32) and the identity $\mathbf{V.C.V} = \mathbf{v}^2$, we obtain for the notch

$$G^{\text{notch}}(\delta) = \bar{V}_1 F_1^{\text{notch}}(\delta). \tag{8.33}$$

Accordingly, for a uniform motion of the points of the notch, we find that the material force driving the notch coincides with the energy released during the notch progress of a unit length inside the body. The relation in (8.33) is meaningful only if $\bar{\mathbf{V}}$ is not a function of $\mathbf{X}$. This shows the intimate relationship between the notion of material configurational force with that of rigid-body ("en bloc") motion. In the limit case of the straight crack, we obtain

$$G^{\text{crack}} = \bar{V}_1 F_1^{\text{crack}}. \tag{8.34}$$

This is the *dissipation rate* due to the crack extension. It is in the classical bilinear form favored in irreversible thermodynamics. It is thus ready for the construction of *crack-extension criteria*, the relationship between $\bar{V}_1$ and $F_1^{\text{crack}}$ (see Maugin, 1992, 1999, for this).

We finally note that (8.33) happily complements (8.24) and (8.15) of the analytical theory of brittle fracture, for it can be established only through passing from the Lagrangian to the Hamiltonian density thanks to the material-momentum contribution and (8.31), which allows the required

*Legendre transformation* between those two quantities. This has not often been acknowledged in the wealth of works on fracture that miss or do not emphasize the importance of working simultaneously with *both* the energy and material momentum (in a sense, reasoning in space–time) so as to keep the consistency between canonical momentum and energy.

## 8.5 Singularities and Generalized Functions

### 8.5.1 The Notion of Generalized Function or Distribution

Special mathematical tools have been devised, starting in the nineteenth century, to deal with singular fields. Noteworthy among these is the notion of the *Cauchy–Hadamard principal valu*e of an integral. But one had to wait until the 1940s to see the appearance of a perfectly adapted notion, that of the *generalized function* or *distribution*, especially formulated by the French mathematician Laurent Schwartz, following pioneering works by Jacques Hadamard and Jean Leray in France and S.L. Sobolev in Russia. By transferring operations of differentiation on sufficiently smooth *test functions* after integration by parts over a compact support, this allows for the weak formulation of solutions of partial differential equations that admit singular behaviors at points or jump discontinuities across surfaces. The principle of virtual power in continuum mechanics may itself be considered an exemplary use of a distributional formulation in which the role of test functions is played by virtual fields of displacements or velocities (see, e.g., Maugin [1980] for this functional setting). The theory of cracks in particular and, more generally, of "elastic defects" should have the theory of distributions as its natural background. But few authors have worked along this line, probably because of a lack of sufficient mathematical education (a notable exception is H.D. Bui and coworkers). Just to give some flavor of what generalized functions are (which we could have exploited in Chapter 7), consider the problem of finding the weak formulation equivalent to the following "nonlinear wave equation" in one dimension of space for the field $u$ (as may occur in continuum mechanics):

$$\frac{\partial u}{\partial t}+\frac{\partial}{\partial x}\left(\frac{1}{2}u^2\right)=0. \tag{8.35}$$

To obtain the looked for *weak* formulation, we multiply (8.35) by an arbitrary sufficiently continuous test function $w(x, t)$, for example, of class $C^1(R^2)$ and of bounded support $K$ on $R^2$ with $w=0$ on the boundary $\partial K$ of $K$ and $w=0$ outside $K$. If $u(x, t)$ is also of class $C^1$ with the initial condition

$u(x,0)=\phi(x)$, $x \in R$, then by integration in space and time of the product of (8.35) with $w$, we obtain

$$\int_{-\infty}^{+\infty}\int_{t=0}^{+\infty}\left(u\frac{\partial w}{\partial t}+\frac{u^2}{2}\frac{\partial w}{\partial x}\right)dxdt+\int_{-\infty}^{+\infty}\phi(x)w(x,0)dx=0. \tag{8.36}$$

Indeed, all derivatives are now applied to the test function. We can, therefore, consider (8.36) as a starting point for solutions $u(x, t)$, which are only piecewise continuous, admitting a finite discontinuity across a shock wave $\Sigma$ of equation $\Sigma(x, t) = 0$ in the $(t, x)$-plane, the local slope being $(dx/dt)_\Sigma$. Call $x = \sigma(t)$ another, explicit, form of the equation of $\Sigma$. Then at $\Sigma$ one has the following Rankine–Hugoniot equation:

$$[u](\langle u\rangle-(d\sigma/dt))=0, \tag{8.37}$$

with the usual meaning of jump and mean value for the symbolisms [..] and < .. > , respectively. Equation 8.37 means that for a truly jump solution the shock speed is the mean value of the "material particle" velocity on both sides of the shock. This peculiar result is due to the simplicity of the starting Equation 8.35.

What we do in the sequel of this section is, following Dascalu and Maugin (1994), show, thanks to the distribution formalism, that (i) the very structure of elasticity theory and the singularity order of elastic solutions dictate the expression of the *energy balance law* in the presence of cracks (or another defect) and (ii) a *Griffith-like surface energy criterion* follows of necessity. The argument applies to cracks but also to other defects such as cavities in expansion or progressing dislocation lines.

### 8.5.2 Basic Equations

We consider the simplest case of pure elasticity in quasistatics in the absence of any local thermomechanical sources. At any regular material point **X** in the body $B$ free of defects, we have the following basic equations of conservation of linear (physical) momentum, moment of momentum, and energy and material momentum:

$$\mathrm{div}_R\,\mathbf{T}=\mathbf{0}, \tag{8.38}$$

$$\mathrm{div}_R(\mathbf{x}\times\mathbf{T})=\mathbf{0}, \tag{8.39}$$

$$\frac{\partial W}{\partial t}-\mathrm{div}_R(\mathbf{T}.\mathbf{v})=0, \tag{8.40}$$

$$\mathrm{div}_R\,\mathbf{b} = \mathbf{0}, \tag{8.41}$$

with

$$\mathbf{T} = \partial W/\partial \mathbf{F}, \quad \mathbf{b} = W\mathbf{1}_R - \mathbf{T}.\mathbf{F}. \tag{8.42}$$

Equations 8.38 through 8.40 can also be written in the sense of distribution theory as

$$\mathrm{Div}_R\,\mathbf{T} + \bar{\mathbf{T}}^d\delta(\partial B) = \mathbf{0}, \tag{8.43}$$

$$\mathrm{Div}_R\,(\mathbf{x}\times\mathbf{T}) + (\mathbf{x}\times\bar{\mathbf{T}}^d)\delta(\partial B) = \mathbf{0}, \tag{8.44}$$

$$D_t W - \mathrm{Div}_R\,(\mathbf{T}.\mathbf{v}) - (\bar{\mathbf{T}}^d.\mathbf{v})\delta(\partial B) = 0, \tag{8.45}$$

where $\mathrm{Div}_R$ and $D_t$ are material gradients and time-derivative distributional operators, $\bar{\mathbf{T}}^d$ is the traction at the boundary $\partial B$, and $\delta(\partial B)$ is the (Dirac) delta distribution with support $\partial B$. The writing of (8.43) through (8.45) is a highly elegant way to incorporate the *natural* boundary conditions in the local statement of balance laws. In the presence of elastic defects (e.g., crack, cavity, dislocation), both Equations 8.43 and 8.44 are left unchanged while (8.45) takes a form including the "energy of the defect." This is what we show in the next section.

### 8.5.3 Case of Cracks

The theory of Griffith (1921) was the first attempt to attribute an energy to a defect in the form of surface tension (energy) on the crack faces. Here the existence of this specific energy of a crack is obtained using the distributional approach, the question being: What is the form taken by the energy equation (8.45) in the presence of an evolving crack?

We consider a straight edge crack in a linear elastic body. We choose a coordinate system centered at the intersection point of the crack with the boundary of $B$ such that the crack lies along the positive $x_1$-axis (Figure 8.4). If the tip of the crack has coordinates $(l,0)$, then the set of defect points $D$ is the closed interval $[0,l]$. We assume that the crack progresses in its own direction with the velocity $c(t) = \dot{l}(t)$. The crack faces $C$ are supposed to be traction free. The general form of the solution of the relevant boundary-value problem at each moment of time is (see Maugin, 1992)

$$\mathbf{u} = \mathbf{u}^s + \mathbf{u}^r, \quad \mathbf{T} = \mathbf{T}^s + \mathbf{T}^r, \tag{8.46}$$

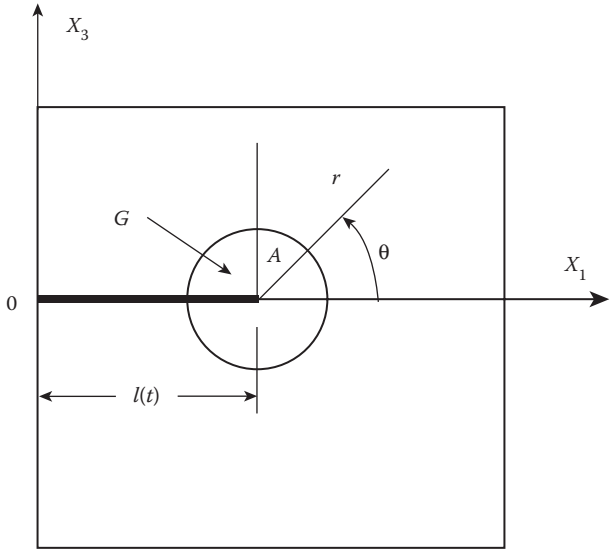


**FIGURE 8.4**
The crack problem revisited (distribution-theory approach). (Adapted from Dascalu, C. and Maugin, G.A., *Proc. R. Soc. London, Ser. A* 445, 23–37, 1994.)

where superscripts indicate the singular and regular contributions in the solution on account of the presence of the crack tip region. If $(r,\theta)$ are polar coordinates with respect to the crack tip, then $\mathbf{u}^S = 0\left(r^{1/2}\right)$, $\mathbf{T}^S = 0\left(r^{-1/2}\right)$—see (8.1) and (8.2)—both the displacement and the traction being continuous at $C$, while $\mathbf{u}^r$ and $\mathbf{T}^r$ are regular on $B$, satisfying the boundary conditions at $\partial B$. The particular expressions of these regular terms for the three modes of fracture give the regularity of the time derivatives:

$$\mathbf{v} = 0\left(r^{-1/2}\right), \quad \dot{W} = 0\left(r^{-2}\right). \tag{8.47}$$

As $W$ and $\mathbf{T}.\mathbf{v}$ have integrable singularities, they generate regular distributions on $R^2$. The function $\dot{W}$ is not integrable, but we can construct a regularization for it, denoted by $\dot{W}\big|_G$, a distribution that, restricted to $R^2 - \{A\}$, coincides with that generated by $\dot{W}$. Let $G$ be a disk centered in $A$ and moving with it (Figure 8.4) and define (cf. Gelfand and Shilov, 1964, Chap. 1):

$$\left\langle \dot{W}\big|_G, \varphi \right\rangle = \int_G \dot{W}\left(\varphi - \varphi(A)\right) da + \int_{R^2-G} \dot{W}\varphi\, da, \tag{8.48}$$

for $\varphi \in C_0^\infty\left(R^2\right)$, this distribution depending on $G$. The existence of the principal value of $W$ permits us to take the limit in (8.48) for $G \to 0$. The first

integral will vanish, and we obtain another distribution that coincides with $\dot{W}$ at regular points of *B*:

$$\left\langle PV\left(\dot{W}\right),\varphi\right\rangle = \lim \int_{R_2-G} \dot{W}\varphi da \quad \text{as} \quad G \to 0. \tag{8.49}$$

By using (8.48) and a differentiation formula on variable domains (Reynolds' theorem), we obtain thus

$$D_t W = \left.\dot{W}\right|_G + \left(\frac{d}{dt}\int_G W da - \int_\Gamma cWN_1 ds\right)\delta(l,0), \tag{8.50}$$

where Γ is the boundary of *G*, $N_1$ is the first component of the outward unit normal to *G*, and δ(*l*,0) is the Dirac distribution concentrated in *A*. The particular expressions giving the singular part of *W* show that the first integral term in the right-hand side of (8.50) vanishes in the limit as $G \to 0$, so that we have the alternate relation

$$D_t W = PV\left(\dot{W}\right) - \left(\lim \int_\Gamma cWN_1 ds\right)\delta(l,0). \tag{8.51}$$

But we continue with Equation 8.50. The vector field **T.v** generates a regular distribution, but div(**T.v**) is not integrable, so that we construct in a similar manner the regularization $\left(\text{div}\left(\mathbf{T}.\mathbf{v}\right)\right)\big|_G$. Then the divergence formula and the boundary condition lead to

$$\text{Div}\left(\mathbf{T}.\mathbf{v}\right) = \left(\text{div}\left(\mathbf{T}.\mathbf{v}\right)\right)\big|_G + \int_\Gamma \mathbf{N}.\mathbf{T}.\mathbf{v} ds\,\delta(l,0) + \bar{\mathbf{T}}^d.\mathbf{v}\,\delta(\partial B). \tag{8.52}$$

We use the traction-free condition to cancel the integral term on *C*. In every regular point the energy equation (8.40) holds, so that

$$\left(\text{div}\left(\mathbf{T}.\mathbf{v}\right)\right)\big|_G = \left.\dot{W}\right|_G, \tag{8.53}$$

and, gathering contributions, we finally have

$$D_t W + G * \delta(l,0) = \text{Div}\left(\mathbf{T}.\mathbf{v}\right) + \bar{\mathbf{T}}^d.\mathbf{v}\,\delta(\partial B), \tag{8.54}$$

where we have set (compare (8.27))

$$G^* = \int_\Gamma (cWN_1 + \mathbf{NT}.\mathbf{v})ds - \frac{d}{dt}\int_G W da. \tag{8.55}$$

Because all terms in (8.55) do not depend on the domain $G$, the same is true for $G^*$, which is the *energy released by the material* during the motion of the tip in a unit of time. The dynamic version of (8.55), already given in previous sections, was obtained by Gurtin and Yatomi (1980). To further transform this formula, we need to use the time-differentiation formula (Gurtin, 1979; Nguyen Quoc Son, 1980) $\dot{\mathbf{u}} = -c\mathbf{u}'_{,1} + \mathbf{u}'$, where $\mathbf{u}'$ has the same singularity as $\mathbf{u}$. Finally, taking the limit as $G \to 0$, the second integral in (8.55) vanishes, and the following result equivalent to (8.34) remains:

$$G^* = cF, \tag{8.56}$$

where $F$ is the driving force or path-independent $J$-integral of Rice and others. In this way, while (8.56) provides the dissipation due to the steady progress of the crack tip in the material, we find that the local balance of energy takes the form:

$$D_t W + \mathbf{c}.\mathbf{N}F\delta(l,0) = \mathrm{Div}(\mathbf{T}.\mathbf{v}) + \bar{\mathbf{T}}^d.\mathbf{v}\,\delta(\partial B). \tag{8.57}$$

The integral driving force $F$, which is an energy released during a unit length extension, is usually involved in a quasistatic fracture criterion $F = F_{\mathrm{cr}}$. If this holds at every time $t$, then the energy relation (8.57) takes on the form:

$$D_t\left(W + F_{\mathrm{cr}}H(l - x_1).\delta(x_2)\right) = \mathrm{Div}(\mathbf{T}.\mathbf{v}) + \bar{\mathbf{T}}^d.\mathbf{v}\,\delta(\partial B); \tag{8.58}$$

This is a *distributional* conservation law. We call the term

$$W_D := G_{\mathrm{cr}}H(l - x_1).\delta(x_2), \tag{8.59}$$

the *energy of the crack.* Here $H(l - x_1)$ is the Heaviside function of the interval $[0, l]$, and the dot in the right-hand side denotes the tensor product of distributions. Equation 8.58 shows, as we announced, that the material-plus-defect system is a *conservative* one. The preceding derivation, in contrast to that of Cherepanov (1967), shows that a quasistatic propagation criterion and the elasticity equations suffice to deduce the existence of the defect energy in (8.58). We also note that although the preceding analysis was carried on linear materials, known crack-tip singularities in nonlinear elastic materials

(see, for example, Knowles and Sternberg, 1972; Stephenson, 1982) conduce to the same result.

Although it was not mentioned since we focused on energy considerations, there also exists a distributional balance of material momentum that includes the driving force at the $ED = S$ set. This will read (proof left by way of exercise)

$$\mathrm{Div}\,\mathbf{b} + F_1^{\mathrm{crack}}\mathbf{E}_1\delta(S) + (\mathbf{N}.\mathbf{b})\delta(\partial B) = \mathbf{0}.$$

## 8.6 Variational Inequality: Fracture Criterion

The global phenomenon of fracture for a whole material specimen $V$, although in the frame of brittle fracture implying locally only an elastic behavior, is a *dissipative* phenomenon. As such, it cannot be reached at that global level through a variational principle that classically expresses a condition of extremum. Only a *variational inequality* evidencing a preferred direction of evolution—in other words, unilateral constraints—can secure a basis for a global formulation. Furthermore, the material character of the forces involved means that such a formulation must involve a $\delta_X$ variation (keeping $\mathbf{x}$ fixed and varying $\mathbf{X}$, a so-called material variation) or a mapping of the material manifold onto itself (a so-called local rearrangement). This was done by Stumpf and Le (1990) and Maugin and Trimarco (1992); see also Maugin (1993, pp. 136–139, 161–163). The proposed variational inequality involves the notion of surface energy, and for a crack of finite extent $\Sigma$ (Figure 8.5) and a homogeneous elastic body, it will read

$$\delta_R\{E(V-\Sigma) + E_S(\Sigma)\} \geq 0, \tag{8.60}$$

where

$$E(V-\Sigma) = \int_{V-\Sigma} W(\mathbf{F})dV, \quad E_S(\Sigma) = \int_{\Sigma} 2\gamma dA. \tag{8.61}$$

Here $2\gamma$ is the surface energy along $\Sigma$ in the tradition of Griffith (1921), for whom the cohesion energy at the crack plays a fundamental role in fracture: We must overcome or at least reach this energy level to have progression of the crack. This is nothing but the "energy of the crack" of the previous section when the crack progresses steadily. The variation denoted $\delta_R$ in (8.60) is to be understood as an infinitesimal variation of the material manifold onto itself at a material point $\mathbf{X}$. Locally, this is represented by the symbol $\delta_X\mathbf{Y}$ (see

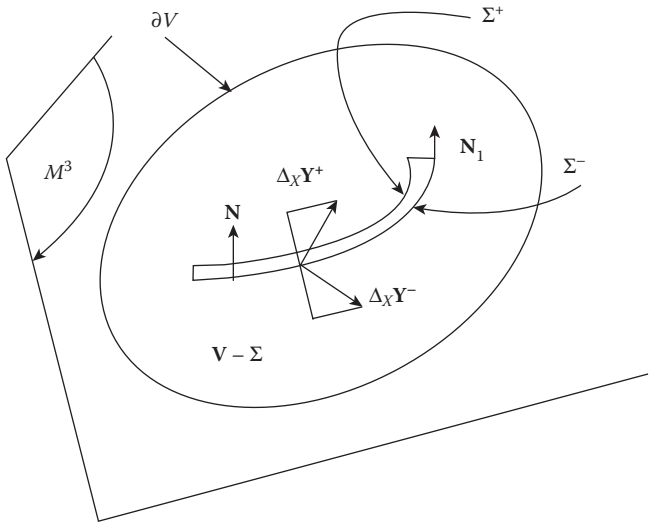


**FIGURE 8.5**
A crack with surface energy (variational formulation). (Adapted from, Maugin, G.A., *Material inhomogeneities in elasticity*. Figure 7.4, p. 163, London: Chapman & Hall. 1993.)

Maugin [1993, pp. 136–139], after Maugin and Trimarco [1992], for a definition of this). Here in fact

$$\delta_X \chi = -\mathbf{F}.\delta_X \mathbf{Y}. \tag{8.62}$$

In this variation the two faces of the crack should not overlap. This imposes a constraint that we can write in an obvious manner as (Figure 8.5)

$$\left|\mathbf{N}.\delta_X \mathbf{Y}^+ - \mathbf{N}.\delta_X \mathbf{Y}^-\right| \geq 0 \quad \text{at} \quad \Sigma. \tag{8.63}$$

The variation $\delta_R$ is also effected at the fixed boundary $\partial V$, so that the work of applied tractions does not appear in (8.60). The variation of the elastic-energy term in (8.60) is done just as in Section 3.9 since we are in quasistatics; that is, it is shown that

$$\delta_R \int_{V-\Sigma} W dV = -\int_{V-\Sigma} \left(\mathrm{div}_R \mathbf{b}\right).\delta_X \mathbf{Y} dV + \int_{\Sigma} \left(\mathbf{N}.\mathbf{b}\right).\delta_X \mathbf{Y} d\Sigma - \int_{\partial\Sigma} \mathbf{F}\left(\partial\Sigma\right).\delta_X \mathbf{Y} dL, \tag{8.64}$$

while the variation of the surface energy term in (8.60) yields (compare (7.169))

$$\delta_R \int_{\Sigma} 2\gamma d\Sigma = -\int_{\Sigma} 2\gamma \Omega \mathbf{N}.\delta_X \mathbf{Y} d\Sigma + \int_{\partial\Sigma} 2\gamma \mathbf{N}_1.\delta_X \mathbf{Y} dL, \tag{8.65}$$

where we accounted for the existence of the edge of the crack ($\mathbf{N}_1$ being defined in Figure 8.5) and the material force $\mathbf{F}(\partial\Sigma)$ is given by

$$\mathbf{F}(\partial\Sigma) = \lim \int_{\Gamma} \mathbf{N}.\mathbf{b}\, d\Gamma \quad \text{as} \quad \Gamma \to 0, \quad \mathbf{b} := W\mathbf{1}_R - \mathbf{T}.\mathbf{F}. \tag{8.66}$$

The proof of (8.64) involves the exploitation of a generalized Green-Gauss theorem for a disklike crack where $\Gamma$ is the normal circular section of a torus-like surface leaning on the contour of the disk (see Figure 7.2 in Maugin, 1993, p. 154). Of course, the force given by (8.66), when projected onto $\mathbf{N}_1$, is none *other* than the path-independent *J*-integral.

Gathering the results (8.64) and (8.65) in (8.60), we deduce from the latter the following results:

$$\mathrm{div}_R \mathbf{b} = \mathbf{0} \quad \text{in} \quad V - \Sigma, \tag{8.67}$$

$$\mathbf{N}.[\![\mathbf{b}]\!] = 2\gamma\Omega\mathbf{N} \quad \text{on} \quad \Sigma, \tag{8.68}$$

$$\{2\gamma\mathbf{N}_1 - \mathbf{F}(\partial\Sigma)\}.\delta_X\mathbf{Y} \geq 0 \quad \text{at} \quad \partial\Sigma, \tag{8.69}$$

to which must be adjoined the unilateral constraint (8.63).

While (8.67) is the now-standard equilibrium form of the balance of material momentum in the absence of external force, both Equations 8.68 and 8.69 deserve special comments. On the one hand, (8.68) clearly reminds us of the *Laplace equation for a membrane* with surface tension (or energy). This result was criticized by Gurtin (1999, p. 197fn) because it essentially deals only with the normal component, leaving a part (the tangential part of $\mathbf{N}.[\![\mathbf{b}]\!]$) indeterminate. A Marangoni-like effect introducing a variation of surface tension along the surface would remove this indeterminacy. On the other hand, (8.69) in fact represents the looked-for *fracture criterion*. For instance, for a plane-through crack of infinite extent in the direction perpendicular to the plane of Figure 8.5, and a possible propagation only in the direction of $\mathbf{N}_1$ (no branching or curving), (8.69) reduces to

$$(2\gamma - J)\delta l \geq 0, \quad \delta l \equiv \mathbf{N}_1.\delta_X\mathbf{Y} \geq 0. \tag{8.70}$$

This yields either

$$2\gamma \equiv J_{\mathrm{cr}} = J \quad \text{for} \quad \delta l \geq 0, \tag{8.71}$$

or

$$J < J_{\mathrm{cr}} = 2\gamma \quad \text{for} \quad \delta l = 0. \tag{8.72}$$

This is nothing but a fracture criterion in the manner of Griffith. That the *J*-integral can be viewed as the main ingredient in a fracture criterion was elaborated on by Landes and Begley (1972).

## 8.7 Dual *I*-Integral of Fracture

All developments so far in this chapter rely on the exploitation of the elastic strain energy function, most often simultaneously with the consideration of the direct-motion description. It was natural, after the introduction of the *J*-integral based on these arguments, that the complementary energy would be used to introduce a *dual* formulation, hence the notion of *I*-integral as introduced originally by Bui (1973) in small strains and quasistatics. In these conditions the *I*-integral reads (using the same definitions as for the *J*-integral)

$$I = \lim \int_{\Gamma} \left( -W_c\left(\boldsymbol{\sigma}\right) n_1 + \mathbf{n}.\frac{\partial \boldsymbol{\sigma}}{\partial x_1}.\mathbf{u} \right) d\Gamma \quad \text{as} \quad \Gamma \to 0, \tag{8.73}$$

where $W_c$, the complementary elastic energy, is related to the strain energy $W$ by the Legendre transformation

$$W(\boldsymbol{\varepsilon}) + W_c\left(\boldsymbol{\sigma}\right) = \boldsymbol{\sigma} : \boldsymbol{\varepsilon} \equiv \mathrm{tr}(\boldsymbol{\sigma}.\boldsymbol{\varepsilon}), \quad \boldsymbol{\sigma} = \frac{\partial W}{\partial \boldsymbol{\varepsilon}}, \quad \boldsymbol{\varepsilon} = \frac{\partial W_c}{\partial \boldsymbol{\sigma}}. \tag{8.74}$$

**EXERCISE:** To prove directly that $I = J$, take the integral over a bounded surface $S$ of unit outward normal n of the first of (8.74) and use the facts that $\boldsymbol{\sigma}$ is symmetric and divergence free.

H.D. Bui has shown that $I$ is none other than the *decrease rate* of the total complementary energy per increase in the length of the crack, that is,

$$I = -\frac{\partial}{\partial l} E_c\left(l\right), \tag{8.75}$$

with

$$E_c\left(V\right) = -\int_V W_c\left(\boldsymbol{\sigma}\right) dV + \int_{\partial V_1} \mathbf{n}.\boldsymbol{\sigma}.\mathbf{u}^d dA, \tag{8.76}$$

where the displacement $\mathbf{u} = \mathbf{u}^d$ is prescribed on the part $\partial V_1$ of $\partial V$, while $\bar{\mathbf{T}}^d$ is a prescribed traction on the complementary part of $\partial V$. With an evolution

of the length of the crack, the expression (8.76) is shown to depend on $l$ as established by Bui.

But the preceding formulation can be generalized to finite strains as shown by Trimarco and Maugin (1995). To do this, one has to account for the developments given in Section 3.8. According to these developments the relevant variational formulation is given by (3.91), where, we remind the reader,

$$\mathbf{E}^{(-2)} = \frac{1}{2}\left(\mathbf{1}_R - \mathbf{C}^{-1}\right) = \frac{1}{2}\left(\mathbf{1}_R - \mathbf{F}^{-1}\mathbf{F}^{-T}\right),$$

with

$$\bar{\mathbf{S}} = J_F^{-1}\partial W_{(3)}/\partial \mathbf{E}^{(-2)}, \quad W_c^* = W_c\left(\bar{\mathbf{S}}, \mathbf{X}\right), \quad \mathbf{E}^{(-2)} = \partial W_c^*/\partial \bar{\mathbf{S}}.$$

Note that $\bar{\mathbf{S}}$ is the covariant associate of the second (contravariant) Piola–Kirchhoff stress.

The variational formulation yields in the bulk (i.e., at regular points)

$$\mathrm{div}\left(J_F^{-1}\bar{\mathbf{S}}\mathbf{F}^{-1}\right) - J_F^{-1}\nabla_R.\left(\mathbf{E}^{(-2)}.\bar{\mathbf{S}} - W_c^*\right) - J_F^{-1}\frac{\partial W_c^*}{\partial \mathbf{X}} = \mathbf{0}.$$

This equation can also be written as

$$\mathrm{div}_R\left(\bar{\mathbf{S}}\mathbf{C}^{-1}\right) - \nabla_R.\left(\mathbf{E}^{(-2)}.\bar{\mathbf{S}} - W_c^*\right) - \frac{\partial W_c^*}{\partial \mathbf{X}} = \mathbf{0}.$$

Now consider the following identity (free running index is the one related to $\partial/\partial\mathbf{X}$):

$$\nabla_R W_c^* - \mathrm{tr}\left(\mathbf{E}^{(-2)}.\frac{\partial \bar{\mathbf{S}}}{\partial \mathbf{X}}\right) - \frac{\partial W_c^*}{\partial \mathbf{X}} = \mathbf{0}. \tag{8.77}$$

By taking the scalar product of this with $\delta_x\mathbf{X} = \delta\mathbf{X}$, and integrating over a domain $D$ included in $V$, and applying the Green–Gauss theorem while noting that $\mathbf{G} = \mathbf{F}^{-1} - \mathbf{1}_R = \nabla\mathbf{U}$, $\mathbf{U} = \mathbf{X} - \mathbf{x}$, we obtain a lengthy expression that expresses the variation of the so-called $H$-integral, that is,

$$H = \int_{\partial\mathbf{D}} \left\{ -W_c^*\,\mathbf{N}.\mathbf{e}_1 - \frac{\partial \bar{\mathbf{S}}}{\partial X_1} : \left(\mathbf{1}_R - \mathbf{E}^{(-2)}\right)\mathbf{N}_D.\mathbf{U} \right\} dS, \tag{8.78}$$

where

$$\mathbf{E}^{(-2)} = -\frac{1}{2}\left(\mathbf{G} + \mathbf{G}^T + \mathbf{G}\mathbf{G}^T\right), \quad \frac{\partial \bar{\mathbf{S}}}{\partial X_1} = \left(\mathbf{e}.\frac{\partial}{\partial \mathbf{X}}\right)\bar{\mathbf{S}}, \quad \delta\mathbf{X} = \mathbf{e}\delta l.$$

It is shown (Trimarco and Maugin, 1995) that sufficient conditions for $\delta H$ to be independent of $\partial D$ read

$$\nabla_R.\delta\mathbf{X} = 0, \quad \mathrm{div}_R\left(\frac{\partial \bar{\mathbf{S}}}{\partial \mathbf{X}}.\delta\mathbf{X}\right)\mathbf{C}^{-1} = \mathbf{0} \quad \text{in} \quad D - \bar{\mathbf{X}} \tag{a}$$

where $\bar{\mathbf{X}}$ is the site of a point-wise inhomogeneity. The second of (a) expresses the requirement for the stress $\left(\partial\bar{\mathbf{S}}/\partial\mathbf{X}\right).\delta\mathbf{X}$ to be statically admissible in finite homogeneous deformations or in infinitesimal deformations. It is then possible to write that

$$H = \mathbf{F}^{\mathrm{inh}}\left(\bar{\mathbf{X}}\right).\mathbf{e} \quad \text{at} \quad \bar{\mathbf{X}} \in D, \quad \text{and} \quad 0 \quad \text{at} \quad \mathbf{X} \in V - \bar{D}, \tag{8.79}$$

with

$$\mathbf{F}^{\mathrm{inh}} = -\int_V \left(\frac{\partial W_c^*}{\partial \mathbf{X}}\right) dV. \tag{b}$$

Assuming that there exists a reference configuration in which the inverse image of the crack line is still a line, that the $H$-integral (8.78) can be defined in the two-dimensional case by supposing that $\bar{\mathbf{X}}$ represents an inhomogeneity, and that the problem is translationally invariant along the orthogonal direction to the plane, the spatial displacement field corresponding to the $\delta\mathbf{X}$ field reads

$$\delta\mathbf{x} = -\left(\mathbf{G} + \mathbf{1}_R\right)^{-1}.\mathbf{e}\delta l.$$

In the small-strain framework the $\mathbf{G}$ present in this expression is disregarded. The rigid translation of the whole body being in the direction $-\mathbf{e}$ while the tip of the crack is kept fixed (this is Bui's assumption), it is equivalent to the elementary displacement $\delta\mathbf{X}$ into the material in the direction $\mathbf{e}$ (see Figure 8.6). Then the conditions (a) are satisfied and (8.79) applies. The $H$-integral reduces to the $I$-integral on noticing that $\mathbf{U} = -\mathbf{u} = -(\mathbf{x} - \mathbf{X})$.

It can also be shown (Trimarco and Maugin, 1995) that

$$H = -\frac{\delta E_c}{\delta l}, \quad I = -\frac{\delta E_c}{\delta l}, \tag{8.80}$$

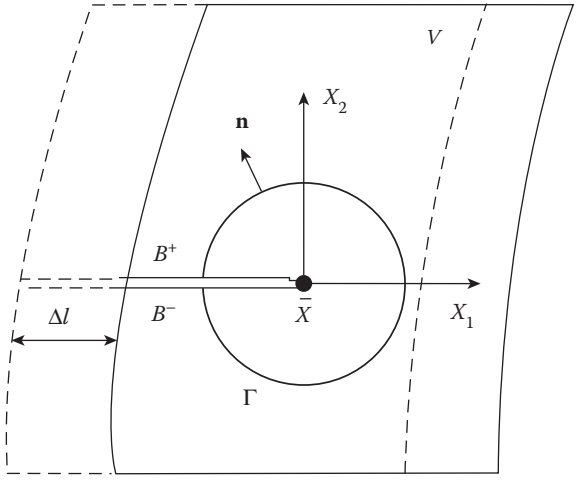


**FIGURE 8.6**
Inverse-motion motion vision of the extension of a crack. (Adapted from Trimarco, C. and Maugin, G.A., *Meccanica,* Figure 1, 30, 139–45, 1995.)

with

$$E_c = -\int_V W_c^* dV - \int_{\partial V_1} \bar{\mathbf{S}} : \mathbf{C}^{-1}\mathbf{N}.\mathbf{U}_0 dS,$$

or

$$E_c = -\int_v w_c dv - \int_{\partial v_1} J_F^{-1}\bar{\mathbf{S}}.\mathbf{F}^{-1}\mathbf{n}.\mathbf{u}_0 ds,$$

with $w_c = J_F^{-1}W_c^*$, and $\mathbf{U}_0$ is a prescribed displacement. The second of (8.80) applies in the small-strain framework. This is none other than one of the results of Bui (1973).

## 8.8 Other Material Balance Laws and Path-Independent Integrals

### 8.8.1 Notion of *L*- and *M*-Integrals

The path-independent *J*-integral and its direct interpretation in terms of a material force issued from the local conservation of material momentum rely

on the *translational* invariance or lack of invariance on the material manifold. This directly fits the notion of extension of a straight crack with the virtual *en-bloc* translation of the region around the tip of the crack generating the extension. But other material balance laws (not necessarily conservation laws, even in the simplest cases) relate to other material motions such as *rotations* and *expansions*. Such laws were established and discussed in Section 4.3. The question naturally arises of their possible implementation in fracture theory and, more generally, in the study of the expansion of various material defects (e.g., spherical cavities in the case of material dilatation). Günther (1962), Knowles and Sternberg (1972), and Fletcher (1976) are responsible for the introduction of the additional material laws (often in statics and generally homogeneous materials). Budiansky and Rice (1973) have associated these balance laws with invariants of *defect mechanics*, called the *L*- and *M*-integrals, respectively. The small-strain approximation for this relationship was recently established by Eischen and Herrmann (1987) by a direct calculation. But here we can support this relationship within the fully nonlinear framework. For this it suffices to consider the global material quantities

$$M^{\text{inh}}(V) = -\int_V \mathbf{X}.\mathbf{f}^{\text{inh}} dV, \quad \mathbf{L}^{\text{inh}}(V) = -\int_V \mathbf{X} \times \mathbf{f}^{\text{inh}} dV, \tag{8.81}$$

in analogy with (quasistatics)

$$\mathbf{F}^{\text{inh}}(V) = -\int_V \mathbf{f}^{\text{inh}} dV = \int_{\partial V} \mathbf{N}.\mathbf{b}\, dA, \quad \mathbf{f}^{\text{inh}} = -\text{div}_R \mathbf{b}. \tag{8.82}$$

In *plane* problems and small strains, which are most often met in engineering, and introducing the contour Γ, these yield (see Herrmann and Kienzler, 2000):

1. **The *M*-integral**:

$$M = \oint_\Gamma x_j n_i b_{ij} d\Gamma \tag{8.83}$$

2. **The *L*-integral**:

$$L = \oint_\Gamma \varepsilon_{3kj} \left( x_k b_{ij} + u_k \sigma_{ij} \right) n_i \, d\Gamma \tag{8.84}$$

3. **The $J_1$- or *J*-integral**:

$$J_1 \equiv J = \oint_\Gamma n_i b_{i1} d\Gamma \tag{8.85}$$

4. **The $J_2$-integral**:

$$J_2 = \oint_\Gamma n_i \, b_{i2} d\Gamma \tag{8.86}$$

while ($8.82_1$) may be referred to as the vectorial ***J***-integral.

In terms of the elastic displacement **u**, we have the following explicit expressions:

$$\mathbf{J} = \oint_\Gamma \left\{ W\mathbf{n} - (\mathbf{n}.\sigma).(\nabla \mathbf{u})^T \right\} d\Gamma, \tag{8.87}$$

$$M = \oint_\Gamma \left\{ W\mathbf{x}.\mathbf{n} - (\mathbf{n}.\sigma).(\nabla \mathbf{u})^T .\mathbf{x} - \frac{1}{2}\mathbf{n}.\sigma.\mathbf{u} \right\} d\Gamma, \tag{8.88}$$

$$\mathbf{L} = -\oint_\Gamma \left\{ W\mathbf{n} \times \mathbf{x} - \left(\mathbf{n}.\sigma.(\nabla \mathbf{u})^T\right) \times \mathbf{x} + \mathbf{u} \times (\mathbf{n}.\sigma) \right\} d\Gamma, \tag{8.89}$$

where we need not emphasize the limit procedure as these integrals are path-independent. We illustrate the appearance of some of these by pursuing the exploitation of the distributional approach started in Section 8.5.

### 8.8.2 Distributional Approach: Energy of Cavities and Inclusions

Here the defect $D$ has the same dimension as the body, like cavities and inclusions. We consider a homogeneous elastic body (plane problem) that contains a circular cavity $C$. Let $S$ the boundary, supposed free of tractions, of $C$:

$$\mathbf{N}.\mathbf{T} = \mathbf{0} \quad \text{on} \quad S. \tag{8.90}$$

The cavity is supposed to expand uniformly with the rate $c(t) = \dot{l}(t)$, $l$ being its radius. At each instant of time the solution (**u**,**T**) is supposed to have no singular behavior in $B$, so that $W$, $\dot{W}$, **T.v**, $\nabla$.(**T.v**) generate regular distributions on $R^2$ by prolongation with the origin outside $B$. Again, we are interested in the relation between the classical and distributional derivatives of $W$ and **T.v**. There is no difficulty to show that (in the notation of Section 8.3)

$$D_t W = \dot{W} - cW\delta(S), \tag{8.91}$$

$$\mathrm{Div}(\mathbf{T}.\mathbf{v}) = \mathrm{div}(\mathbf{T}.\mathbf{v}) - \mathbf{N}.\mathbf{T}.\mathbf{v}\,\delta(\partial B), \tag{8.92}$$

where, for the last one, we used the condition (8.90). The energy relation in (8.40) and the formulas (8.91) and (8.92) yield

$$D_t W + cW\delta(S) = \mathrm{Div}(\mathbf{T}.\mathbf{v}) + \bar{\mathbf{T}}^d.\mathbf{v}\,\delta(\partial B), \tag{8.93}$$

which is a relation similar to (8.57). But in the present case the set $S = ED$ of extension points of the defect does not reduce to a single point so that the new term in (8.93) is a distribution concentrated on $S$. By applying (8.93) to $\phi$, using (8.90) and the relation $x_i = lN_i$ at $S$, we get

$$\frac{d}{dt}\int_B W da + (\dot{l}/l)M = \int_{\partial B} \bar{\mathbf{T}}^d.\mathbf{v}\,dA, \tag{8.94}$$

with (compare (8.88))

$$M = \int_S \left\{W\mathbf{x}.\mathbf{N} - \left(\mathbf{N}.\mathbf{T}.(\nabla\mathbf{u})^T\right).\mathbf{x}\right\} dA. \tag{8.95}$$

The relation (8.94) was obtained by Budiansky and Rice (1973). Its form recalls the expressions (8.21), valid also for a crack. Thus the second term in the left-hand side of (8.94) is the energy-release rate in the expansion of the cavity.

The propagation criterion that fits the formulation in (8.93) will necessarily involve a critical specific energy $W_{cr}$ of the material, that is, $W = W_{cr}$ on $S$, so that (8.93) becomes

$$D_t W + c\,W_{cr}\delta(S) = \mathrm{Div}(\mathbf{T}.\mathbf{v}) + \bar{\mathbf{T}}^d.\mathbf{v}\,\delta(\partial B). \tag{8.96}$$

Let us suppose now that a Griffith-type surface energy exists on the cavity boundary $S$. If $(r, \theta)$ are polar coordinates centered in 0, then $\delta(S) = \delta(r - l)$. Denoting by $H(l - r)$ the Heaviside function of $C$, by $\delta'(r - l)$ the normal derivative of $\delta(r - l)$ on $S$, and by $D_l$ the derivative with respect to the radius $l$ of the cavity, we have

$$D_t\left(W_{cr}\delta(r-l)\right) = cW_{cr}\,D_l\,\delta(r-l) = cW_{cr}\delta'(r-l). \tag{8.97}$$

By supposing that the energy of $B$ consists of the elastic energy $W$ and the surface energy $W_{cr}\delta(r - l)$, the obtained energy balance will read

$$D_t W + cW_{cr}\delta'(S) = \mathrm{Div}(\mathbf{T}.\mathbf{v}) + \bar{\mathbf{T}}^d.\mathbf{v}\,\delta(B). \tag{8.98}$$

This obviously differs from (8.96) in what concerns the described behavior in the points of $S$. This means that the existence of an energy distribution on $S$, such as considered by Sih and Liebowitz (1967), contradicts the balance laws of elasticity. We note that the same difference exists between (8.98) and (8.93), in which the propagation criterion is not used. Returning to our result in (8.96), we note that

$$D_t\left(W_{\mathrm{cr}}H\left(l-r\right)\right)=cW_{\mathrm{cr}}D_l\,H\left(l-r\right)=cW_{\mathrm{cr}}\delta\left(r-l\right). \tag{8.99}$$

Accordingly, the energy equation (8.96) reads

$$D_t\left(W+W_{\mathrm{cr}}H\left(l-r\right)\right)=\mathrm{Div}\left(\mathbf{T}.\mathbf{v}\right)+\bar{\mathbf{T}}^{d}.\mathbf{v}\,\delta\left(\partial B\right). \tag{8.100}$$

Thus, the obtained energy of $B$ consists of the elastic energy $W$ and the energy of the cavity $W_{\mathrm{cr}}H(l-r)$. The latter is distributed over the cavity $C$, and its density represents the energy expended to extend the defect by a unit area. Every new point of the cavity is endowed with the energy consumed for it.

In conclusion, we first note that the incompatibility of the Griffith-type energy with the elasticity equations is not particular to circular flaws (cavities). This is also true for the notch problem considered in Section 8.4 to introduce the problem of fracture (see Dascalu and Maugin, 1994, pp. 31–33). Also, a similar analysis applies to an inclusion of one elastic material into another one. Physical situations of this type with migrating interfaces were considered by Eshelby (1970). In this case the notion of defect is relative: one material is a defect with respect to another. Equation 8.93 remains valid, but the distribution concentrated on $S$ now takes the form $c[W]\delta(S)$, $[W]$ being the jump of $W$ across $S$. This reminds us of phase-transition progression. The corresponding propagation criterion is $[W]=W_{\mathrm{cr}}$ depending on the two materials. The energy of the relative defect is given by the same formula, but $W_{\mathrm{cr}}$ represents the energy needed to transform one material phase into another.

### 8.8.3 Distributional Approach: Dislocations

The dislocation motion was one reason that led Eshelby to introduce the notion of force on an elastic singularity. It is thus salient to revisit this problem using distribution theory and obtaining the "energy of a dislocation" in that formalism. To that purpose we consider a straight-edge or screw dislocation in a linear homogeneous elastic body. We choose a coordinate system so that the dislocation line is parallel to the $x_3$-axis and pierces the $x_1x_2$-plane at the point $(l, 0)$. The dislocation is supposed to glide with the speed $c(t)=\dot{l}(t)$ along the $x_1$-axis. The situation is the same as in Figure 8.3, but now $C$ is

the intersection of the dislocation slip plane with the $x_1$ $x_2$-plane. If $\tilde{\mathbf{b}}$ is the Burgers vector, then

$$\left[\mathbf{u}\right] = \tilde{\mathbf{b}} \quad \text{on} \quad C. \tag{8.101}$$

The structure of the solution is the same as that given by (8.46), with (cf. Mura, 1982; Teodosiu, 1982)

$$\mathbf{T}^S = 0\left(r^{-1}\right), \quad \left(\nabla\mathbf{u}\right)^S = 0\left(r^{-1}\right), \tag{8.102}$$

and $\mathbf{u}^r$ and $\mathbf{T}^r$ finite on $B$. The singular terms $\mathbf{u}^s$ and $\mathbf{T}^s$ do not depend explicitly on time, so that the order of singularity of their time derivatives is the same as that of their gradient. Because $W$ and $\mathbf{T}.\mathbf{v}$ are not integrable we need to construct for them the regularizations $W\big|_G$ and $\mathbf{T}.\mathbf{v}\big|_G$ defined as in (8.48). These distributions depend on $G$ and, restricted to $R^2 - \{A\}$, coincide with $W$ and $\mathbf{T}.\mathbf{v}$, respectively. Applying $W\big|_G$ to $\phi_1$ (a test function defined everywhere but with value *one* in the domain of interest), we get

$$\left\langle W\big|_G, \varphi_1 \right\rangle = \int\limits_{B-G} W\, dA. \tag{8.103}$$

This is the elastic energy of $B$ without a circular hole centered in $A$.

Without giving the tedious mathematical details (see Dascalu and Maugin, 1994, pp. 33–36 for these), we mention that we have to evaluate $D_t\left(W\big|_G\right)$ and $\mathrm{Div}\left(\mathbf{T}.\mathbf{v}\big|_G\right)$. Then, writing the energy conservation law for these two terms, after some lengthy computations, we arrive at a distributional energy conservation in the form:

$$D_t\left(W\big|_G\right) + \left(W_1 - \frac{d}{dt}\int_G (x_1 - l) W dA\right)\delta_{,1}(l,0) + \left(W_2 - \frac{d}{dt}\int_G x_2 W dA\right)\delta_{,2}(l,0)$$
$$+ \int_\Gamma cWN_1 + \mathbf{N}.\mathbf{T}.\mathbf{v}\, d\Gamma\, \delta(l,0) = \mathrm{Div}\left(\mathbf{T}.\mathbf{v}\big|_G\right) + \bar{\mathbf{T}}^d.\mathbf{v}\,\delta(\partial B), \tag{8.104}$$

wherein

$$W_1 := \int_\Gamma (x_1 - l)\left(WN_1 - \mathbf{N}.\mathbf{T}.\mathbf{u}_{,1}\right) d\Gamma \quad , \quad W_2 := \int_\Gamma x_2 \left(WN_1 - \mathbf{N}.\mathbf{T}.\mathbf{u}_{,1}\right) d\Gamma, \tag{8.105}$$

Equation 8.104 is an energy equation depending on $G$, which applied to $\phi_1$ gives the energy balance on $B$-$G$. To obtain the dislocation energy we have to consider the limit as $G \to 0$. The limit

$$\lim \left\langle D_t \left( W\big|_G \right), \varphi \right\rangle \quad \text{as} \quad G \to 0 \tag{8.106}$$

exists. This is essentially given by the principal value of $W$ in $A$. On the other hand, the limit as $G \to 0$ of the last contribution in the left-hand side in (8.104) is none other than $cJ$, where $J$ is the Cherepanov–Eshelby–Rice path-independent integral. Furthermore, the implicit dependence on time of the singular parts of **u** and **T** is such that

$$\lim \frac{d}{dt} \int_G (x_1 - l) W dA = \lim \frac{d}{dt} \int_G x_2 W dA = 0 \quad \text{as} \quad G \to 0, \tag{8.107}$$

so that the other distributions concentrated in $A$ are also convergent, their limit depending on the singular parts of the fields. The integrals (8.105) are calculated only for these singular parts. In the end, in the limit, (8.103) will take the following reduced form:

$$D_t W + c f^{(\mathrm{PK})} \delta(l, 0) = \mathrm{Div}(\mathbf{T}.\mathbf{v}) + \bar{\mathbf{T}}^d.\mathbf{v}\, \delta(\partial B), \tag{8.108}$$

where the integral $f^{(\mathrm{PK})}$ gives the Peach–Koehler force on a dislocation (Eshelby, 1951). Then the energy-like criterion is obtained from (8.108) in the form $f^{(\mathrm{PK})} = f_{\mathrm{cr}}$. Such a *criterion of activation* is usually encountered in dislocation theory. On account of this, we can state the following energy conservation

$$D_t \left( W + f_{\mathrm{cr}} H(l - x_1).\delta(x_2) \right) = \mathrm{Div}(\mathbf{T}.\mathbf{v}) + \bar{\mathbf{T}}^d.\mathbf{v}\, \delta(\partial B). \tag{8.109}$$

The second contribution in the time derivative represents the energy of the dislocation, which is uniformly distributed on its slip plane. The material "force" $f_{\mathrm{cr}}$ represents the energy expended in the dislocation glide with a unit length. A similar calculation can be carried out for edge dislocations.

## 8.9 Generalization to Inhomogeneous Bodies

Case of smoothly materially inhomogeneous elastic materials. In this case ($8.15_2$) and (8.22) contain a material inhomogeneity force contribution

in their right-hand side. This modifies the expression (8.26) accordingly. Then it is shown that for materially inhomogeneous elastic bodies, (8.26) is replaced by

$$F_1^{\text{crack}} = \int_\Gamma \left( (\mathbf{N}.\mathbf{b})_1 + P_1 \left( \bar{\mathbf{V}}.\mathbf{N} \right) \right) dA - \left( \frac{\partial}{\partial t} \int_G P_1 \, dV - \int_G f_1^{\text{inh}} dV \right). \quad (8.110)$$

Such an expression has been exploited in quasistatics by Haddi and Weichert (1994). It shows that the crack driving force is a material force in its own right; it plays the same role as a spatially integrated true inhomogeneity force. Numerical applications and illustrations of (8.110) are given by Haddi and Weichert (1995), Mueller and Maugin (2002), and Steinmann et al. (2000). However, it is already quite instructive to examine simple cases of smooth inhomogeneities as was done by Eischen (1987) and Herrmann and Kienzler (2000) and Hermman and Kienzler (2001) in quasistatics and small strains, for which (8.110) reduces to

$$F_1^{\text{crack}} = \int_\Gamma \left( W N_1 - \mathbf{t}.\frac{\partial \mathbf{u}}{\partial x_1} \right) d\Gamma + \int_G f_1^{\text{inh}} dV, \quad (8.111)$$

where $\mathbf{t}$ is the traction at $\Gamma$ and $N_1 = \mathbf{N}.\mathbf{E}_1$ where $\mathbf{N}$ is the unit normal to the contour $\Gamma$. Here the first contribution is the celebrated $J = J_1$ *path-independent* integral of fracture, but the second integral introduces a domain-dependent term. Eischen, Kienzler, and Herrmann were able to introduce an extended path-independent integral, $J_e$, for *plane* problems of *strains* in linear isotropic elasticity for specific smooth elastic inhomogeneities. For instance, one may consider an exponential variation of the shear modulus such that

$$\mu(x_1, x_2) = \mu_0(x_2) \exp(\alpha x_1), \quad (8.112)$$

where $\mu_0$ is an arbitrary function of $x_2$, and $\alpha$ is an arbitrary constant, with the obvious restriction that $\mu$ must be positive and the condition $(\lambda_{,1}/\lambda) = (\mu_{,1}/\mu)$ guaranteeing that the Poisson ratio is independent of $x_1$. From (8.111) the following integral is then shown to be path-independent:

$$J_e = J - \alpha U \quad , \quad U := \frac{1}{2} \int_\Gamma \mathbf{t}.\mathbf{u} \, d\Gamma, \quad (8.113)$$

where a 2-D divergence theorem has been used to convert the inhomogeneity-force surface integral of (8.111). In the case of plane stresses, the result (8.113)

is still valid under the condition that Poisson's ratio remains independent of $x_1$, and the shear modulus is such that, instead of (8.112),

$$\mu(x_1, x_2, x_3) = \mu_0(x_2, x_3)\exp(\alpha x_1), \tag{8.114}$$

with $\mu_0$ an arbitrary function of its arguments.

Another possibility studied by the same authors for plane strains is that the shear modulus varies as

$$\mu = \mu_0(mx_1 + 1)^\alpha, \tag{8.115}$$

where $\mu_0$ is a mere material constant. Again, by use of the divergence theorem applied to the last contribution in (8.111), it is shown that the following extended integral is path-independent:

$$J_e = J + m(M - \alpha U), \tag{8.116}$$

where $U$ has already been defined in (8.113) and $M$ is none other than the $M$-integral of fracture, here given by

$$M = \int_\Gamma (W\mathbf{x}.\mathbf{n} - \mathbf{x}.(\nabla\mathbf{u}).\mathbf{t})d\Gamma. \tag{8.117}$$

The homogeneous case is recovered by setting $m = 0$. The formal result (8.116) is valid for plane stresses under the condition (since there remains some three-dimensionality in the problem) that $M$ be replaced by its three-dimensional analog. It is remarkable that the result (8.116) mixes the classical $J$- and $M$-integrals, but this could be figured out since a representation of the type (8.115) introduced a moment (multiplication by a certain power of $x_1$) of the elastic energy of the homogeneous case (in particular for $\alpha = 1$)—compare the definition (8.83) of the $M$-integral. More can be found on this matter for structural members in Kienzler (1993) and Herrmann and Kienzler (2001).

## 8.10 Generalization to Dissipative Bodies

### 8.10.1 The Problem of Thermal Brittle Fracture

It should again be clear to the reader that at any *regular* material point **X** the local equations of momentum (5.2) and (5.31)—in the absence of variable

$\alpha$ and setting $\mathbf{f}_0 = \mathbf{0}$ (for the sake of simplicity) in materially homogeneous materials—are, through the Noether–Ericksen identity, direct consequences of one another. However, if we integrate each of these over a regular (simply connected) **homogeneous** material body $B$—of boundary $\partial B$ equipped with unit outward normal $\mathbf{N}$—thanks to the trivial commuting of material integration and material time differentiation and the mathematically justified use of the divergence theorem, we obtain the following two global equations:

$$\frac{\partial}{\partial t}\int_B \mathbf{p}\,dV = \int_{\partial B} \mathbf{N}.\mathbf{T}\,dS, \tag{8.118}$$

$$\frac{\partial}{\partial t}\int_B \mathbf{P}dV = \int_{\partial B} \mathbf{N}.\mathbf{b}\,dS + \int_B \mathbf{f}^{\text{th}}dV, \quad \mathbf{f}^{\text{th}} = S\nabla_R\theta, \tag{8.119}$$

respectively, where the second must be understood *component-wise* (on the material manifold) because, in contrast to what happens in (8.118), the quantities involved in the integrands in (8.119) are material *covectors*, and the material manifold $M^3$ does not play the same neutral role as that played by the Euclidean physical manifold $E^3$ in (8.118). Obviously, in writing the global forms, we have again lost the convection property relating the two equations of linear momentum. This means that (8.118) and (8.119) can be used for different purposes, essentially (8.118) for *solving* the physical boundary-value, initial-value problem and (8.119) for another purpose that becomes clear in two instances. The first of these is exploited during numerical computations using a certain scheme. Not only must this scheme (e.g., *finite-difference scheme* in nonlinear wave propagation, or *finite-element method* in structural computations; see Chapter 13) be compatible with energy conservation, that is, the global equation obtained by summing over the relevant regular material region,

$$\frac{\partial}{\partial t}\int_B H dV = \int_{\partial B} \mathbf{N}.\big(\mathbf{T}.\mathbf{v} - \mathbf{Q}\big)dS, \tag{8.120}$$

but it must also be compatible with the additional balance law (another form of the energy conservation) obtained by summing the second of (5.31) over $B$, that is,

$$\frac{\partial}{\partial t}\int_B S\theta dV + \int_{\partial B} \mathbf{N}.\mathbf{Q}\,dS = \int_B h^{\text{th}}dV, \quad h^{\text{th}} = S\dot{\theta}. \tag{8.121}$$

Equations 8.119 and 8.120 or 8.121 are the relevant equations to study the progress of fracture in the thermoelasticity of conductors because they

capture thermomechanical singularities; that is, they give rise to nonvanishing quantities that characterize this singularity: the driving force and the energy-release rate. We will not repeat here the analysis given in the purely elastic case. It suffices, accounting for the singularity order of temperature in the neighborhood of the crack tip (singularity of the Laplacian operator), to mention the thermal generalizations of Equations 8.26 and 8.27:

$$\frac{\partial}{\partial t}\int_B P_1 dV + F_1^{\text{crack}} = \int_{\partial B}\left(\mathbf{N}.\mathbf{b}\right)_1 dS + \int_B \left(\mathbf{f}^{\text{th}}\right)_1 dV, \tag{8.122}$$

and

$$\frac{\partial}{\partial t}\int_B H dV + G^{\text{crack}} = \int_{\partial B}\mathbf{N}.\left(\mathbf{T}.\mathbf{v}-\mathbf{Q}\right)dS, \tag{8.123}$$

where we were cautious to write the first in component (1) form, and we observe the appearance of source terms due to the inward motion of the crack front. These are given the same formulas as those for pure elasticity except that $L^{\text{th}}$ replaces the previous $L$. Accounting for these expressions, we finally obtain the global balance of material momentum and energy over the subbody $C$ with surrounding surface $S$ as

$$F_1^{\text{crack}} = \int_\Gamma \left(\left(\mathbf{N}.\mathbf{b}\right)_1 + P_1\left(\bar{\mathbf{V}}.\mathbf{N}\right)\right)dS + \int_G \left(\mathbf{f}^{\text{th}}\right)_1 dV - \frac{\partial}{\partial t}\int_G P_1 dV \tag{8.124}$$

and

$$G^{\text{crack}} = \int_\Gamma \left(H\left(\bar{\mathbf{V}}.\mathbf{N}\right) + \mathbf{N}.\left(\mathbf{T}.\mathbf{v}-\mathbf{Q}\right)\right)dS - \frac{\partial}{\partial t}\int_G H dV. \tag{8.125}$$

We recognize in the last expression minus the change in *potential energy* (*dynamic thermoelastic, homogeneous case*) that is, the *dissipation rate* in the progress of the notch inside the material body. Accordingly, there must be a relationship between the latter quantity and the *power expended* irreversibly by the *material force* of component $F_1^{\text{crack}}$. Because of the universal form of the expressions for $F^{\text{crack}}$ and $G^{\text{crack}}$, just the same as before it is shown that

$$\bar{V}_1 F_1^{\text{crack}} = G^{\text{crack}} \geq 0, \tag{8.126}$$

where the inequality sign indicates the thermodynamic irreversibility of the crack growth phenomenon. This corresponds to the presence of a *hot heat*

*source* at the crack tip, an effect that can be observed by means of infrared thermography.

Note that if the temperature field in the neighborhood of the crack-tip line satisfies the following condition

$$\bar{\mathbf{V}}.\nabla_{\mathrm{R}}\theta = -\left.\frac{\partial\theta}{\partial t}\right|_{\mathrm{x}} + \text{regular term}, \tag{8.127}$$

then the heat source localized at the crack tip is related to entropy and the material thermal force by (Maugin and Berezovski, 1999)

$$Q_{\text{tip}} \equiv \lim_{\Gamma\to 0}\int_{\Gamma}\mathbf{N}.\mathbf{Q}\,dS = \lim_{\Gamma\to 0}\left(\frac{\partial}{\partial t}\int_{G}\left(-S\theta\right)dV\right) - \lim_{\Gamma\to 0}\int_{G}\left(\bar{\mathbf{V}}.\mathbf{f}^{\text{th}}\right)dV. \tag{8.128}$$

**COMMENTS:** The perspicacious reader will have noticed that the expression (8.124)—component along the crack direction—is a dynamic thermoelastic generalization of the celebrated *Eshelby–Cherepanov–Rice J*-integral of brittle fracture if we remember the expression of the dynamic Eshelby tensor b. The preceding formulation is strictly based on thermomechanical arguments on the material manifold.

### 8.10.2 Fracture in Anelasticity

This is sometimes called *ductile fracture* in opposition to the *brittle fracture* that occurs during the elastic behavior of a material. Here we suppose that anelasticity is appropriately accounted for by internal variables of state collectively called $\alpha$. According to the thermomechanical developments in Chapter 5, the presence of this last variable has practically the same consequences as temperature effects, for example, the existence of the "intrinsic" material force $\mathbf{f}^{\text{intr}}$ and heat source $h^{\text{intr}}$ that cannot be eliminated and will be added as volume contributions in (8.119) and (8.121).

Equations 5.1 through 5.3 are left formally unchanged. But, obviously, there exists now an *intrinsic dissipation* so that the entropy equation is generalized to

$$\theta\frac{\partial S}{\partial t} + \nabla_{R}.\mathbf{Q} = \Phi^{\text{int}} \equiv A\left.\frac{\partial\alpha}{\partial t}\right|_{X}. \tag{8.129}$$

The balance of material momentum is accordingly modified and was obtained in Chapter 5. Its local form at regular material points reads

$$\left.\frac{\partial\mathbf{P}}{\partial t}\right|_{X} - \left(\text{div}_{R}\mathbf{b} + \mathbf{f}^{\text{inh}}\right) = \mathbf{f}^{\text{th}} + \mathbf{f}^{\text{intr}}, \quad \mathbf{f}^{\text{intr}} := A\left(\nabla_{R}\alpha\right)^{T}. \tag{8.130}$$

Clearly, insofar as this equation is concerned, internal variables produce a source term—a material force—that resembles $\mathbf{f}^{\text{th}}$ in both general expression and effects! In particular, (8.129) can also be written as (cf. Chapter 5)

$$\left.\frac{\partial(S\theta)}{\partial t}\right|_X + \nabla_R.\mathbf{Q}=\mathbf{\Phi}^{\text{th}} + \mathbf{\Phi}^{\text{intr}}, \quad \mathbf{\Phi}^{\text{th}} := S\frac{\partial\theta}{\partial t}. \tag{8.131}$$

The similarity between variables $\alpha$ and $\theta$ is thus enhanced, but while the latter is governed by the *heat equation*, the former has to be governed by a pure *evolution equation* subjected to the second law of thermodynamics (non-negative dissipation).

In the *thermo-anelastic fracture problem*, because of the already noticed similarity between source terms in the right-hand side of (8.130), the proof of the consistency relation (8.126) will be facilitated. Indeed, for instance, we shall have

$$\bar{\mathbf{V}}.\lim_{\Gamma\to 0}\int_G \mathbf{f}^{\text{intr}}\,dV \approx -\lim_{\Gamma\to 0}\int_G\left(A\left.\frac{\partial\alpha}{\partial t}\right|_X\right)dV, \tag{8.132}$$

if $\alpha$ verifies a lemma such as in (8.127). We recognize in the right-hand side of (8.132) the limit, changed of sign, of the global intrinsic dissipation in the material domain $G$.

**Energy-release rate in fracture**. We let the reader show that in fracture (neglecting thermal effects and considering a materially homogeneous material), we can obtain the expression of the *energy-release rate* as

$$G^{\text{crack}} = \int_\Gamma\left(H\left(\bar{\mathbf{V}}.\mathbf{N}\right)+\mathbf{N}.\mathbf{T}.\mathbf{v}\right)dA - \left(\frac{\partial}{\partial t}\int_G H dV + \int_G A\left.\frac{\partial\alpha}{\partial t}\right|_X dV\right), \tag{8.133}$$

while (8.130) yields, component-wise, a *global material force*, the driving force acting on the crack tip,

$$F_1^{\text{crack}} = \int_\Gamma\left(\left(\mathbf{N}.\mathbf{b}\right)_1 + P_1\left(\bar{\mathbf{V}}\mathbf{N}\right)\right)dS - \frac{\partial}{\partial t}\int_G P_1\,dV + \int_G f_1^{\text{intr}}dV, \tag{8.134}$$

with, in the limit as $G$ shrinks to the crack tip, the *global dissipative inequality*

$$G^{\text{crack}} = F_1^{\text{crack}}\bar{V}_1 \geq 0 \tag{8.135}$$

in which we have accounted for the fact that in these limits we have the following local behavior: $\mathbf{v}\approx -\bar{\mathbf{V}}.\mathbf{F}^{-T}$, $\dot{\alpha}\approx -\bar{\mathbf{V}}.\nabla_R\alpha$, $A\dot{\alpha}\approx -\bar{\mathbf{V}}.\mathbf{f}^{\text{intr}}$. The

bilinear form (8.135) governs the irreversible thermodynamics of the extension of $C$ independently of the precise physical *significance* of $\alpha$.

**REMARK:** Dual integral in elastoplasticity

In Equation 8.130 one can perform a Legendre transformation with respect to deformation and internal variables of the energy present in the definition of $\mathbf{b}$—following what is done in Maugin (2000; Equations 66 through 69)—in order to recur to a generalized $I$-integral in the manner of Bui (see Section 8.7) in the presence of anelasticity effects described by variable $\alpha$. This was discussed by Stolz (2008a, 2008b) in small strains without reference to previous relevant works.

## 8.11 A Curiosity: "Nondissipative" Heat Conductors

### 8.11.1 Conservation Equations

It was shown in previous sections that unavoidable source terms related to temperature gradients hinder the a priori existence of path-independent integrals in thermoelasticity. But it happens that a rather curious theory of continuum thermoelasticity was proposed by Green and Naghdi (1993) with a view to formulate a fully hyperbolic system (bounded speed of wave propagation) for such a theory. It also happens that this theory a priori presents only strict conservation laws. The absence of source terms, which renders the theory *dissipation free*, is favorable for the existence of path-independent integrals for fracture in such a theory. This was shown by Dascalu and Maugin (1995). The main idea is to introduce in the energy density a variable, the *thermal displacement*, that accounts for the past history of the temperature field, and also its material gradient. Thus we introduce a scalar variable $\gamma$ such that

$$\theta(\mathbf{X},t)=\frac{\partial}{\partial t}\gamma(\mathbf{X},t)\quad\text{or}\quad\gamma=\int_0^t\theta(\mathbf{X},t')dt'. \tag{8.136}$$

A variational formulation based on a the direct-motion description will consider a Lagrangian density per unit reference volume in the form:

$$L^{\text{th}}=\frac{1}{2}\rho_0\mathbf{v}^2-\bar{W}(\mathbf{F},\dot{\gamma},\nabla_R\gamma), \tag{8.137}$$

where no inertia term is isolated for the field $\gamma$, which does not appear just by itself. We skip the details of the derivation (see Kalpakides and Maugin, 2004a).

The two field equations at regular material points $\mathbf{X}$ are readily obtained as the linear (physical) momentum equation and the entropy equation in the form

$$\frac{\partial \mathbf{p}}{\partial t} - \mathrm{div}_R \mathbf{T} = \mathbf{0}, \quad \mathbf{p} := \rho_0 \mathbf{v}, \quad \mathbf{T} = \partial \bar{W} / \partial \mathbf{F}, \tag{8.138}$$

and

$$\frac{\partial S}{\partial t} + \nabla_R . \mathbf{S} = 0, \quad S = -\frac{\partial \bar{W}}{\partial \dot{\gamma}} = -\frac{\partial \bar{W}}{\partial \theta}, \quad \mathbf{S} = -\frac{\partial \bar{W}}{\partial (\nabla_R \gamma)}. \tag{8.139}$$

The first of (8.139) has no source term although $S$ is obviously identified as the entropy density (cf. second of (8.139)). That is the reason why this theory is called a theory of thermoelasticity "without dissipation." Application of Noether's theorem to the present variational formulation for space–time translations in material space yields the canonical equations of (material) momentum and energy in the form:

$$\left.\frac{\partial \mathbf{P}^{\mathrm{th}}}{\partial t}\right|_X - \mathrm{div}_R \mathbf{b}^{\mathrm{th}} = \mathbf{0}, \quad \left.\frac{\partial H^{\mathrm{th}}}{\partial t}\right|_X - \nabla_R . \mathbf{Q}^{\mathrm{th}} = 0, \tag{8.140}$$

where we have set

$$\mathbf{P} = \mathbf{P}^{\mathrm{mech}} - S \nabla_R \gamma, \quad \mathbf{P}^{\mathrm{mech}} := -\mathbf{p}.\mathbf{F}, \tag{8.141}$$

$$\mathbf{b}^{\mathrm{th}} = -\left(L^{\mathrm{th}} + \mathbf{T}.\mathbf{F} - \mathbf{S} \otimes \nabla_R \gamma\right), \tag{8.142}$$

$$H^{\mathrm{th}} = \frac{1}{2} \rho_0 \mathbf{v}^2 + E, \quad E = \bar{W} + S\theta, \quad \mathbf{Q}^{\mathrm{th}} = \mathbf{T}.\mathbf{v} - \theta \mathbf{S}. \tag{8.143}$$

These results deserve several comments. First, the equations (8.140) have no source term, which is the desired result. Second, the classical material heat flux is identified as $\mathbf{Q} = \theta \mathbf{S}$, that is, a highly classical relationship between heat flux and entropy flux. As a result, the energy equation given by the second of (8.140) cannot be distinguished from the classical one (in the absence of body force; cf. Chapter 2). Third, the formula for the Eshelby stress (8.142) captures the effect of the gradient of $\gamma$. Finally, the canonical momentum is made of two parts, a now-classical mechanical part and a part due to the gradient of $\gamma$. This may look strange, but it was remarked by Dascalu and Maugin (1995) that such a term can indeed be interpreted as a momentum

in some physical theories (e.g., in the two-fluid theory of superfluid helium, this term can be transformed into a term proportional to the relative velocity between the two fluid components). What is important here is the absence of source terms in the right-hand side of *both* Equations 8.140 and $8.139_1$. Our marked interest in these equations is such that we could have started with the variational formulation based on the consideration of the inverse motion, for which the initial Lagrangian density is taken as (cf. Maugin and Kalpakides, 2002)

$$J_F^{-1}L = \frac{1}{2}\rho\mathbf{V}.\mathbf{C}.\mathbf{V} - \bar{w}\left(\mathbf{F}^{-1}, \partial\gamma(\mathbf{x},t)/\partial\mathbf{x}, \nabla\gamma = \partial\gamma/\partial\mathbf{x}\right). \tag{8.144}$$

In this case the Euler–Lagrange equations are directly the equation of canonical momentum in $(8.140_1)$ and the entropy equation $(8.139_1)$, while the standard linear momentum equation $(8.138_1)$ and the energy equation $(8.140_2)$ are obtained by application of Noether's theorem. The reader will find the Hamiltonian equations for this theory in Maugin and Kalpakides (2002) and the construction of additional conservation laws in Kalpakides and Maugin (2004a). In particular, under certain conditions (material homogeneity, Lagrangians that are homogeneous of degree two in the deformation gradient), there holds a balance law of *action* in the form

$$\frac{\partial}{\partial t}\left(\mathbf{P}^{\text{th}}.\mathbf{X} - H^{\text{th}}t\right) - \nabla_R.\left(\mathbf{X}.\mathbf{b}^{\text{th}} - \mathbf{Q}t\right) = 2L^{\text{th}}. \tag{8.145}$$

This has the same structure as Equation 3.107.

### 8.11.2 The Problem of Thermoelastic Fracture

This was considered by Dascalu and Maugin (1995). We need not duplicate the arguments in Section 8.4. We simply note that with the requirements that

$$\mathbf{N}.\mathbf{T}^{\pm} = \mathbf{0}, \quad \mathbf{N}.\mathbf{Q}^{\pm} = 0 \tag{8.146}$$

along the faces of the crack, equations similar to (8.26) and (8.27) will be obtained but with quantities noted with superscript *th*:

$$\mathbf{F}^{\text{th}}_{\text{crack}} = \lim \int_{\Gamma} \left(\mathbf{P}^{\text{th}}(\bar{\mathbf{V}}.\mathbf{N}) + \mathbf{N}.\mathbf{b}^{\text{th}}\right) d\Gamma \quad \text{as} \quad \Gamma \to 0, \tag{8.147}$$

$$G_{\text{crack}} = \lim \int_{\Gamma} \left(H^{\text{th}}\left(\bar{\mathbf{V}}.\mathbf{N}\right) + \mathbf{N}.\left(\mathbf{T}.\mathbf{v} - \mathbf{Q}\right)\right) d\Gamma \quad \text{as} \quad \Gamma \to 0. \tag{8.148}$$

These two are compatible, yielding the local statement of the second law of thermodynamics:

$$G_{\text{crack}} = \bar{\mathbf{V}}.\mathbf{F}^{\text{th}}_{\text{crack}} \geq 0, \tag{8.149}$$

when we have the following asymptotic behavior of the fields at the crack tip:

$$\dot{\gamma}(\mathbf{X},t) \approx -(\bar{\mathbf{V}}.\nabla_R)\gamma(\mathbf{X},t), \tag{8.150}$$

$$\theta \approx -\bar{\mathbf{V}}.\nabla_R\gamma, \quad \mathbf{v} \approx -\bar{\mathbf{V}}.\mathbf{F}^T,$$

while

$$S\bar{\mathbf{V}}.\nabla_R\gamma \approx -S\theta, \quad \bar{\mathbf{V}}.\mathbf{P}^{\text{mech}} \approx \rho_0\mathbf{v}^2. \tag{8.151}$$

Note that the result (8.149) is general, being in fact independent of the considered thermolasticity theory. An equivalent form of (8.148) is obtained as

$$G_{\text{crack}} = \int_\Lambda (\mathbf{N}.(\mathbf{b}^{\text{th}} + (\bar{\mathbf{V}}.\mathbf{P}^{\text{th}})\mathbf{1}_R).\bar{\mathbf{V}})ds - \frac{d}{dt}\int_A \bar{\mathbf{V}}.\mathbf{P}^{\text{th}}dA, \tag{8.152}$$

where $\Lambda$ is another contour encircling the domain $A$ that contains the crack tip and moves together with it. In quasistatics, this reduces to

$$G_{\text{crack}} = \int_\Lambda \mathbf{N}.\mathbf{b}^{\text{th}}.\bar{\mathbf{V}}ds, \tag{8.153}$$

where the kinetic energy is no longer involved in the Eshelby stress $\mathbf{b}^{\text{th}}$. This is compatible with (8.149).

### 8.11.3 Recovery of Classical Thermoelasticity

We are obviously aware of the amount of artificiality in the Green and Naghdi (1993) construct. All is based on the assumptions made regarding the free energy functional dependence. An approximation yielding the classical theory of thermoelasticity has, therefore, to be obtained from an approximation of that energy. With $\beta = \nabla_R\gamma$, we can write a Taylor series expansion with respect to that material vector about its zero value. Thus

$$W(\mathbf{F},\theta=\dot{\gamma},\beta=\nabla_R\gamma) = \hat{W}(\mathbf{F},\theta,\beta=\mathbf{0}) + \frac{\partial W}{\partial\beta}(\beta=\mathbf{0}).\beta + 0(\beta^2). \tag{8.154}$$

We let the reader evaluate all the derivatives of $W$ needed in the theory, with

$$\hat{S} = -\frac{\partial \hat{W}}{\partial \theta}, \ \hat{\mathbf{S}} = -\frac{\partial W}{\partial \beta}(\beta = \mathbf{0}), \ \hat{\mathbf{Q}} = \theta \hat{\mathbf{S}}. \tag{8.155}$$

It is checked that ($7.138_1$), ($7.139_1$), and (8.140) yield the equations (Kalpakides and Maugin, 2004a, Section 6):

$$\frac{\partial \mathbf{p}}{\partial t} - \mathrm{div}_R \hat{\mathbf{T}} = \mathbf{0}, \tag{8.156}$$

$$\frac{\partial \hat{S}}{\partial t} + \nabla_R . \hat{\mathbf{S}} = -\theta \hat{\mathbf{S}} . \nabla_R \theta = -\hat{\mathbf{Q}} . \nabla_R \theta, \tag{8.157}$$

$$\frac{\partial \mathbf{P}^{\mathrm{mech}}}{\partial t} - \mathrm{div}_R \hat{\mathbf{b}} = \hat{\mathbf{f}}^{\mathrm{th}} = \hat{S} \nabla_R \theta, \tag{8.158}$$

$$\frac{\partial \hat{H}}{\partial t} - \nabla_R . \left( \hat{\mathbf{T}} . \mathbf{v} - \hat{\mathbf{Q}} \right) = 0, \tag{8.159}$$

where all symbols with a superimposed caret are indeed those of the classical theory, for example, in $\hat{H}$, $\hat{E} = \hat{W} + \hat{S}\theta$, and $\mathbf{P}^{\mathrm{mech}}$ is none other than the classical purely mechanical term. In the fracture problem one has to focus attention on the additional terms that were involved in the Eshelby stress of the Green–Naghdi theory. In this limit a source term will appear in the expression of the driving force. This will be none other than the bulk integral of the material thermal force present in the right-hand side of (8.159). Thus in Equations 8.155 through 8.160 one has simply to forget about the way the entropy flux was introduced (the second of (8.155)) and then construct a constitutive equation for it or for $\hat{\mathbf{Q}}$ as is usually done.

***Note on the Bibliography***

The bibliography on fracture, even limited to theoretical works, is enormous. The main technical journal in the field is the *International Journal of Fracture*. But many works are published in general journals on continuum mechanics or applied mathematics. The *essential books* with a theoretical bias older than the present work are the books by Cherepanov (1979), Bui (1978), Freund (1990), Maugin (1992), and Cherepanov (1998), the later where all main actors are called on the stage as witnesses of the developments over a period of 50 years. Now, in addition to the works already cited in the body of this chapter, we note the following. *General questions* on fracture were approached in

the works of Sanders (1960), Atkinson and Eshelby (1968), and Cherepanov (1968). *Dynamic fracture* is dealt with by Nilsson (1973), Chen and Shield (1977), Casal (1978), Nishioka (1989, 1998), Ehrlacher (1981), Mura (1981), Nishioka and Atluri (1983, 1984), Atluri and Nishioka (1983, 1984, 1985), Rice (1985), Russo (1986), Van Vroonheven (1992), Maugin (1994b), Kalpakides and Agiasofitou (2002), and Agiasofitou and Kalpakides (2004). *Path-independent integrals and invariants* are examined in detail in Chen and Shield (1977), Casal (1978), Freund (1978), Buggisch et al. (1981), De Lorenzi (1982), Golebiewska-Herrmann (1982), Cherepanov (1989), Bank-Sills and Sherman (1992), Ioakimidis and Anastasselou (1993), and Chen and Lu (2003). Propagation of cracks in *inhomogeneous bodies* receives some attention in Atkinson (1975a, 1975b), Rongshun Li and Chudnovky (1993), Haddi and Weichert (1995), Weichert and Schultz (1993), Mueller and Maugin (2002), and Maugin and Kalpakides (2005). *Fracture in anelastic solids* (plastic or viscoelastic) is considered by Atluri (1982), Schapery (1984, 1990), Carpenter et al. (1986), and Maugin (1994a). *Thermoelastic fracture* is the subject of the following works: Bui et al. (1979, 1987), Bui and Proix (1984), and Francfort and Golebiewska-Herrmann (1982, 1986). An interesting mathematically founded variational approach to fracture has been developed by Bourdin, Francfort, and Marigo (see their review paper, 2008).

# 9

# *Generalized Continua*

## Object of the Chapter

Where polar solid continua and other generalizations are introduced, showing what is a true multifield theory where conservation laws of the Eshelbian framework acquire their true status as relevant to a system wider than classical continuum mechanics.

## 9.1 Introduction

Polar continua, also referred to as *micropolar continua* (in Eringen's classification) or *Cosserat continua* (acknowledging the pioneering role played by the Cosserat brothers, 1909), provide the simplest, while most developed, example of generalized continuum mechanics in which a microstructure, although simple, is granted to each material point **X**. This microstructure here is equivalent to a rigidly rotating microbody, so that the generalized medium under scrutiny will be equipped with six degrees of freedom at each point—the classical three degrees of *translation* giving rise to the classical notions of *displacement*, deformation field, and *stresses* (cf. Chapter 2), and three additional degrees of rotation yielding the new notions of *microrotation*, wryness (see later on), and *couple stresses*—and no more. Such bodies possess the means to respond not only to classical forces but also to local couples. The microrotation may be mathematically represented by any appropriate means for $SO(3)$, such as Euler angles, orthogonal transformations, quaternions, and spinors. Here we use orthogonal transformations, which are by far the most convenient representation while vividly illustrating the physical situation, because the associated energy changes are contained in transformations. If the microbody at each **X** was a completely deformable body, such as a small ellipsoid of variable size, then there would be six additional degrees of freedom (a *true* microdeformation), instead of three more, at each **X**. We would then be dealing with *micromorphic media* (for these see Section 9.6). The basics

of polar media are exposed at length in various synthetic works (e.g., Eringen and Kafadar, 1976; Nowacki, 1986; Eringen, 1999; the first work emphasizes the linear theory, and the other two provide a comprehensive introduction to nonlinear theory—finite deformation and microrotation). The modern presentation owes much to the paper of Kafadar and Eringen (1971). The general structure exposed in this chapter, with a clear distinction between balance laws and conservation laws (in the Eshelbian framework), follows a contribution of the author (Maugin, 1998). Of course, the contents of the present chapter are necessarily related to those of Section 5.5, where the abstract additional variable $\alpha$ was an unspecified additional degree of freedom. Here it should be equated to the microrotation, an orthogonal tensor, or else in a more generalized continuum theory.

Although polar media and generalized continua have been the subject of numerous works exhibiting solutions and attempts at identifying the material coefficients (see the formidable bibliography in Nowacki [1986] in the case of Cosserat media), very few works have considered their invariance properties and general geometric framework except recent works with a renewed attention caused by the conception of artificial polar solids and the relationship to new materials such as nanomaterials. The situation concerning various modelings and their application is well described in Maugin and Metrikine (2010).

## 9.2 Field Equations of Polar Elasticity

### 9.2.1 Elements of Kinematics

In addition to the classical motion already introduced in Chapter 2, we consider a micromotion described by *orthogonal* transformations noted

$$\kappa = \bar{\kappa}(\mathbf{X}, t) = \left\{\kappa^i_{.K}\right\}, \tag{9.1}$$

such that

$$\kappa^{-1} = \kappa^T = \left\{\kappa^K_{.i}\right\}, \quad \det\kappa = +1, \quad \kappa.\kappa^{-1} = \mathbf{1}, \quad \kappa^{-1}.\kappa = \mathbf{1}_R. \tag{9.2}$$

Material finite deformation measures called the Cosserat and wryness tensors are defined by

$$\bar{\mathbf{C}} := \mathbf{F}^T.\kappa, \quad \Gamma := \frac{1}{2}\kappa^{-1} \dot{\times} \left(\nabla_R \kappa\right), \tag{9.3}$$

where the symbolism introduced is such that $\bar{\mathbf{C}}$ is the material pull back of $\kappa$, and $\Gamma$ is a geometric object that is axial on its first index, being associated by duality with the skew quantity obtained by taking the material gradient of (9.1). In *components* these material covariant objects are given by

$$\bar{C}_{KL} = \delta_{ij} F^i_{.K} \kappa^j_{.L}, \quad \Gamma_{QL} = \frac{1}{2} \varepsilon^{..P}_{QK} \kappa^K_{.i} \kappa^i_{.P,L}. \tag{9.4}$$

It is more than a curiosity to note that

$$\mathbf{C} = \bar{\mathbf{C}}.\bar{\mathbf{C}}^T. \tag{9.5}$$

The physical velocity associated with κ is obviously defined by

$$\dot{\kappa} := \left.\frac{\partial \bar{\kappa}}{\partial t}\right|_X = \bar{\nu}.\kappa, \quad \bar{\nu} = \dot{\kappa}.\kappa^{-1} = -\bar{\nu}^T. \tag{9.6}$$

The axial vector ν associated with the skew tensor velocity $\bar{\nu}$ is given by

$$\nu = -\frac{1}{2}\text{dual}\,\bar{\nu}, \quad \text{i.e.,} \quad \nu_k = -\frac{1}{2}\varepsilon^{..q}_{kp}\bar{\nu}^p_{.q}. \tag{9.7}$$

Reciprocally,

$$\bar{\nu} = -\text{dual}\,\nu, \quad \text{i.e.,} \quad \bar{\nu}^{km} = -\varepsilon^{kmn}\nu_n. \tag{9.8}$$

In conclusion of these kinematic developments, the *direct* generalized motion of the polar continuum is given by

$$\{\chi(\mathbf{X},t),\, \kappa(\mathbf{X},t)\}, \tag{9.9}$$

with velocity set $\{\mathbf{v}, \dot{\kappa}\}$ or {ν, ν}, *first* material gradients (deformations) {**F**, $\nabla_R$ κ}, and independent finite strains $\{\bar{\mathbf{C}}, \Gamma\}$ in terms of the space–time parametrization (**X**, *t*). We are thus unequivocally equipped for a *first-gradient field theory of polar elastic media*. Kinetic energy will be introduced later on.

### 9.2.2 Lagrange Equations of Motion

We shall consider the following general Lagrangian density per unit volume of the reference configuration, limiting ourselves to quasistatics for the moment:

$$L = \bar{L}(\mathbf{x}, \mathbf{v}, \mathbf{F}, \kappa, \dot{\kappa}, \nabla_R \kappa) = -\bar{W}(\mathbf{F}, \kappa, \nabla_R \kappa; \mathbf{X}). \tag{9.10}$$

Making abstraction of boundary conditions, initial conditions, and external data, we obtain the Euler–Lagrange equations of motion in the form:

$$E_\chi := \frac{\partial \bar{L}}{\partial \mathbf{x}} - \nabla_R \cdot \frac{\partial \bar{L}}{\partial (\nabla_R \chi)} = \mathrm{div}_R \mathbf{T} = 0 \tag{9.11}$$

and

$$E\kappa := \frac{\partial \bar{L}}{\partial \kappa} - \nabla_R \cdot \frac{\partial \bar{L}}{\partial (\nabla_R \kappa)} = \mathrm{div}_R \bar{\mathbf{M}} + \bar{\mathbf{N}} = 0, \tag{9.12}$$

in which we have defined the two-point tensor fields $\mathbf{T}$, $\bar{\mathbf{M}}$, and $\bar{\mathbf{N}}$ of components $T^K_{.i}$, $\bar{M}^{KL}_{..i}$, and $\bar{N}^{Ki}$ or $\bar{N}^K_{.i}$ by, respectively,

$$\mathbf{T} := \frac{\partial \bar{W}}{\partial \mathbf{F}}, \quad \bar{\mathbf{M}} := \frac{\partial \bar{W}}{\partial (\nabla_R \kappa)}, \quad \bar{\mathbf{N}} := -\frac{\partial \bar{W}}{\partial \kappa}, \tag{9.13}$$

where the first is none other than the first *Piola–Kirchhoff stress* and the second and third may be referred to as the *Piola–Kirchhoff microstress* and the *microinternal force*, respectively. Here the material divergence is not a covariant operator but just the partial derivative with respect to the material coordinates, taken with respect to the first index.

The second invariance of continuum mechanics is the rotational invariance in the actual frame. Here this is equivalent to the invariance of the strain function $W$ under infinitesimal rotation of the actual frame. This reads

$$\left( \mathbf{TF} - \bar{\mathbf{N}} . \kappa + \bar{\mathbf{M}} : (\nabla_R \kappa)^T \right)_{skew} = \mathbf{0}. \tag{9.14}$$

Here *skew* means the skewsymmetric part of the corresponding *spatial* tensor. Equation 9.14 is a direct generalization of (2.88). This suggests taking the material inner product of (9.12) with $\kappa$ and then the skew part of the resulting spatial tensor, that is

$$C_\kappa := \left( \kappa . \left( \mathrm{div}_R \bar{\mathbf{M}} + \bar{\mathbf{N}} \right) \right)_{skew} = \mathbf{0}, \tag{9.15}$$

and combine the result with (9.14) to yield

$$\mathrm{div}_R \mathbf{M} + \mathbf{F} \hat{\times} \mathbf{T} = \mathbf{0}, \tag{9.16}$$

where the symbolism $\hat{\times}$ has the opposite operational meaning to the symbolism $\dot{\times}$, meaning the vector product in physical space and then inner product in material space, and the two-point tensor field $\mathbf{M}$ of tensorial component $M^K_{.i}$ is defined by

$$\mathbf{M} := \left\{ M^K_{.i} = \varepsilon^{ipq} \bar{M}^{KL}_{..p} \kappa_{qL} \right\}. \tag{9.17}$$

Equation 9.16 is the balance of physical moment of momentum, in quasistatic form. In particular, whenever $W$ does not depend on the microstructure, this reduces to the classical equation

$$\mathbf{F}\hat{\times}\mathbf{T}=\mathbf{0},\quad \text{i.e.,}\quad \varepsilon_{ijk}F^{j}_{.K}T^{Kk}=0\quad\text{or}\quad \left(\mathbf{F}.\mathbf{T}\right)_{skew}=\mathbf{0}, \tag{9.18}$$

which reflects the symmetry of the Cauchy stress.

The reasoning just made means that in field theory, (9.16) is not a direct field equation but the result of a manipulation that takes the *isotropy of physical space* into account. But this does not exhaust the possible conservation laws, as we said nothing about the fact that

$$\left(\frac{\partial\bar{L}}{\partial t}\right)_{\text{expl}}=0,\quad \mathbf{f}^{\text{inh}}:=-\left(\frac{\partial\bar{W}}{\partial\mathbf{X}}\right)_{\text{expl}}\neq\mathbf{0}. \tag{9.19}$$

These relates to the canonical balance laws of energy and material momentum.

### 9.2.3 Canonical Balance Laws

At this point there are two ways to establish the canonical balance laws of interest. The sophisticated one is to implement Noether's theorem for time and material space translations. The "poor man" one uses algebraic manipulations of the already known equations. Here, for a change, we briefly illustrate the latter. For that purpose, aiming first at the balance of energy, we add up the inner product of (9.11) with $\mathbf{v}$ to the contracted product of (9.12) with $\dot{\kappa}$, and therefore envisage the vanishing scalar quantity

$$\mathbf{v}.E_{\chi}+\text{tr}\left(\dot{\kappa}.E_{\kappa}\right)=0. \tag{9.20}$$

This, by using commutation rules and accounting for the obvious identity

$$\text{tr}\left(\bar{\nu}.C_{\kappa}\right)=0$$

deduced from (9.15), yields, after some algebra that we leave to the reader,

$$\left.\frac{\partial W}{\partial t}\right|_{X}-\nabla_{R}.\left(\mathbf{T}.\mathbf{v}+\mathbf{M}.\nu\right)=0. \tag{9.21}$$

It is readily verified that this can also be written in the form:

$$\left.\frac{\partial W}{\partial t}\right|_{X}-\nabla_{R}.\left(\mathbf{T}.\dot{\chi}+\bar{\mathbf{M}}:\dot{\kappa}\right)=0, \tag{9.22}$$

because of the trivial identity $\mathbf{M}.\nu\equiv\bar{\mathbf{M}}:\dot{\kappa}$.

We can perform a parallel space-like operation on (9.11) and (9.12) by forming the following vanishing material covector (compare to (9.20)):

$$E_{\chi}.\mathbf{F}+E_{\kappa}.\left(\nabla_{R}\boldsymbol{\kappa}\right)^{T}=0. \tag{9.23}$$

Again exploiting commutations rules, the constitutive equations (9.13) and the definition given by the second of (9.19) will result in the following fully material balance law:

$$\mathrm{div}_{R}\mathbf{b}+\mathbf{f}^{\mathrm{inh}}=\mathbf{0}, \tag{9.24}$$

in which the generalized (but quasistatic) *Eshelby stress* has the expression

$$\mathbf{b}=W\mathbf{1}_{R}-\mathbf{T}.\mathbf{F}-\mathbf{M}:\left(\nabla_{R}\boldsymbol{\kappa}\right)^{T} \tag{9.25}$$

There is no surprise here, as the Eshelby material stress is a machinery that captures all gradient effects present in the energy density. The intermediate equation (9.23) is a generalization of the *Ericksen identity* of standard hyperelasticity (see Chapter 3), but it is also a direct statement of Noether's identity in field theory (see Chapter 4). Of course, (9.21) and (9.24) should be compatible since they are the canonical conservation equations for energy and linear momentum. This is indeed true as can be shown by performing the exercise that consists in showing that (9.21) is equivalent to the equation

$$\mathbf{V}.\left(\mathrm{div}_{R}\mathbf{b}+\mathbf{f}^{\mathrm{inh}}\right)=0. \tag{9.26}$$

One may finally wonder what the symmetry condition is that is imposed on $\mathbf{b}$ so that the original law of moment of momentum, here (9.16), is verified. A direct computation shows that the following material equation holds:

$$\mathrm{div}_{R}\hat{\mathbf{B}}+\hat{\mathbf{C}}=\left(\mathbf{C}\mathbf{b}\right)_{skew}, \tag{9.27}$$

where we have defined an *Eshelby material hyperstress tensor* $\hat{\mathbf{B}}$ and a material couple tensor $\hat{\mathbf{C}}$ in components by

$$\hat{B}^{K}_{.PQ}\equiv\hat{B}^{K}_{.[PQ]}=\bar{C}_{[P|L|}M^{LK}_{..i}F^{i}_{.Q]},\quad \hat{C}_{PQ}\equiv\hat{C}_{[PQ]}=-\left(\bar{C}_{[P|K|}F^{i}_{.Q]}\right)_{,L}M^{LK}_{..i}. \tag{9.28}$$

**Objective Form of Constitutive Equations**

This can be obtained through a direct reasoning on the functional form in (9.10) or, since there are no dissipative processes, by integrating the condition in

(9.14)—a set of three first-order partial differential equations—along characteristics, yielding a first integral in the objective form:

$$W = \hat{W}\left(\bar{\mathbf{C}}, \Gamma; \mathbf{X}\right), \tag{9.29}$$

so that the basic two constitutive equations become

$$T^{Ki} = \frac{\partial \hat{W}}{\partial \bar{C}_{KL}} \kappa^{i}_{.L}, \quad M^{Ki} = \frac{\partial \hat{W}}{\partial \Gamma_{LK}} \kappa^{i}_{.L}. \tag{9.30}$$

### 9.2.4 Accounting for Inertia

If inertia is accounted for, then we must consider the true Lagrangian density per unit volume of $K_R$, $L = K - W$. For a classical type of inertia, for example, without gyroscopic term, $K$ is taken as a homogeneous function of degree two in the set of velocities $\left\{\mathbf{v}, \dot{\boldsymbol{\kappa}}\right\}$ or {**v**, ν}.That is,

$$2K = \frac{\partial K}{\partial \mathbf{v}} \cdot \mathbf{v} + \frac{\partial K}{\partial \dot{\boldsymbol{\kappa}}} \cdot \dot{\boldsymbol{\kappa}}. \tag{9.31}$$

The simplest solution of this functional equation reads

$$K = \frac{1}{2} \rho_0 \left(\mathbf{X}\right) \left( \mathbf{v}^2 \left(\mathbf{X}, t\right) + I^{::KL}_{ij} \left(\mathbf{X}\right) \dot{\kappa}^{i}_{.K} \dot{\kappa}^{j}_{.L} \right), \tag{9.32}$$

where the geometric object ***I*** is symmetric in both pairs of indices. Of course, this can also be written as the apparently simpler form

$$K = \frac{1}{2} \rho_0 \left(\mathbf{X}\right) \left( \mathbf{v}^2 + \sigma\left(\mathbf{X}, t\right).\nu\left(\mathbf{X}, t\right) \right), \tag{9.33}$$

where the (axial and spatial) *spin vector* σ and the *inertia tensor* of the microstructure ***j*** (a symmetric spatial tensor with six independent components at most) are defined by

$$\sigma = j.\nu, \tag{9.34}$$

and (in components)

$$j^{pq} = \varepsilon^{p}_{.ik} \varepsilon^{q}_{.jl} L^{ijKL}\left(\mathbf{X}\right) \kappa^{k}_{.K} \kappa^{l}_{.L}. \tag{9.35}$$

It was shown by Eringen (1964) that if the material inertia tensor $J^{PQ} = j^{pq}\boldsymbol{\kappa}^{P}_{.p}\boldsymbol{\kappa}^{Q}_{.q}$ satisfies the material conservation law (conservation of microinertia)

$$\left.\frac{\partial J^{PQ}}{\partial t}\right|_{X} = 0, \tag{9.36}$$

then, in turn, $\boldsymbol{j}$ satisfies the following "spatial" balance law (parentheses around a set of indices indicate symmetrization):

$$\frac{dj^{kl}}{dt} - 2\, j^{(k}_{.m}\overline{\mathbf{v}}^{l)m} = 0. \tag{9.37}$$

Then it is trivial to show that in addition to (9.36) or (9.37), the three basic balance laws of physical linear momentum, angular momentum, and energy (in the absence of dissipation and external sources) are obtained as the Euler–Lagrange equations of motion, and the application of Noether's theorem for time-translation, as

$$\left.\frac{\partial}{\partial t}\left(\rho_0\mathbf{v}\right)\right|_{X} - \operatorname{div}_R\mathbf{T} = \mathbf{0}, \tag{9.38}$$

$$\left.\frac{\partial}{\partial t}\left(\rho_0\boldsymbol{\sigma}\right)\right|_{X} - \operatorname{div}_R\mathbf{M} - \mathbf{F}\,\hat{\times}\,\mathbf{T} = \mathbf{0}, \tag{9.39}$$

$$\left.\frac{\partial}{\partial t}\left(K+W\right)\right|_{X} - \nabla_R.\left(\mathbf{T}.\mathbf{v} + \mathbf{M}.\boldsymbol{\nu}\right) = 0. \tag{9.40}$$

It remains to establish the dynamic form of the conservation of material momentum for these polar media. Of course, the energy $W$ will be replaced by $-L$ in the Eshelby stress, but, what may be more surprising to most readers, the material (in fact, here, *canonical*) momentum includes the microrotational degree of freedom although it is, per se, a linear momentum. Indeed, on applying the general formula (4.33), we obtain a canonical material momentum in the form

$$\mathbf{P} = \rho_0\left(\mathbf{C}.\mathbf{V} + \mathbf{G}.\boldsymbol{\nu}\right), \tag{9.41}$$

where the two-point tensor field $\mathbf{G}$ is given in components by

$$G^{\,n}_{L} = -\boldsymbol{\kappa}^{i}_{.K,L}\boldsymbol{\varepsilon}_{jmn}I^{..KQ}_{ij}\boldsymbol{\kappa}^{m}_{.Q}. \tag{9.42}$$

The conservation of canonical momentum reads thus

$$\left.\frac{\partial \mathbf{P}}{\partial t}\right|_X - \mathrm{div}_R \mathbf{b} = \mathbf{f}^{\mathrm{inh}}, \tag{9.43}$$

with **P** given by (9.41) and

$$\mathbf{b} = -\left(L\mathbf{1}_R + \mathbf{T}.\mathbf{F} + \hat{\mathbf{M}} : \left(\nabla_R \boldsymbol{\kappa}\right)^T\right), \quad \mathbf{f}^{\mathrm{inh}} = \left(\frac{\partial L}{\partial \mathbf{X}}\right)_{\mathrm{expl}}. \tag{9.44}$$

This completes the set of fundamental balance and conservation laws for nondissipative polar materials, based on the direct-motion description and the Piola–Kirchhoff format. Note that a variational principle in the spatial framework was given by Maugin (1970) for the more general case of *micromorphic* materials, thus including the present case. Insofar as the inverse-motion description is concerned, one should consider a Lagrangian density per unit volume of the actual configuration $K_t$ in the form

$$\hat{L} = \frac{1}{2}\rho\left(\mathbf{V}.\mathbf{C}.\mathbf{V} + L_{ij}^{.KL}\dot{\kappa}^i_{.K}\dot{\kappa}^j_{.L}\right) - J_F\hat{W}, \tag{9.45}$$

since the notion of inverse motion applies only to the classical motion. The Hamiltonian-mechanics definition of **P** is $\mathbf{P} = \partial L/\partial \mathbf{V}$. Still, (9.45) will yield the expression (9.41) if we note that

$$\dot{\kappa}^i_{.K} := \left.\frac{\partial \kappa^i_{.K}}{\partial t}\right|_X = \left.\frac{\partial \kappa^i_{.K}}{\partial t}\right|_x - \mathbf{V}.\nabla_R \kappa^i_{.K}. \tag{9.46}$$

The last contribution in this equation will provide the microrotation contribution in the definition in Equation 9.45, now written per unit of actual volume.

The accompanying chart (Figure 9.1) gives a flowchart of the whole set of basic conservation laws according to Maugin (1998). Also included here are the equations obtained by inner, vectorial, and tensorial multiplication of the balance of canonical momentum by **X**. With the last operation and taking the skew part of the result, one should obtain an equation of the type of (9.27) (cf. Maugin, 1998) involving Eshelby hyperstresses.

### 9.2.5 Dissipative Case

In this case we have no variational principle at our disposal, and we must resort to a statement of the global balance laws of thermomechanics and their localization as achieved by, for example, Kafadar and Eringen (1971).

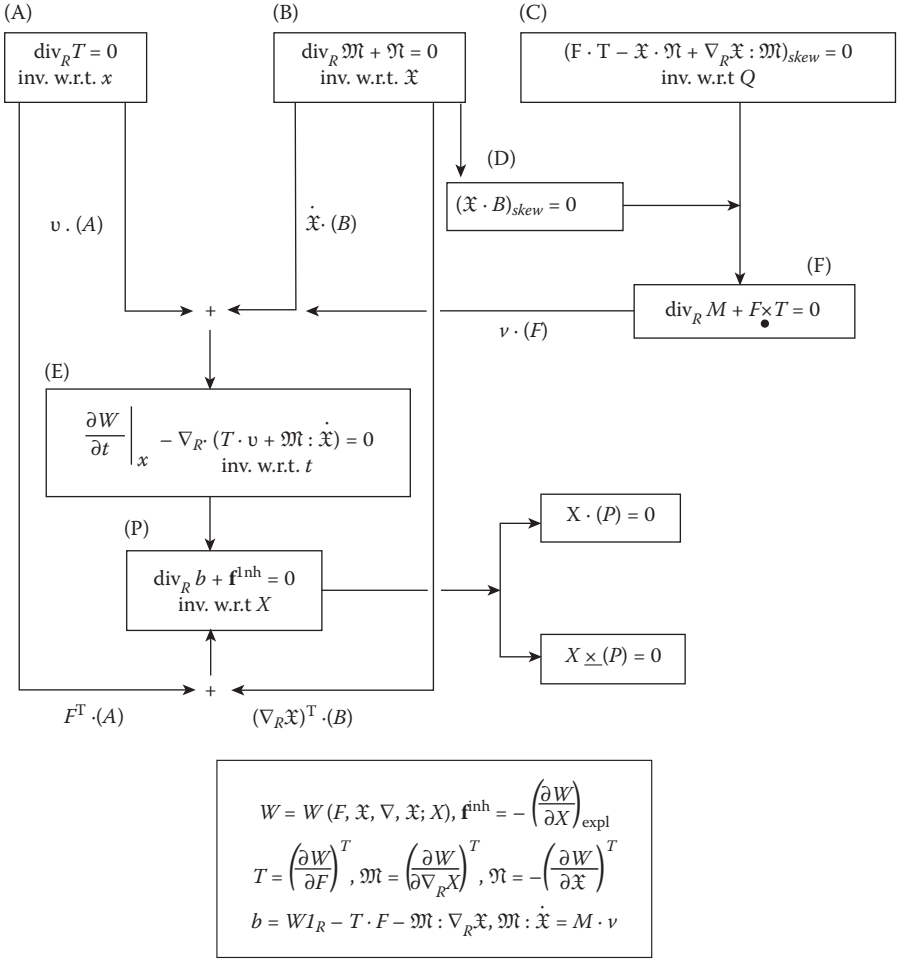


**FIGURE 9.1**
Flowchart of the formal structure of the set of field and conservation equations of polar media (quasistatics). The notation is slightly different from the one used in the present book but the one-to-one correspondence between symbols and operations is easily established; in particular, some tensors are defined by their transposed. (Reproduced from Maugin, G.A., *Philos. Trans. R. Soc. London, Ser., A* 356, 1367–1395, 1998.)

The balance of *material momentum* will then be deduced for large classes of dissipative materials, just as was done for dissipative materials in Chapter 5. Accordingly, we just list the local standard balance laws in their Piola–Kirchhoff format in the absence of external sources:

$$\left.\frac{\partial}{\partial t}\rho_0\right|_X = 0, \tag{9.47}$$

$$\left.\frac{\partial J^{PQ}}{\partial t}\right|_X = 0, \tag{9.48}$$

$$\left.\frac{\partial}{\partial t}(\rho_0 \mathbf{v})\right|_X - \mathrm{div}_R \mathbf{T} = \mathbf{0}, \tag{9.49}$$

$$\left.\frac{\partial}{\partial t}(\rho_0 \boldsymbol{\sigma})\right|_X - \mathrm{div}_R \mathbf{M} - \mathbf{F} \hat{\times} \mathbf{T} = \mathbf{0}, \tag{9.50}$$

$$\left.\frac{\partial}{\partial t}(K+E)\right|_X - \nabla_R . (\mathbf{T}.\mathbf{v} + \mathbf{M}.\nu - \mathbf{Q}) = 0. \tag{9.51}$$

$$\theta \left.\frac{\partial}{\partial t} S\right|_X + \nabla_R . \mathbf{Q} = 0, \tag{9.52}$$

where $E$ is the internal energy per unit of reference volume, $S$ is the entropy per unit of reference volume, $\theta$ is the thermodynamic temperature, and $\mathbf{Q}$ is the material heat flux. Equation 9.52 can also be written as

$$\left.\frac{\partial S}{\partial t}\right|_X + \nabla_R . \left(\frac{\mathbf{Q}}{\theta}\right) = \frac{d}{\theta}, \quad d = -\mathbf{Q}.\nabla_R (\ln \theta). \tag{9.53}$$

Limiting ourselves to the case of thermoelastic conductors, the second law of thermodynamics imposes that $d \geq 0$, while the constitutive equations for nondissipative processes have been deduced, by use of the "thermodynamic admissibility" argument, as

$$\mathbf{T} = \frac{\partial \bar{W}}{\partial \mathbf{F}}, \quad \bar{\mathbf{M}} = \frac{\partial \bar{W}}{\partial (\nabla_R \kappa)}, \quad S = -\frac{\partial \bar{W}}{\partial \theta}, \quad \mathbf{M} \equiv \bar{\mathbf{M}} \dot{\times} \kappa, \tag{9.54}$$

with free energy density

$$W = \bar{W}(\mathbf{F}, \kappa, \nabla_R \kappa, \theta; \mathbf{X}) = E - S\theta. \tag{9.55}$$

Insofar as $\mathbf{Q}$ is concerned, it is subjected only to the nonnegativeness condition imposed on $d$ and to the continuity condition

$$\mathbf{Q}(\mathbf{F}, \kappa, \nabla_R \kappa, \theta, \nabla_R \theta; \mathbf{X}) \to \mathbf{0} \quad \text{as} \quad \nabla_R \theta \to \mathbf{0}. \tag{9.56}$$

The set of Equations 9.47 through 9.56 leaves us with very little room to maneuver. To obtain the local balance of material (canonical) momentum, we must apply **F** to the right of Equation 9.49 and account for the other equations, including the constitutive equations (9.54) and (9.55) to arrive finally at the equation:

$$\left.\frac{\partial}{\partial t}\mathbf{P}\right|_X - \mathrm{div}_R\,\mathbf{b} = \mathbf{f}^{\mathrm{inh}} + \mathbf{f}^{\mathrm{th}}, \tag{9.57}$$

where **P** is defined by (9.41) and we have set

$$\mathbf{b} = -\left(L^{\mathrm{th}}\mathbf{1}_R + \mathbf{T}\mathbf{L} + \bar{\mathbf{M}} : \left(\nabla_R \boldsymbol{\kappa}\right)^T\right), \quad L^{\mathrm{th}} := K - \bar{W}\left(.,.,.,\theta;\mathbf{X}\right), \tag{9.58}$$

$$\mathbf{f}^{\mathrm{inh}} := \left(\frac{\partial L^{\mathrm{th}}}{\partial \mathbf{X}}\right)_{\mathrm{expl}}, \quad \mathbf{f}^{\mathrm{th}} := S\nabla_R\theta. \tag{9.59}$$

The last two material covectors are the material force of inhomogeneity and the material thermal force, respectively.

## 9.3 Small-Strain and Small-Microrotation Approximation

In many situations it is sufficient to envisage the case of small strains and, here, in addition, small microrotations. Notice, however, that there are situations where strains may be small but microrotations may remain mathematically finite, yielding a micromotion that exhibits interesting nonlinear effects such as solitary wave solutions, while small strains accompany these (cf. Maugin and Miled, 1986). But here we consider both macro- and micromotions "small." In this case we naturally introduce a relative Cosserat tensor by

$$\tilde{\mathbf{C}} = \bar{\mathbf{C}} - \mathbf{1}_R. \tag{9.60}$$

The direct-motion gradient **F** and the microrotation $\boldsymbol{\kappa}$ can be approximated by

$$\mathbf{F} = \mathbf{1}_S + \left(\nabla_R \mathbf{u}\right)^T, \quad \boldsymbol{\kappa} = \mathbf{1}_S + \boldsymbol{\Phi}, \tag{9.61}$$

where $\mathbf{1}_s$ is a so-called shifter, **u** is the displacement field, and $\boldsymbol{\Phi}$ is skewsymmetric and of infinitesimally small magnitude. We therefore have the following linearized measures:

$$\tilde{\mathbf{C}} \cong \left(\nabla_R \mathbf{u}\right)^T + \Phi, \quad \Gamma \cong \frac{1}{2}\mathbf{1}_S \dot{\times}\left(\nabla_R \Phi\right). \tag{9.62}$$

Define $\phi$, the vector dual to the skewsymmetric tensor $\Phi$, by

$$\phi_K = \frac{1}{2}\varepsilon_{KLM}\Phi_{ML}, \quad \Phi_{KL} = -\varepsilon_{KLM}\phi_M. \tag{9.63}$$

Then instead of the measures in (9.62) we can, as well, use the following infinitesimal measures of generalized deformation for a linear polar elastic solid (we no longer distinguish between lower- and uppercase Latin indices):

$$\mathbf{e} := \left(\nabla \mathbf{u}\right)^T + \operatorname{dual}\phi = \left\{e_{ji} = u_{i,j} - \varepsilon_{jik}\phi_k\right\}, \quad \gamma := \nabla\phi = \left\{\gamma_{ji} = \phi_{i,j}\right\}. \tag{9.64}$$

In this approximation, the tensors $\mathbf{T}$ and $\mathbf{M}$ reduce to the usual (but here nonsymmetric) *Cauchy stress* tensor $\sigma$ and *couple-stress* tensor $\boldsymbol{m}$ with constitutive equations

$$\sigma = \frac{\partial \hat{W}}{\partial \mathbf{e}}, \quad \mathbf{m} = \frac{\partial \hat{W}}{\partial \gamma}, \quad S = -\frac{\partial \hat{W}}{\partial \theta}, \quad W = \hat{W}\left(\mathbf{e}, \gamma, \theta; \mathbf{x}\right).$$

The two basic laws of motion (9.49) and (9.50) take on the following form (compare to Eringen, 1968; Nowacki, 1986):

$$\rho_0 \frac{\partial^2 \mathbf{u}}{\partial t^2} - \operatorname{div}\sigma = \mathbf{0}, \quad \rho_0 j. \frac{\partial^2 \phi}{\partial t^2} - \operatorname{div} m - \left(\mathbf{1} \dot{\times} \sigma\right) = \mathbf{0}. \tag{9.65}$$

In components the last equation reads

$$\rho_0 j_{ij} \frac{\partial^2 \phi_j}{\partial t^2} - \frac{\partial m_{ji}}{\partial x_j} - \varepsilon_{ipq}\sigma_{pq} = 0. \tag{9.66}$$

Isotropic microinertia, $\mathbf{j} = I\mathbf{1}$ , that is, $j_{ij} = I\delta_{ij}$, is often assumed for the sake of simplicity or as an evident conclusion from a true microanalysis, but this restriction is not imposed by the formulation.

On account of the approximations introduced in the preceding, the canonical balance equations of energy and momentum take on the following form ($e$ = internal energy per unit mass):

$$\frac{\partial}{\partial t}\left(\rho_0\left(e+\frac{1}{2}\dot{\mathbf{u}}^2+\frac{1}{2}\dot{\phi}.j.\dot{\phi}\right)\right)-\nabla.\left(\boldsymbol{\sigma}.\dot{\mathbf{u}}+m.\dot{\phi}-\mathbf{q}\right)=0, \tag{9.67}$$

and

$$\frac{\partial}{\partial t}\mathbf{P}^{\text{tot}.f}-\operatorname{div}\mathbf{b}=\mathbf{f}^{\text{inh}}+\mathbf{f}^{\text{th}}, \tag{9.68}$$

wherein

$$\mathbf{P}^{\text{tot}.f}=-\rho_0\left((\nabla\mathbf{u}).\dot{\mathbf{u}}+(\nabla\phi).j.\dot{\phi}\right),\quad \mathbf{f}^{\text{inh}}=\left(\frac{\partial\hat{L}}{\partial\mathbf{x}}\right)_{\text{expl}},\quad \mathbf{f}^{\text{th}}=S\nabla\theta, \tag{9.69}$$

$$\mathbf{b}=\left(\hat{W}-\frac{1}{2}\rho_0\dot{\mathbf{u}}^2-\frac{1}{2}\rho_0\dot{\phi}.j.\dot{\phi}\right)\mathbf{1}-\boldsymbol{\sigma}.(\nabla\mathbf{u})^T-m.(\nabla\phi)^T. \tag{9.70}$$

**REMARK: Constrained theory of Cosserat continua**

The first measure introduced in (9.49) compares the displacement gradient and the microrotation, an expression that can be written as

$$e_{ij}=u_{(j,i)}+u_{[j,i]}-\varepsilon_{ijk}\phi_k. \tag{9.71}$$

The skewsymmetric tensor $\omega_{ji}=u_{[i,j]}$ is called the (macro-)rotation. If we impose that the macro- and microrotations coincide, that is, $\omega_{ji}=\varepsilon_{jik}\phi_k$, then the two measures of deformation introduced in (9.64) reduce to

$$e_{ij}=\varepsilon_{ij}=u_{(i,j)},\quad \gamma_{ij}=\frac{1}{2}\varepsilon_{ipq}u_{[p,q]j}, \tag{9.72}$$

In plain words, the Cosserat theory becomes a very special *second-gradient theory* of the displacement. Of course, there is then a difficulty in interpreting the expression of the total kinetic energy.

## 9.4 Discontinuity Surfaces in Polar Materials

For the sake of illustration, we consider only the case of coherent phase-transition fronts (Maugin, 1998b). Already in classical thermoelasticity it is assumed that both temperature and material velocity are continuous at a

discontinuity front Σ, because the transition occurs at a temperature where the two phases coexist, and lattice sites (in the discrete picture) at the front belong to the two phases, so that Σ does not exhibit dislocations, a very ideal situation we admit. The conditions to be imposed in the case of polar crystals are even more severe since the microrotations of material points belonging to the two crystalline systems at Σ must obviously be synchronized in time. Otherwise, we would have some kind of disclinations (rotation dislocations) present at Σ. Therefore $\theta(\mathbf{X}, t)$ and the generalized velocities based on $\chi^{-1}(x, t)$ and $\kappa(\mathbf{x}, t)$—*not* $\kappa(\mathbf{X}, t)$—are to be continuous at Σ, that is,

$$\left[\theta\right] = 0, \quad \left[\mathbf{V}\right] = \mathbf{0}, \quad \left[\left(\frac{\partial \kappa}{\partial t}\right)_x\right] = 0. \tag{9.73}$$

A direct consequence of the last of these is the relation

$$\left[\left(\frac{\partial \kappa}{\partial t}\right)_X\right] = -\bar{\mathbf{V}}.\left[\nabla_R \kappa\right]. \tag{9.74}$$

Now, following the illustrative case of complex media in Section 7.7 and based on the equations valid at any regular material points for polar media (in the Piola–Kirchhoff format)—Equations 9.47 through 9.53 and 9.57—we can write down the following set of jump conditions at Σ:

$$\bar{V}_N\left[\rho_0\right] = 0, \tag{9.75}$$

$$\bar{V}_N\left[J_{KL}\right] = 0, \tag{9.76}$$

$$\mathbf{N}.\left[\bar{\mathbf{V}} \otimes \mathbf{p} + \mathbf{T}\right] = \mathbf{0}, \tag{9.77}$$

$$\mathbf{N}.\left[\bar{\mathbf{V}} \otimes \rho_0 \sigma + \mathbf{M}\right] = \mathbf{0}, \tag{9.78}$$

$$\mathbf{N}.\left[\bar{\mathbf{V}}\left(K + E\right) + \left(\mathbf{T}.\mathbf{v} + \mathbf{M}.\nu - \mathbf{Q}\right)\right] = 0, \tag{9.79}$$

which are all homogeneous (vanishing sources), and the set relating to dissipative and pseudo-inhomogeneous processes:

$$\mathbf{N}.\left[\bar{\mathbf{V}} S\theta - \mathbf{Q}\right] - q_\Sigma = 0, \tag{9.80}$$

$$\mathbf{N}.\left[\bar{\mathbf{V}}\mathbf{S} - (\mathbf{Q}/\theta)\right] = \sigma_\Sigma \geq 0, \tag{9.81}$$

$$\mathbf{N}.\left[\bar{\mathbf{V}} \otimes \mathbf{P} + \mathbf{b}\right] + \mathbf{f}_\Sigma = \mathbf{0}, \tag{9.82}$$

where $q_\Sigma$, $\sigma_\Sigma$, and $\mathbf{f}_\Sigma$ are, respectively, a surface heat source, a surface dissipation rate, and a surface pseudo-inhomogeneity force. Because of the choice of entropy flux $\mathbf{S} = \mathbf{Q}/\theta$ and of the first of (9.73), we obviously have

$$q_\Sigma = \theta_\Sigma \sigma_\Sigma \geq 0. \tag{9.83}$$

Just as in previous chapters, we now have to evaluate the power expended by the material surface force $\mathbf{f}_\Sigma$. We give the detail of this only in *quasistatics* (see the comments at the end of Section 7.7). This is none other than a special case of the proof given in that section. Thus we simply note the essential steps with the following sequence of equations:

$$p_\Sigma = \mathbf{f}_\Sigma.\bar{\mathbf{V}} = -\mathbf{N}.\left[\mathbf{b}\right].\bar{\mathbf{V}}, \tag{9.84}$$

$$\mathbf{N}.\left[\mathbf{Q}\right] = \mathbf{N}.\left[\bar{\mathbf{V}}E + \mathbf{T}.\mathbf{v} + \mathbf{M}.\nu\right] = \mathbf{N}.\left[\bar{\mathbf{V}}S\theta\right] - q_\Sigma, \tag{9.85}$$

$$q_\Sigma = -\mathbf{N}.\left[\bar{\mathbf{V}}W + \mathbf{T}.\mathbf{v} + \mathbf{M}.\nu\right], \tag{9.86}$$

$$\mathbf{N}.\left[\mathbf{T}.\mathbf{v} + \mathbf{M}.\nu\right] = -\mathbf{N}.\left[\mathbf{T}.\mathbf{F} + \mathbf{M} : \left(\nabla_R \kappa\right)^T\right].\bar{\mathbf{V}}, \tag{9.87}$$

so that

$$p_\Sigma = \mathbf{f}_\Sigma.\bar{\mathbf{V}} = q_\Sigma. \tag{9.88}$$

But the jump relations (9.77) and (9.78) reduce here to

$$\mathbf{N}.\left[\mathbf{T}\right] = \mathbf{0}, \quad \mathbf{N}.\left[\mathbf{M}\right] = \mathbf{0}. \tag{9.89}$$

Consequently,

$$\mathbf{N}.\left[\mathbf{T}.\mathbf{F} + \mathbf{M} : \left(\nabla_R \kappa\right)^T\right] = \left\langle \mathbf{N}.\mathbf{T} \right\rangle.\left[\mathbf{F}\right] + \left\langle \mathbf{N}.\mathbf{M} \right\rangle : \left[\left(\nabla_R \kappa\right)^T\right]. \tag{9.90}$$

Finally, using the Maxwell–Hadamard lemma for jumps of gradients of $\chi$ and $\kappa$, we can write that

$$\left[\mathbf{F}\right]^i_{.K} = f^i N_K, \quad \left[\nabla_R \kappa\right]^i_{.KL} = g^i_{.K} N_L, \tag{9.91}$$

and thus

$$\langle \mathbf{N}.\mathbf{T} \rangle . [\mathbf{F}].\bar{\mathbf{V}} + \langle \mathbf{N}.\mathbf{M} \rangle . \left[ \left( \nabla_R \boldsymbol{\kappa} \right)^T \right] . \bar{\mathbf{V}} = \left\lfloor tr \left\{ \langle \mathbf{T} \rangle . \mathbf{F} + \langle \mathbf{M} \rangle : \left( \nabla_R \boldsymbol{\kappa} \right)^T \right\} \right\rfloor \bar{V}_N . \tag{9.92}$$

Gathering these results we obtain that

$$q_\Sigma = -\text{Hugo}_{\text{PT}} \bar{V}_N \geq 0, \tag{9.93}$$

where we have defined the so-called Gibbs–Hugoniot driving force by

$$\text{Hugo}_{\text{PT}} = \mathbf{N}.[\mathbf{b}].\mathbf{N} = \left\lfloor W - \text{tr} \left( \langle \mathbf{T} \rangle . \mathbf{F} + \langle \mathbf{M} \rangle : \left( \nabla_R \boldsymbol{\kappa} \right)^T \right) \right\rfloor . \tag{9.94}$$

whence

$$\theta_\Sigma \sigma_\Sigma = f_\Sigma \bar{V}_N \geq 0, \tag{9.95}$$

along with the surface balance of material forces

$$f_\Sigma + \text{Hugo}_{\text{PT}} = 0. \tag{9.96}$$

The expression (9.94) has a peculiar form that is a consequence of the working hypothesis of quasistatic evolution. Had we considered the full dynamic case including kinetic energy related to both macro- and micromotions, we would have shown that (9.94) would be replaced by the more general expression:

$$\text{Hugo}_{\text{PT}} = [W] - \langle \mathbf{N}.\mathbf{T} \rangle . \mathbf{f} - \langle \mathbf{N}.\mathbf{M} \rangle : \mathbf{g}, \tag{9.97}$$

where **f** and **g** are none other than the physical vector and two-point tensor field introduced in components in (9.91). Remarkably enough, although this is proved in full dynamics, the kinetic energy is *not* involved in (9.97).

If we impose the vanishing condition

$$\text{Hugo}_{\text{PT}} \equiv 0, \tag{9.98}$$

this would correspond to a *nondissipative* progressing phase transition if $\bar{V}_N \neq 0$, hence a phase transition *à la* Landau.

## 9.5 Fracture of Solid Polar Materials

Because of the canonical form of most relations, we do not need to give the detail of the proof of the following results. Considering a straight-through

crack just like in Section 8.4, in the pure homogeneous elasticity of nonlinear polar materials, we obtain the driving force acting on the tip of the crack in its own direction and the accompanying energy-release rate in the same form as (8.26) and (8.27) (cf. Maugin, 1998), that is,

$$F_1^{\text{crack}} = \int_\Gamma \Big( (\mathbf{N}.\mathbf{b})_1 + P_1 \left( \bar{\mathbf{V}}.\mathbf{N} \right) \Big) dA - \frac{\partial}{\partial t} \int_G P_1 \, dV, \tag{9.99}$$

and

$$G^{\text{crack}} = \int_\Gamma \left( H \left( \bar{\mathbf{V}}.\mathbf{N} \right) + \mathbf{N}.\mathbf{T}.\mathbf{v} + \mathbf{N}.\mathbf{M}.\nu \right) dA - \frac{\partial}{\partial t} \int_G H dV, \tag{9.100}$$

where it is understood that **b**, **P**, and $H$ contain the necessary additional micropolar contributions due to kinetic energy, gradients of $\kappa$, and rotational kinetic energy. The relationship (8.34) will hold true if the micromotion satisfies at the crack tip a condition such as (compare to (9.74))

$$\dot{\kappa} = -\bar{\mathbf{V}}.\nabla_R \kappa + \text{regular term}. \tag{9.101}$$

There are no difficulties to generalize the expressions (9.99) and (9.100) to the inhomogeneous and thermally conducting cases (cf. Maugin, 1998).

In the much simpler case of the quasistatics in small strains and small rotation angles, Equation 9.99 provides the generalization of the *J*-integral as (compare to (8.29))

$$J = \int_\Gamma \left( W N_1 - \mathbf{t}.\frac{\partial \mathbf{u}}{\partial X_1} - \mathbf{m}.\frac{\partial \phi}{\partial X_1} \right) dL, \tag{9.102}$$

where $\mathbf{t} = \mathbf{N}.\mathbf{T}$ and $\mathbf{m} = \mathbf{N}.\mathbf{M}$ along the contour $\Gamma$, while the Eshelby stress has the following quasistatic canonical definition:

$$b_{ji} = W\delta_{ji} - \sigma_{jk} u_{k,i} - m_{jk} \phi_{k,i}, \tag{9.103}$$

where $m_{ji}$ are the components of the reduction of **M** to this linearized case. The result (9.102) was obtained quite early by Atkinson and Leppington (1974). This *J*-integral and the corresponding *L*- and *M*-integrals were discussed by Jaric (1978). Lubarda and Markenscoff (2000) rediscovered some of these results. Lazar and Maugin in the period 2004–2007 have carefully studied the viewpoint of Lie groups and conservation laws for micropolar materials and their derivatives in comparison with gradient and so-called nonlocal theories.

## 9.6 Other Microstructure Modelings

As indicated in Section 9.1, micropolar media constitute but a special case of *micromorphic* continua (according to Eringen's classification). Readers interested in a general nonlinear presentation of micromorphic continua may consult the original work of Eringen and Suhubi (1964), Eringen's book (1999), and, for the application to plasticity, the works of Sievert (1992), Sansour (1998), and Forest (2006). Here we shall limit the presentation to the case of small strains and to the examination of the problem of compatibility of generalized measures of deformation in the presence of defects—which may now be dislocations, disclinations, and point defects or microvoids—as well as the corresponding expression of the Eshelby stress and the various material forces in action in such defective media. To proceed by comparison, we remind the reader of Kroener's incompatibility theory (1958), already given in Section 3.11. There we called $\beta_{ji} = u_{i,j}$ the infinitesimal distortion. In the case of incompatibilities due to plasticity, it was noticed that if the total distortion is compatible by definition, the plastic and elastic distortion are not compatible simultaneously, and we had

$$\beta_{ij} = \beta^e_{ij} + \beta^p_{ij} = u_{i,j} \tag{9.104}$$

and

$$\varepsilon_{jkl}\beta_{li,k} = 0 \Rightarrow \alpha_{ji} := \varepsilon_{jkl}\beta^e_{li,k} \neq 0, \quad \alpha_{ji,j} = 0, \tag{9.105}$$

where the last equation represents Bianchi's identity. The density of dislocation was then essentially identified to the torsion of the material manifold. This can be compared to the finite-strain formulation in Section 6.4.

### 9.6.1 Micromorphic Compatible Case

We consider a sufficiently general case but in small strains and quasistatics to alleviate the notation. This is the theory of *micromorphic media*, that is, media whose material point itself presents a deforming microstructure, so that a six-order tensor $\phi_{ij}$ has to be added to the usual three components $u_i$ of the displacements to fully describe the kinematics of the material (cf. Eringen, 1999), so that kinematics becomes nine-dimensional. Accounting for the gradients of these yields a large number of generalized deformation measures. Then a large number of generalized "internal" forces are necessarily involved by duality. Such a theory was developed essentially by Eringen and Suhubi in 1964, and independently by Mindlin in the same years (e.g. Mindlin, 1964). A variational Hamiltonian principle (Maugin, 1970) can be used to formulate the theory in the absence of dissipation. The principle of virtual power, however,

is the safest tool to construct such a theory without any ambiguity in the concepts, the duality between deformation fields and generalized forces, and the formulation of natural boundary conditions (cf. Germain, 1973; Maugin, 1980; Forest, 2006). We note $u_{i,j}$ for the displacement gradient, $\phi_{ij}$ for the micro-deformation tensor and $\kappa_{ij} = \phi_{ij,k}$ for its gradient. For compatible fields, the relevant infinitesimal deformation measures are the relative deformation (nine components) $\gamma_{ji}$ (which replaces the classical distortion $\beta_{ji}$), the microstrain (six components) $e_{ij}$, and the microwryness tensor (27 components) $\kappa_{kij}$ such that

$$\gamma_{ji} = u_{i,j} - \phi_{ij}, \quad e_{ij} = e_{ji} = \phi_{(ij)}, \quad \kappa_{kij} = \phi_{ij,k}. \tag{9.106}$$

These admit themselves canonical decompositions such as

$$\gamma_{ij} = \gamma_{(ij)} + \gamma_{[ij]}, \quad \gamma_{(ij)} = \gamma\delta_{ij} + \overline{\gamma}_{ij}, \tag{9.107}$$

$$e_{(ij)} = e\delta_{ij} + \overline{e}_{ij}\,, \tag{9.108}$$

$$\kappa_{kij} = \delta_{ij}\kappa_k + \kappa_{k[ij]} + \overline{\kappa}_{k(ij)}, \quad \kappa_k := \kappa_{kii}/3. \tag{9.109}$$

Each of the measures in (9.106) admits a dual in *internal-force* space. For an elastic solid with volume energy $W = \overline{W}\left(\gamma_{ij}, e_{ij}, \kappa_{kij}\right)$, these are the force stress (Cauchy stress) $\sigma_{ji}$, the microstress $s_{ji}$, and the micro-hyperstress $\mu_{kji}$ such that

$$\sigma_{ji} = \frac{\partial \overline{W}}{\partial u_{i,j}}, \quad s_{ji} = \frac{\partial \overline{W}}{\partial e_{ij}} = s_{ij}, \quad \mu_{kij} = \frac{\partial \overline{W}}{\partial \kappa_{ijk}}, \tag{9.110}$$

which satisfy jointly the following equilibrium equations at each regular material point (cf. Eringen and Suhubi, 1964; Eringen, 1999, in a different notation):

- Balance of linear (physical) momentum:

$$\sigma_{ji,j} + f_i \ = 0 \tag{9.111}$$

- Balance of micromotion (here equilibrium form):

$$\mu_{kij,k} + \sigma_{ji} - s_{ji} + l_{ji} = 0, \tag{9.112}$$

where bulk data are the body force $f_i$ and the body moment tensor $l_{ji}$. The micro-hyperstress $\mu_{kij}$ naturally admits a decomposition similar to that of $\kappa_{kij}$, that is, in the antisymmetric part, its trace, and its symmetric traceless part:

$$\mu_{kij} = \mu_{k[ij]} + \frac{1}{3}\mu_k\delta_{ij} + \overline{\mu}_{k(ij)}. \tag{9.113}$$

### 9.6.2 Micromorphic Incompatible Case

In this case the "elastic" parts of the deformation measures $\gamma_{ji}$, $e_{ij}$, and $\kappa_{kij}$ are *incompatible*, which means they are not gradients, and we can introduce the *total* same measures—which, then, are compatible—by (we follow Forest and Sievert, 2003; Lazar and Maugin, 2007)

$$\gamma_{ji} := \gamma^e_{ji} + \gamma^p_{ji} = u_{i,j} - \phi_{ij}, \tag{9.114}$$

$$e_{ij} = \phi_{(ij)} = e^e_{ij} + e^p_{ij}, \tag{9.115}$$

$$\kappa_{kij} = \phi_{ij,k} = \kappa^e_{kij} + \kappa^p_{kij}. \tag{9.116}$$

Accordingly, the "plastic" parts denoted by a superscript $p$ are not compatible. The total quantities are compatible and, therefore, satisfy the following compatibility conditions (cf. Eringen, 1999):

$$\varepsilon_{jkl}\left(\gamma_{li,k} + \kappa_{kil}\right) = 0, \quad \varepsilon_{jkl}\kappa_{lin,k} = 0, \quad 2e_{ij,k} - \kappa_{kij} - \kappa_{kji} = 0. \tag{9.117}$$

The "plastic" parts—or the "elastic" parts—will have to fulfill incompatibility conditions. These will read (e.g., for the "elastic" parts)

$$\alpha_{ji} = \varepsilon_{jkl}\left(\gamma^e_{li,k} + \kappa^e_{ilk}\right), \quad \Theta_{nji} = \varepsilon_{jkl}\kappa^e_{\ln i,k}, \quad Q_{kij} = -\left(2e^e_{ij,k} - \kappa^e_{kji} - \kappa^e_{kij}\right), \tag{9.118}$$

and the nonvanishing objects introduced in the left-hand side of these equations must be given a geometric interpretation if we want to have at hand a generalization of Kroener's vision of incompatibility. The first of these, just like in Kroener's theory, is the *dislocation density tensor*, which is identified with the linearized version of the *Cartan torsion* tensor $\tilde{T}_{ijk}$ according to (nine independent components)

$$\alpha_{ji} = \frac{1}{2}\varepsilon_{jkl}\tilde{T}_{ikl}. \tag{9.119}$$

The second object introduced in (9.118) can be identified with the (linearized) *Riemann–Cartan curvature* $R_{ijkl}$ by (27 independent components)

$$\Theta_{kij} = \frac{1}{2}\varepsilon_{kmn}R_{ijmn}, \tag{9.120}$$

hence it is a curvature tensor. This can also be decomposed in such a way that

$$\Theta_{kij} = \Theta_{k(ij)} + \Theta_{k[ij]} = \Theta_{k(ij)} - \varepsilon_{ijl}\Theta_{lk}, \quad \Theta_{ij} = -\frac{1}{2}\varepsilon_{ikl}\Theta_{jkl} = -\frac{1}{4}\varepsilon_{ikl}\varepsilon_{jmn}R_{klmn}. \tag{9.121}$$

The last defined quantity is the *disclination density* tensor. In effect, it seems natural in this theory to associate the rotational internal degree of freedom with this type of defect (cf. Clauss and Eringen, 1969). As for the geometric quantity $\Theta_k = \Theta_{jjk}/3$, it is called the Weyl "distance curvature" (Schouten, 1954).

Finally, the third object introduced in (9.118) is the *tensor of nonmetricity*. The last of the equations in (9.118) therefore means that the microstrain $e_{ij}$ is *nonmetric*. The quantity $Q_k = Q_{kjj}/3$ is called the *Weyl covector* and will describe defects of the *dilatation* type. In all we can say from a differential-geometric viewpoint that $\gamma_{ij}$, $\kappa_{kij}$, and $e_{ij}$ are, respectively, a coframe, a connection, and a metric. The allied torsion, curvature, and nonmetricity fulfill the following *Bianchi identities* (cf. Schouten, 1954):

- First identity:

$$\alpha_{ji,j} = \Theta_{ji,j} \tag{9.122}$$

- Second identity:

$$\Theta_{jin,j} = 0 \tag{9.123}$$

- Third identity:

$$\varepsilon_{klm} Q_{mij,l} = 2\Theta_{k(ij)} \tag{9.124}$$

The first of these means that dislocations can interact with both disclinations and point defects. The second is just a divergence-free condition. And the last shows that one part of the curvature is given in terms of the nonmetricity tensor that describes point defects. Of course, this greatly simplifies if there are only dislocations present in the material (classical Kroener's theory).

What about the Eshelby stress? We can write it down at once since its formula is canonical, capturing all gradients of the theory. That is, from the energy $W = \bar{W}(\gamma_{ji}, e_{ij}, \kappa_{kij}; x_i)$ where we envisage a possibility of standard material inhomogeneity:

$$b_{ji} = \bar{W}\delta_{ji} - \sigma_{jk}\left(u_{k,i} - \gamma^p_{ik}\right) - \mu_{jkl}\phi_{lk,i}. \tag{9.125}$$

To evaluate the corresponding configurational-material forces, we must compute the divergence of this Eshelby stress. The result of this lengthy computation is as follows:

$$b_{ij,i} + f^{(m)}_j = 0, \tag{9.126}$$

where the *material force source* is given by

$$f^{(m)}_j = -f^{(PK)}_j - f^{(M)}_j + \frac{1}{2} s_{mn} Q_{jmn} + \sigma_{lk}\kappa^P_{kjl} - f_i\left(u_{i,j} - \gamma^p_{ij}\right) - l_{kl}\kappa_{jkl} + f^{\text{inh}}_j, \tag{9.127}$$

where the various contributions are, respectively, the negative of the Peach–Koehler force in the theory of continuously distributed dislocations (compare to Equation 1.83) and the negative of the so-called Mathisson–Papapetrou force introduced by Maugin in defect theory by analogy with gravitational theories with spin (cf. Maugin, 1993). The contribution of nonmetricity is original to micromorphic theory; then there is the convected part of the body force changed of sign with a convection effected with an effective distortion; an equivalent term for the body couple follows, and finally the standard material inhomogeneity force given by the negative of the explicit gradient of $\bar{W}$. Here,

$$f_j^{(PK)} = \varepsilon_{jkl}\sigma_{kp}\alpha_{pl}, \quad f_j^{(M)} = \varepsilon_{jkl}\mu_{kmn}\Theta_{mnl}, \quad f_j^{\text{inh}} = -\left.\frac{\partial \bar{W}}{\partial x_j}\right|_{\text{expl}}. \tag{9.128}$$

### 9.6.3 Special Cases

Several cases of great interest can be extracted from the general micromorphic scheme. These are (in the classification of Eringen, 1999):

i. *Microstretch elasticity*: Only dilatational degrees of freedom are kept in addition to the rotational and translational ones. Therefore, this is both a generalization of micropolar elasticity (Cosserat continua) and a special case of the micromorphic elasticity. The relevant equations can be deduced from the micromorphic ones by setting to zero the shear parts of the microfields. This can be represented by directors with stretch and rotation only, and no microshear of them.
ii. *Micropolar (Cosserat) elasticity*: Only the rotational degrees of freedom in addition to the translational ones are kept. This is the most popular case. This will obviously raise some interest when dealing with defects such as disclinations.
iii. *Dilatation elasticity* (also called elasticity with voids; Cowin and Nunziato, 1983): Only the dilatation of the microstructure is kept in addition to the macrodisplacement. We can easily imagine the interest for this scheme for defects such as microvoids or vacancies.

We briefly examine the last two cases.

i. **Case of micropolar (Cosserat) elasticity** (see Lazar and Maugin, 2007). In this case the equilibrium equations read as follows at any regular material point:

$$\sigma_{ji,j} + f_i = 0, \quad m_{ji,j} + \varepsilon_{ikj}\sigma_{kj} + l_i = 0, \tag{9.129}$$

where $m_{ji}$ is the moment-stress or couple-stress tensor and $l_i$ is the body couple. The standard elastic constitutive equations are given by

$$\sigma_{ji} = \frac{\partial \bar{W}}{\partial \gamma_{ij}}, \quad m_{ji} = \frac{\partial \bar{W}}{\partial \kappa_{ij}}, \quad W = \bar{W}\left(\gamma_{ij}, \kappa_{ij}; x_i\right). \tag{9.130}$$

The total fields are considered to be the sum of elastic and plastic parts (elastic parts without superscript *e*), that is,

$$\gamma_{ji} = \gamma^e_{ji} + \gamma^p_{ji} = u_{i,j} + \varepsilon_{ijk}\phi_k, \quad \kappa_{ji} = \kappa^e_{ji} + \kappa^p_{ji} = \phi_{i,j}. \tag{9.131}$$

The total fields satisfy compatibility conditions (Eringen, 1999) such as

$$\varepsilon_{jkl}\left(\gamma_{li,k} + \varepsilon_{ikm}\kappa_{lm}\right) = 0, \quad \varepsilon_{jkl}\kappa_{li,k} = 0. \tag{9.132}$$

The incompatibility conditions then read (we write them for the elastic parts)

$$\alpha_{ji} = \varepsilon_{jkl}\left(\gamma^e_{li,k} + \varepsilon_{ikm}\kappa^e_{lm}\right), \quad \Theta_{ji} = \varepsilon_{jkl}\kappa^e_{li,k}. \tag{9.133}$$

The Bianchi identities for such micropolar media are obtained by differentiating these equations, yielding the result of Clauss and Eringen (1969):

$$\alpha_{ji,j} = \varepsilon_{imk}\Theta_{km}. \tag{9.134}$$

The canonical writing of the Eshelby stress produces the following formula in the incompatible case:

$$b_{ji} = \bar{W}\delta_{ji} - \sigma_{jk}\bar{\gamma}_{ik} - m_{jk}\kappa_{ik} \tag{9.135}$$

and in the compatible case:

$$b_{ji} = \bar{W}\delta_{ji} - \sigma_{jk}u_{k,i} - m_{jk}\phi_{k,i}. \tag{9.136}$$

The last formula corresponds to the result known from repeated studies (Jaric, 1978; Atkinson and Leppington, 1974; Lubarda and Markenscoff, 2000; and Maugin, 1998, for finite strains and rotations). Computing the divergence of the Eshelby stress in the incompatible case, we find Equation 9.126 but with

$$f^{(m)}_j = -f^{(\mathrm{PK})}_j - f^{(\mathrm{discl})}_j + \varepsilon_{jki}\sigma_{lk}\kappa^p_{il} - f_i\,\bar{\gamma}_{ji} - l_i\,\kappa_{ji} + f^{\mathrm{inh}}_j, \tag{9.137}$$

with

$$f_j^{(\mathrm{PK})} = \varepsilon_{jkl}\sigma_{ki}\alpha_{il}, \quad f_j^{(\mathrm{discl})} = \varepsilon_{jkl}m_{ki}\Theta_{il}, \quad f_j^{\mathrm{inh}} = -\left.\frac{\partial \bar{W}}{\partial x_j}\right|_{\mathrm{expl}}, \tag{9.138}$$

in which we recognize the Peach–Koehler force, an analogous force acting on the disclination density, and the pure inhomogeneity force. In the compatible case (9.139) reduces to

$$f_j^{(m)} = -f_i\, u_{i,j} - l_i\, \phi_{i,j} + f_j^{inh}. \tag{9.139}$$

**ii. Case of dilatation elasticity** (see Lazar and Maugin, 2007). In this case the equilibrium equations at each regular material point are reduced to

$$\sigma_{ji,j} + f_i = 0, \quad \mu_{k,k} + \sigma - s + l = 0, \tag{9.140}$$

along with the constitutive equations

$$\sigma_{ji} = \frac{\partial \bar{W}}{\partial \gamma_{ji}}, \quad s - \sigma = \frac{\partial \bar{W}}{\partial \phi}, \quad \mu_k = \frac{\partial \bar{W}}{\partial \kappa_k}, \quad W = \bar{W}\left(\gamma_{ji}, \phi, \kappa_k; x_i\right). \tag{9.141}$$

In the presence of incompatibilities, the total fields are given by

$$\gamma_{ji} = u_{i,j} - \phi\delta_{ij} = \gamma_{ij}^e + \gamma_{ji}^p, \quad e = e^e + e^p = \phi, \quad \kappa_k = \kappa_k^e + \kappa_k^p = \phi_{,k}. \tag{9.142}$$

The compatibility conditions for these total fields read

$$\varepsilon_{jkl}\left(\gamma_{li,k} - \delta_{il}\kappa_k\right) = 0, \quad \varepsilon_{jkl}\kappa_{l,k} = 0, \quad -e_{,k} + \kappa_k = 0. \tag{9.143}$$

The incompatibility conditions (here written for the elastic parts) read

$$\alpha_{ji} = \varepsilon_{jkl}\left(\gamma_{li,k}^e - \delta_{il}\kappa_k^e\right), \quad \Theta_j = \varepsilon_{jkl}\kappa_{l,k}^e, \quad Q_k = 2\left(e_{,k}^e - \kappa_k^e\right), \tag{9.144}$$

and the Bianchi identities are given by

$$\alpha_{ji,j} = \Theta_i, \quad \Theta_{k,k} = 0, \quad \varepsilon_{klm}Q_{m,l} = 2\Theta_k. \tag{9.145}$$

Finally, in presence of incompatibilities, the Eshelby stress is given by

$$b_{ji} = \bar{W}\delta_{ji} - \sigma_{jk}\bar{\gamma}_{ik} - \mu_j\kappa_i, \tag{9.146}$$

and the material force source in the equilibrium version of the conservation of material momentum is given by

$$f_j^{(m)} = -f_j^{(\mathrm{PK})} - f_j^{(\mathrm{PD})} + \frac{1}{2} s Q_j + \sigma_{jl} \kappa_l^p - f_i \, \overline{\gamma}_{ji} - l \kappa_j + f_j^{\mathrm{inh}}, \tag{9.147}$$

where

$$f_j^{(\mathrm{PK})} = \varepsilon_{jkl} \sigma_{ki} \alpha_{il}, \quad f_j^{(\mathrm{PD})} = \varepsilon_{jkl} \mu_k \Theta_l, \quad f_j^{\mathrm{inh}} = -\left. \frac{\partial \bar{W}}{\partial x_i} \right|_{\mathrm{expl}}, \tag{9.148}$$

are, respectively, the Peach–Koehler force, the material force acting on *point defects/microvoids* (see also Appendix 9.2) and the material force of pure inhomogeneity. In the compatible case, (9.146) reduces to

$$b_{ji} = \bar{W} \delta_{ji} - \sigma_{jk} u_{k,i} - \mu_j \phi_{,i}. \tag{9.149}$$

This, of course, is nothing but the tensor defined in (9.103).

This concludes our excursion into the world of material and configurational forces, originally discovered by J.D. Eshelby, in relation to the theory of defects and the generalization of Kroener's geometric incompatibility theory to modern theories of complex continua. The reader familiar with modern gauge theories of gravitation will have identified some analogy between the present developments in their geometric background and those in gauge theory. For the case of plasticity, distributed dislocations, and the corresponding Peach–Koehler force, we recommend the works of Lazar (2000, 2002) in a modern geometric framework. The recent work of Lazar and Anastasiadis (2006) seems to bring a final answer in the case of a linear theory (quadratic energies).

## Appendix A9.1: Liquid Crystals

Liquid crystals (cf. de Gennes, 1974) partake of two visions, as they may flow, exhibiting thus a fluid-like property, but also present a tendency to ordering that is akin to a solid-crystal-like property, for example, in their so-called nematic phase. This ordering may present "defects," such as disclinations. The natural question therefore arises of the "motion" of such defects and, by the duality inherent in mechanics, of associated configurational forces. But in most of this book these forces are dealt with in reference configurations, while a standard property of many fluids is to possess

no such privileged configuration; most fluids respond instantaneously to external loading, sometimes with a type of delay related to viscosity, but they usually forget any initial configuration. In addition, liquid crystals are more *elastic fluids* than usual fluids, and, compared to classical perfect fluids that are Eulerian in nature (that is, present at most a pressure at equilibrium), liquid crystals are *not* Eulerian fluids, presenting most of the time a nonisotropic structure, even at rest. Of course, it is not forbidden to formulate fluid mechanics, say, in Lagrangian coordinates, but this is seldom used except in some astrophysics and explosion problems. The anisotropic characteristic of liquid crystals is best represented at a mesoscopic level by a field of unit directions $\mathbf{n}(\mathbf{x}, t)$, a so-called *director* field, which represents a kind of average direction of a bunch of elongated particles. An accepted kinematic representation therefore consists in considering at each point (placement) of a fluid $\mathbf{x}$ in its actual configuration $K_t$ the field $\mathbf{n}(\mathbf{x}, t)$, hence two additional degrees of freedom if the vector $\mathbf{n}$ is normalized to unity. Accordingly, during the process of flow and deformation, the point of application of $\mathbf{n}$ is displaced and $\mathbf{n}$ can at most rotate. If a reference configuration $K_R$ is introduced with some arbitrariness, with initial vector *director* field of component $N^K$, the components of $\mathbf{n}$ are related to the $N^K$ by a rotation, hence an orthogonal transformation, that is

$$n^i = \kappa^i_K N^K. \tag{A9.1}$$

Accordingly, liquid crystals of this type are true Cosserat or micropolar continua. A consistent theory basing on this remark (and the use of $\kappa$) can be expanded (cf. Eringen, 2001). But to exhibit something quite different from the contents of the present chapter, we consider here the kinematic description given by the couple $\{\mathbf{x}, \mathbf{n}(\mathbf{x}, t)\}$ or, with a parametrization of the solid type,

$$\left\{\mathbf{x} = \chi(\mathbf{X}, t), \quad \mathbf{n} = \bar{\mathbf{n}}(\mathbf{X}, t)\right\}. \tag{A9.2}$$

and

$$\left\{\mathbf{X} = \chi^{-1}(\mathbf{x}, t), \quad \mathbf{n} = \hat{\mathbf{n}}(\mathbf{x}, t)\right\}. \tag{A9.3}$$

These two parametrizations provide the basis for several variational formulations in which we emphasize the quasistatic case. The following energies may be considered, noting that the fluid nature of a liquid crystal is reflected in the fact that energy will depend on the direct or inverse deformation gradient only through the density:

$$W(\rho, \mathbf{n}, \nabla_R \bar{\mathbf{n}}) = \bar{W}(\mathbf{F}, \mathbf{n}, \nabla_R \bar{\mathbf{n}}) \quad \text{as} \quad \rho = \rho_0 J_F^{-1}, \tag{A9.4}$$

$$w(\rho, \mathbf{n}, \nabla\hat{\mathbf{n}}) = \bar{w}(\mathbf{F}^{-1}, \mathbf{n}, \nabla\hat{\mathbf{n}}) \quad \text{as} \quad \rho = \rho_0 J_{F^{-1}}, \tag{A9.5}$$

$$W = \hat{W}(\mathbf{F}, \mathbf{n}, \nabla\hat{\mathbf{n}}) \quad \text{as} \quad \nabla_R \bar{\mathbf{n}} = \mathbf{F}^T . \nabla\hat{\mathbf{n}}, \tag{A9.6}$$

$$w = \hat{w}(\mathbf{F}^{-1}, \mathbf{n}, \nabla_R \bar{\mathbf{n}}) \quad \text{as} \quad \nabla\hat{\mathbf{n}} = \mathbf{F}^{-T} . \nabla_R \bar{\mathbf{n}}, \tag{A9.7}$$

and also

$$\phi(\rho, \mathbf{n}, \nabla\hat{\mathbf{n}}) = w/\rho. \tag{A9.8}$$

Here, $W$, $\bar{W}$, and $\hat{W}$ are per unit *volume* in the reference configuration while $w$, $\bar{w}$, and $\hat{w}$ are per unit *volume* of the actual configuration, and $\phi$ is more traditionally per unit *mass* of the actual configuration. Following Maugin and Trimarco (1995), in the absence of body forces and couples, we can state the following *natural* variational formulations for the hydrostatics of nematic liquid crystals:

$$\delta_X \int_{V_R} \bar{W} dV = 0, \quad \delta_x \int_V \bar{w} dv = 0. \tag{A9.9}$$

These are *natural* in the sense that the variation may commute with the integral sign and the arguments of the integrand are expressed in terms of the appropriate space–time parametrization. Stranger (unnatural) variational formulations are given by

$$\delta_X \int_V w dv = 0, \quad \delta_x \int_{V_R} W dV = 0. \tag{A9.10}$$

Only the first in (A9.9) is commonly considered. It is of interest to note some intermediary results, for example,

$$\delta_X (\nabla\mathbf{n}) = \nabla(\delta_X \mathbf{n}) - (\nabla(\delta_X \chi))^T . \nabla\mathbf{n}, \tag{A9.11}$$

$$\delta_X \rho = -\rho\, \mathbf{F}^{-T} \nabla_R (\delta_X \chi) = \rho\, \mathbf{F} . \delta_X \mathbf{F}^{-1}. \tag{A9.12}$$

From the first of (A9.9), one obtains the following Euler–Lagrange equations:

$$\mathrm{div}_R \mathbf{T} = \mathbf{0}, \quad \Gamma \equiv -\frac{\delta \bar{W}}{\delta \mathbf{n}} = \mathbf{0}, \tag{A9.13}$$

with

$$\mathbf{T} = \frac{\partial \bar{W}}{\partial \mathbf{F}}, \quad \frac{\delta \bar{W}}{\delta \mathbf{n}} := \frac{\partial \bar{W}}{\partial \mathbf{n}} - \mathrm{div}_R\left(\frac{\partial \bar{W}}{\partial(\nabla_R \bar{\mathbf{n}})}\right); \tag{A9.14}$$

while from the second of (A9.9) we obtain

$$\mathrm{div}\bar{\mathbf{T}} = \mathbf{0}, \quad \gamma \equiv -\frac{\delta \bar{w}}{\delta \mathbf{n}} = \mathbf{0}, \tag{A9.15}$$

with

$$\bar{\mathbf{T}} = \frac{\partial \bar{w}}{\partial \mathbf{F}^{-1}}, \quad \frac{\delta \bar{w}}{\delta \mathbf{n}} := \frac{\partial \bar{w}}{\partial \mathbf{n}} - \mathrm{div}\left(\frac{\partial \bar{w}}{\partial(\nabla \hat{\mathbf{n}})}\right), \tag{A9.16}$$

respectively, at regular points $\mathbf{X}$ and $\mathbf{x}$ related by the static relation $\mathbf{x} = \chi(\mathbf{X})$. But we note that in truth $W$ depends on $\mathbf{F}$ only through $J_F$ in order to respect the *fluidic* nature of the medium. Furthermore, in most, if not all, cases, liquid crystals are *incompressible*, but we discard this constraint for the sake of illustration. Therefore,

$$\mathbf{T} = -p\mathbf{F}^{-1}, \quad p \equiv \rho\frac{\partial W}{\partial \rho}. \tag{A9.17}$$

In like manner,

$$\bar{\mathbf{T}} = -\pi\mathbf{F}, \quad \pi = \rho\frac{\partial w}{\partial \rho}. \tag{A9.18}$$

Here, both $\mathbf{T}$ and $\bar{\mathbf{T}}$ have the *perfect-fluid* nature in that they are just proportional to the appropriate "unit" tensor in their respective algebra, that is, $\mathbf{F}^{-1}$ and $\mathbf{F}$. Thus the fact that the nematic liquid crystal is an oriented fluid that does not obey Euler's hydrostatics at rest is not transparent in these "natural" variational formulations. Had we considered the energies $\hat{W}$ and $\hat{w}$, we would have obtained more complex expressions for $\mathbf{T}$ and $\bar{\mathbf{T}}$. We let the reader show that then (cf. Maugin and Trimarco, 1995)

$$\mathbf{T} = \mathbf{F}^{-1}.\left\{-\hat{p}\mathbf{1} - \frac{\partial \hat{W}}{\partial(\nabla \hat{\mathbf{n}})}.(\nabla \hat{\mathbf{n}})^T\right\}, \quad \hat{p} = \rho\frac{\partial \hat{W}}{\partial \rho}. \tag{A9.19}$$

But this hints at looking for the (purely spatial) *Cauchy stress* as

$$\sigma = J_F^{-1}\mathbf{F}.\mathbf{T} = -\rho J_F^{-1}\frac{\partial \hat{W}}{\partial \rho}\mathbf{1} - J_F^{-1}\frac{\partial \hat{W}}{\partial(\nabla \hat{\mathbf{n}})}.(\nabla \hat{\mathbf{n}})^T, \tag{A9.20}$$

but since $w/\rho = \hat{W}/\rho_0$, we have $\hat{W} = \rho_0 \hat{\phi}(\rho, \mathbf{n}, \nabla\hat{\mathbf{n}})$, and thus

$$\boldsymbol{\sigma} = -\bar{p}\mathbf{1} - \rho \frac{\partial \phi}{\partial(\nabla\hat{\mathbf{n}})}.(\nabla\hat{\mathbf{n}})^T, \quad \bar{p} = \rho^2 \frac{\partial \phi}{\partial \rho}, \tag{A9.21}$$

or

$$\boldsymbol{\sigma} = -\left(\rho \frac{\partial w}{\partial \rho} - w\right)\mathbf{1} - \frac{\partial w}{\partial(\nabla\hat{\mathbf{n}})}.(\nabla\hat{\mathbf{n}})^T. \tag{A9.22}$$

By the same token the first of (A9.13) yields

$$\mathrm{div}\boldsymbol{\sigma} = 0. \tag{A9.23}$$

This is the "Eulerian" equilibrium equation of a "non-Eulerian" fluid. Equations A9.22 and A9.23 are precisely the recognized expressions of the Cauchy stress in the Ericksen–Leslie (and Oseen–Frank) theory of nonviscous nematic liquid crystals. The stress tensor in (A9.21) or (A9.22) is sometimes referred to as the *Ericksen tensor* in liquid crystals.

Now we let the reader check by a dual computation to the previous one that if one defines a completely material tensor $\mathbf{b}$ by

$$\mathbf{b} := J_F \mathbf{F}^{-1}.\bar{\mathbf{T}}, \tag{A9.24}$$

then it satisfies the conservation law

$$\mathrm{div}_R\, \mathbf{b} = \mathbf{0}. \tag{A9.25}$$

The computation shows that (cf. Maugin and Trimarco, 1995)

$$\mathbf{b} = \left(W - \rho \frac{\partial W}{\partial \rho}\right)\mathbf{1}_R - \frac{\partial W}{\partial(\nabla_R \bar{\mathbf{n}})}.(\nabla_R \bar{\mathbf{n}})^T, \tag{A9.26}$$

or

$$\mathbf{b} = \bar{W}\mathbf{1}_R - \frac{\partial \bar{W}}{\partial \mathbf{F}}.\mathbf{F} - \frac{\partial \bar{W}}{\partial(\nabla_R \bar{\mathbf{n}})}.(\nabla_R \bar{\mathbf{n}})^T. \tag{A9.27}$$

Thus $\mathbf{b}$ is none other than the canonical (material) stress tensor, or *Eshelby stress* for nondissipative nematic liquid crystals.

We can sum up the "natural" variational formulations in the accompanying flowchart (Figure A9.1). The upper left and lower right formulations are just these two formulations; the lower left and upper right formulations

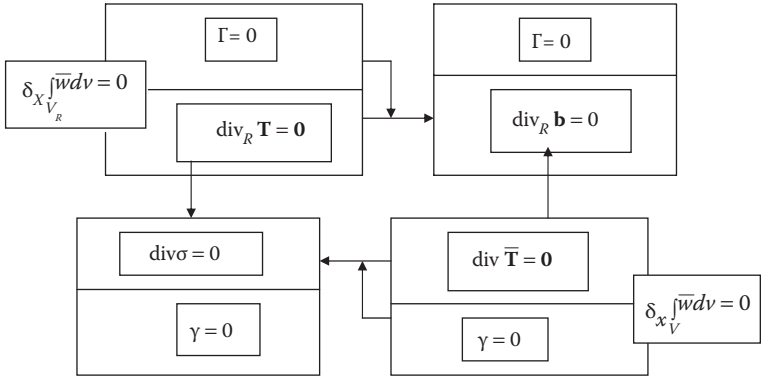


**FIGURE A9.1**
Flowchart of the basic quasistatic equations of nematic liquid crystals. (Adapted from Maugin, G.A., and Trimarco, C., *Int. J. Eng. Sci.*, 33, 1663–78, 1995.)

are those that would follow directly from the variational expressions (A9.10). Of course, because of the identification of (A9.25) and (A9.27), another way to obtain these equations, perhaps an equivalent but purely spatial one, is to apply Noether's theorem to the preceding formulations. In particular, Noether's identity here takes one of the following two forms:

$$\left(\mathrm{div}_R \mathbf{T}\right).\mathbf{F} + \mathrm{div}_R \mathbf{b} = \mathbf{0} \tag{A9.28}$$

and

$$\left(\mathrm{div}\overline{\mathbf{T}}\right).\mathbf{F}^{-1} + \mathrm{div}\sigma = \mathbf{0}. \tag{A9.29}$$

Then it is found through this canonical way that **b** is indeed given by (A9.27) or (A9.26), while (A9.21) or (A9.22) is obtained in the form

$$\mathrm{div}\sigma = \mathbf{0}, \quad \sigma = W\mathbf{1} - \frac{\partial W}{\partial \mathbf{F}^{-1}}.\mathbf{F}^{-1} - \frac{\partial W}{\partial(\nabla\hat{\mathbf{n}})}.\left(\nabla\hat{\mathbf{n}}\right)^T. \tag{A9.30}$$

In the dynamic case, $W$ is replaced by $-L$. The inertia of the microstructure here is reduced to a single scalar $I$ so that we have the following two essential Lagrangian densities depending on whether we use a direct- or inverse-motion description:

$$L = \frac{1}{2}\rho_0\left(\mathbf{v}^2 + I\dot{\mathbf{n}}^2\right) - \overline{W}\left(\mathbf{F}, \mathbf{n}, \nabla_R \overline{\mathbf{n}}\right), \tag{A9.31}$$

or

$$J_{\overline{F}}^{-1} L = \frac{1}{2}\rho\left(\mathbf{V}.\mathbf{C}.\mathbf{V} + I\dot{\mathbf{n}}^2\right) - \overline{w}\left(\mathbf{F}^{-1}, \mathbf{n}, \nabla\hat{\mathbf{n}}\right). \tag{A9.32}$$

Then we obtain the dynamic equations

$$\frac{\partial}{\partial t}(\rho_0 \mathbf{v})\Big|_X - \mathrm{div}_R \mathbf{T} = \mathbf{0}, \quad \frac{\partial}{\partial t}(\rho_0 I \dot{\mathbf{n}})\Big|_X - \Gamma = \mathbf{0}, \tag{A9.33}$$

while the conservation of canonical momentum is given by

$$\frac{\partial}{\partial t}\mathbf{P}^{\mathrm{tot}}\Big|_X - \mathrm{div}_R \mathbf{b} = \mathbf{0}, \quad \mathbf{P}^{\mathrm{tot}} = -\rho_0 \left(\mathbf{v}.\mathbf{F} + I\left(\nabla_R \bar{\mathbf{n}}\right).\dot{\mathbf{n}}\right), \tag{A9.34}$$

where the expression of $\mathbf{T}$ has been given before and, in that for $\mathbf{b}$, $W$ is replaced by $-L$. Here we have another example where the canonical momentum includes all inertial effects, including those of the microstructure.

### REMARK ON THE CASE OF LIQUID CRYSTALS

The example just presented is not gratuitous. It illustrates the ambiguity that may exist between the notions of Cauchy stress and Eshelby-like stress depending on the energy chosen and its specific arguments. The confusion is such that even sharp observers of the physical scene (Kroener, 1993; Nabarro, 1986, 1987; and Eshelby, 1980, himself) were at a loss with the case of liquid crystals in which, logically, there is no reference configuration such as in elastic solids. Here we obtained an answer by considering artificially a reference configuration and introducing a dependence on the density, an often nonrealistic hypothesis. This allowed us to exhibit the primitive, but enlightening, expressions (A9.17) and (A9.18) that the Ericksen tensor, although basically a Cauchy stress, is an Eshelby-like tensor from a different viewpoint. The fact that both Cauchy and Eshelby formats may be introduced even in solid mechanics was emphasized in the works of Steinmann and coworkers, while liquid crystals illustrate this fact by their very nature. Of course, this is a mark of both the richness of and the difficulty in dealing with the notion of *force*. From general definitions, physical forces are those quantities that contribute to the motion or equilibrium equations whose components are in the physical framework. As a consequence, the physical (Newtonian) surface force associated with the static balance law on the left-hand side in the flowchart in Figure A9.1 is indeed given by the surface integral of the Cauchy–Ericksen tensor; that is, when no field singularity contained within $S$ hinders the application of the Green–Gauss theorem,

$$\mathbf{F}(S) = \int_S \mathbf{n}_S.\sigma\, da = -\int_S \left\{\left(\rho\frac{\partial W}{\partial \rho} - W\right)\mathbf{n}_S + \mathbf{n}_S.\frac{\partial W}{\partial(\nabla\hat{\mathbf{n}})}.(\nabla\hat{\mathbf{n}})^T\right\} da, \tag{A9.35}$$

where $\mathbf{n}_S$ is the unit outward to $S$ in $K_t$.

But the total material or configurational surface force associated with the static balance of canonical momentum is given by the surface integral, in material space, of the Eshelby stress tensor; that is, again in the absence of singularities within the integration domain,

$$\mathbf{F}(S_R) = \int_{S_R} \mathbf{N}_S.\mathbf{b}\,dA = -\int_{S_R} \left\{ \left( \rho \frac{\partial \bar{W}}{\partial \rho} - \bar{W} \right) \mathbf{N}_S + \mathbf{N}_S . \frac{\partial \bar{W}}{\partial (\nabla_R \bar{\mathbf{n}})} . (\nabla_R \hat{\mathbf{n}})^T \right\} dA. \quad \text{(A9.36)}$$

The expressions (A9.35) and (A9.36) are formally identical, although, in general, not "taking place in the same space." But then the question arises of the existence and introduction of a reference configuration. Any configuration that preserves the volume is as good as another one to serve as a reference. In particular, the actual configuration itself is often considered as an instantaneously re-actualized reference configuration. With such a picture in mind Equations A9.35 and A9.36 become not only *formally* but also *physically* identical, and one is entitled to say that Ericksen's tensor and Eshelby's tensor (for nematic liquid crystals) are *one*, and only one, concept.

## Appendix A9.2: Material Force Acting on a Center of Dilatation

In the preceding, point defects are associated with the microstructure of a nonclassical continuum, that is, through an additional degree of freedom of the dilatation type. But one can also express the configurational force acting on such a defect in the classical continuum mechanics framework but in the presence of an anelastic strain related to the dilatation effect. Thus, in small strains, we can write

$$\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}^e + \boldsymbol{\varepsilon}^a = (\nabla \mathbf{u})_S, \quad \boldsymbol{\varepsilon}^a = \alpha \mathbf{1} \delta(\mathbf{x} - \mathbf{x}_0), \quad \text{(A9.37)}$$

and

$$\mathbf{b} = \bar{W}(\boldsymbol{\varepsilon}^e)\mathbf{1} - \boldsymbol{\sigma}.(\nabla \mathbf{u})^T, \quad \boldsymbol{\sigma} = \partial \bar{W} / \partial \boldsymbol{\varepsilon}^e. \quad \text{(A9.38)}$$

Here, the scalar $\alpha$ denotes the strength of the center of dilatation (that creates an obviously incompatible isotropic strain whose center is located at $\mathbf{x}_0$). The case $\alpha > 0$ represents indeed a center of dilatation (e.g., a *foreign* atom in the discrete vision), and $\alpha < 0$ might be called a center of contraction (e.g., a *vacancy* in the discrete vision). The inhomogeneity force acting on this is

obtained by the formula (equilibrium in material space in the absence of other effects than elasticity):

$$\mathbf{F}^{\text{inh}} = \mathbf{F}^{(\text{PD})} = -\int_B \left(\operatorname{div}\mathbf{b}\right) dV, \tag{A9.39}$$

where $B$ is a material volume enclosing the center of dilatation (or point defect). Applying (A9.38), we have

$$b_{ji,j} = \sigma_{pq}\varepsilon^{e}_{pq,i} - \sigma_{jk,j}u_{k,i} - \sigma_{jk}u_{k,ij},$$

where we can exploit (A.9.37), the equilibrium equation in physical space ($\sigma_{jk,i} = 0$) and the symmetry of the Cauchy stress to change the order of indices in the spatial derivatives, obtaining thus

$$b_{ji,j} = \alpha\left(tr\sigma\right)\left(\delta\left(\mathbf{x} - \mathbf{x}_0\right)\right)_{,i}. \tag{A9.40}$$

Finally, by integration this yields

$$\mathbf{F}^{(\text{PD})}\left(\mathbf{x}_0\right) = \mathbf{f}^{(\text{PD})} = -\alpha\nabla\left(tr\,\sigma\right)\big|_{\mathbf{x}=\mathbf{x}_0}. \tag{A9.41}$$

If $\bar{\mathbf{V}}$ is the material velocity of this defect, then the associated dissipation is given by

$$D = \mathbf{f}^{(\text{PD})}.\bar{\mathbf{V}} \geq 0. \tag{A9.42}$$

Accordingly, such a point defect with positive $\alpha$ (foreign atom) will try to migrate toward regions where the hydrostatic pressure (trace of the stress) is high. Obviously, then, a vacancy will have a tendency to move toward a region of low hydrostatic pressure.

If, in addition to this, the singular point $\mathbf{x}_0$ has attached to it a foreign electric charge $\beta$ so that we have a charge density $q_f = \beta\delta(\mathbf{x} - \mathbf{x}_0)$, then it is easily shown that a term

$$-\beta\nabla\varphi\big|_{\mathbf{x}=\mathbf{x}_0}, \tag{A9.43}$$

where $\varphi$ is the electrostatic potential, will be added to the right-hand side of (A9.41). This force has the classical form of an electric force acting on a charge in an electric field $\mathbf{E} = -\nabla\varphi$ (cf. Section 11.1). This has been exploited by R. Mueller et al. in examining the influence of foreign atoms in electrodeformable crystals (Schrade et al., 2007a, 2007b).

# 10

# *Systems with Mass Changes and/or Diffusion*

### Object of the Chapter

Where we discover that volumetric growth is governed by an Eshelby-like stress tensor and that binary mixtures of solid and fluid constituents also belong in the Eshelbian view of the material to the posthumous satisfaction of both J.D. Eshelby and M. Biot—of porous media fame—while the Eshelby stress is a natural tensorial generalization of the notion of chemical potential.

## 10.1 Introduction

Systems with variable mass have always been the object of conceptual difficulties. Of course, Newton's equation of balance of linear momentum for a point particle, written as

$$\frac{d}{dt}\left(m\dot{\mathbf{x}}\right) = \mathbf{F}, \tag{10.1}$$

contains the potentiality of a time-varying mass $m$. This has the effect that (10.1) is also valid in special relativity with a well-known formula for the varying mass in terms of the velocity. In Chapter 12 we shall uncover other examples of point mechanics with a more complicated or an unusual formula for mass-versus-velocity when some steadily propagating nonlinear waves are reinterpreted as quasiparticles. But here we are more interested in cases that are more akin to the "rocket problem" translated to a continuum, in which one species, or the continuum itself, can modify its mass even in its reference configuration. We have alluded to this in Chapter 5 when we spoke of the growth phenomenon. That is, we may be concerned with a single continuum with a mass balance law (in a reference configuration) written as

$$\frac{\partial}{\partial t}\rho_0(\mathbf{X},t)\Big|_{\mathbf{x}} \neq 0. \tag{10.2}$$

A nonvanishing right-hand side in this equation suggests that some external source is present such as occurs in biological growth where nutriments provide this source. More classically for most readers, the theory of so-called *mixtures* provides a modeling of the same type but for each of the constituents. For example, in a mixture of fluids, with the classical Eulerian representation, we have equations of mass balance written as

$$\left(\frac{\partial}{\partial t} + \mathbf{v}_\alpha . \nabla\right)\rho_\alpha + \rho_\alpha(\nabla . \mathbf{v}_\alpha) = m_\alpha \neq 0, \tag{10.3}$$

where subscript $\alpha = 1, 2, ..., n$ labels specifically the constituents. As compared to (10.2), when the velocity of the global mixture is defined for the centroid (the center of mass), the global mixture has a mass balance law without a source term in the right-hand side, because it is assumed that there is no net production or consumption of mass, viz.

$$\sum_{\alpha=1}^{n} m_\alpha = 0. \tag{10.4}$$

While in (10.2) the mass exchange takes place with the outside (the system is thermodynamically *open*), in the case of (10.3) and (10.4) these exchanges occur only between constituents, sometimes called *species.* While (10.2) does not at first bring conceptual problems, the concepts underlying the formulation in (10.3) and (10.4) remain a difficult and debated subject matter. The essential reason for this is that some basic working hypothesis of continuum physics is readily overthrown. This is posed by the assumed possible simultaneous presence of various species (in different amounts) at the same physical point while different species a priori belong to different material manifolds! This matter is of special importance in the framework of this book, which places a strong emphasis on material configurations. This will be treated with caution. But to remind the reader of other difficulties, one may mention the evident difficulty presented by the definition of some thermodynamic quantities such as temperature and internal energy. Should these be defined for the whole mixture or for each species, and then how does one pass from the latter to the former? For a discussion of these questions we recommend the fundamental works of Bowen (1967, 1976) and the book of Rajagopal and Tao (1995) after the fundamental contribution of Truesdell revisited in Truesdell (1984).

There is an additional ingredient that means that systems with mass exchange have their due place in this book. Classically, in fluids one introduces Gibbs free enthalpy as the quantity

$$h = \psi + (p/\rho) = \psi + p\tau, \tag{10.5}$$

where $p$ is the thermodynamic pressure and $\tau$ is the specific volume. This is the relevant scalar thermodynamic potential in many discussions related to phase changes in fluids. In previous chapters we have introduced the Eshelby stress *tensor*. If we write it for a perfect fluid of pressure $p$ and discard inertia, considering the actual configuration as a reference one, the said tensor yields

$$b^j_{.i} = W\delta^j_i - (-p\delta^j_k\delta^k_i) = \rho h\delta^j_i. \tag{10.6}$$

It is thus a tensorial generalization of the notion of Gibbs free energy. This was remarked by several authors (Bowen, 1976; Grinfeld, 1991; Müller, 1999; Buratti et al., 2003) so that the Eshelby stress was even referred to as the *chemical tensor* (Truskinovskii, 1983). No wonder that the Eshelby stress plays such a predominant role in the study of phase transitions in deformable solids. Herein after we shall examine how this tensor appears naturally when considering cases governed by equations such as (10.2) or (10.3), often limiting the second case of mixtures to that of binary mixtures for the sake of example.

## 10.2 Volumetric Growth

Here we are concerned with the *growth of bodies in the bulk*. We must understand precisely what this means. In classical continuum mechanics we consider that the set of "material particles" composing a given body does not vary. These "particles" are neither annihilated nor created ex nihilo. Growing or shrinking bodies are not so. One may think of volumetric growth as the local structural rearrangement that consists in pushing in more material particles of the same type at a given material point. These are not foreign ones. They look just the same as those previously there. The result of this is a change in the matter density in the reference configuration as stated in (10.2). The biological processes by which many tissues grow or shrink are of this type when examined at a phenomenological level. This is more difficult to figure out than the growth of material bodies by *accretion* or *degradation* at their surfaces. The first process, accretion, can occur through crystal growth, spray deposition, casting solidification, or filament winding. The second takes place when corrosion, wear, ablation, erosion, or decay occurs. Accretion of deformable bodies has been analyzed and modeled in several more or less successful attempts, for example, by the Arutyunyan school (Arutyunyan et al., 1987; Arutyunyan and Naumov, 1993; Naumov, 1994; Naumov et al., 1995) or by Gurtin (see the appropriate chapters in Gurtin, 1999). Wear has been studied by Dragon-Luiset (2001). Gurtin and Dragon-

Luiset show that accretion and wear have as their driving force the Eshelby stress or something close to it (normal jump, tangential component, Mandel stress). Cherepanov (1987), with his usual insight, has clearly perceived that accretion and ablation (e.g., during machine tooling) fit in the paradigm of Eshelbian mechanics (but he does not use this wording).

The present section does not consider accretion or surface growth. It focuses on volumetric growth in the spirit of works by Takamizawa and Matsuda (1990), Rodriguez et al. (1994), Taber (1995), Epstein and Maugin (1999, 2000a, 2000b), Klisch and Hoger (2001), Kuhl et al. (2003), Kuhl and Steinmann (2003a, 2003b, 2003c), Kuhl (2004), Imatani and Maugin (2001a, 2001b, 2002), Di Carlo (2004), Di Carlo and Quiligotti (2002), and Quiligotti (2002). We will follow essentially Epstein and Maugin (2000b) but with diffusion neglected. We have, therefore, the following *basic equations*:

*Balance of mass:*

$$\frac{d}{dt}\int_{B_R}\rho_0(\mathbf{X},t)dV=\int_{B_R}\Pi dV, \tag{10.7}$$

*Balance of linear (physical) momentum:*

$$\frac{d}{dt}\int_{B_R}\mathbf{p}_R dV=\int_{B_R}\left(\mathbf{f}^0+\mathbf{f}^\Pi\right)dV+\int_{\partial B_R}\mathbf{N}.\mathbf{T}dA, \tag{10.8}$$

where $\mathbf{f}^0$ is the external body force per unit reference volume, and $\mathbf{f}^\Pi$ is a source term due to the fact that (10.7) contains a mass source term in its right-hand side because of volumetric growth. The Cauchy argument has already been used, and $\mathbf{T}$ is none other than the first Piola–Kirchhoff stress, while $\mathbf{p}_R=\rho_0\mathbf{v}$. Localization of (10.7) yields (10.2) in the form

$$\left.\frac{\partial}{\partial t}\rho_0\right|_{\mathbf{x}}=\Pi(\mathbf{X},t), \tag{10.9}$$

while localization of (10.8) yields

$$\left.\frac{\partial}{\partial t}\mathbf{p}_R\right|_{\mathbf{x}}=\mathbf{f}^0+\mathbf{f}^\Pi+\mathrm{div}_R\mathbf{T}. \tag{10.10}$$

This allows us to identify

$$\mathbf{f}^\Pi=\Pi\mathbf{v}, \tag{10.11}$$

since by expanding the left-hand side of (10.10) on account of (10.9), we must recover the balance of linear momentum for a classical continuum.

The balance of angular momentum does not bring anything new (no new concept) and simply yields the symmetry of **T** with respect to **F**, that is, (cf. (2.88))

$$\mathbf{F}.\mathbf{T} = \mathbf{T}^T.\mathbf{F}^T. \tag{10.12}$$

The writing down of the laws of thermodynamics requires a bit more caution. However, on account of (10.10), we can write these two laws in global form as

$$\frac{d}{dt}\int_{B_R}\left(K+E\right)dV = \int_{B_R}\left(\left(\mathbf{f}^0.\mathbf{v}+\rho_0 h_0\right)+\frac{\Pi}{\rho_0}\left(K+E\right)+\Pi_E\right)dV + \int_{\partial B_R}\mathbf{N}.\left(\mathbf{T}.\mathbf{v}+\mathbf{M}_E-\mathbf{Q}\right)dA \tag{10.13}$$

and

$$\frac{d}{dt}\int_{B_R} S dV \geq \int_{B_R}\left(\theta^{-1}\left(\rho_0 h_0+\Pi_E\right)+\frac{\Pi}{\rho_0}S\right)dV - \int_{\partial B_R}\mathbf{N}.\left(\theta^{-1}\mathbf{Q}\right)dA. \tag{10.14}$$

In these equations,

$$K=\frac{1}{2}\rho_0\mathbf{v}^2, \quad E=\rho_0 e, \quad S=\rho_0\eta,$$

while $e$, $\eta$, $h_0$, and $\mathbf{Q}$ have their usual meaning, and we have introduced irreversible volume and surface contributions to the internal energy, $\prod_E$ and $\mathbf{M}_E$, for the sake of generality since we would obviously be tempted to do so a priori (this is a line to be pursued further). However, these shall be put equal to zero in the sequel since we do not envisage chemical processes in the bulk and surface accretion or influx of matter at the surface. On account of this, the localization of (10.13) and (10.14) yields the equations

$$\rho_0\dot{e} = \mathrm{tr}\left(\mathbf{T}.\left(\nabla_R\mathbf{v}\right)^T\right) - \nabla_R.\mathbf{Q}+\rho_0 h_0, \tag{10.15}$$

and

$$\rho_0\dot{\eta} \geq \theta^{-1}\rho_0 h_0 - \nabla_R.\left(\theta^{-1}\mathbf{Q}\right), \tag{10.16}$$

that is, the standard equations! But if we use the volume densities of internal energy and entropy, these will take the following more interesting forms

$$\frac{\partial}{\partial t}E\Big|_{\mathbf{x}} = tr\left(\mathbf{T}.\left(\nabla_R \mathbf{v}\right)^T\right) + \frac{\Pi}{\rho_0}E + \rho_0 h_0 - \nabla_R.\mathbf{Q}, \tag{10.17}$$

and

$$\frac{\partial}{\partial t}S\Big|_{\mathbf{x}} \geq \theta^{-1}\left(\rho_0 h_0 - \nabla_R.\mathbf{Q}\right) + \frac{\Pi}{\rho_0}S + \theta^{-2}\mathbf{Q}.\nabla_R\theta. \tag{10.18}$$

Introducing the free energy $W$ per unit reference volume by $W = E - \theta S$, we can also write (10.17) in the following "*canonical* form" (compare to (5.8) in Chapter 5):

$$\frac{\partial}{\partial t}\left(\theta S\right)\Big|_{\mathbf{x}} + \nabla_R.\mathbf{Q} = h^{\text{int}} + h^{g} + h^{\text{ext}} \tag{10.19}$$

and (10.18) in the form of the *Clausius–Duhem inequality*:

$$-\left(\dot{W} + S\dot{\theta}\right) + tr\left(\mathbf{T}.\dot{\mathbf{F}}\right) + \frac{\Pi}{\rho_0}W - \theta^{-1}\mathbf{Q}.\nabla_R\theta \geq 0, \tag{10.20}$$

where we have defined the following sources of energy:

$$h^{\text{int}} := tr\left(\mathbf{T}.\dot{\mathbf{F}}\right) - \frac{\partial W}{\partial t}\Big|_{\mathbf{x}}, \quad h^{g} := \frac{\Pi}{\rho_0}\left(W + \theta S\right), \quad h^{\text{ext}} = \rho_0 h_0, \tag{10.21}$$

of which the second is related to volumetric growth. Remarkably enough, (10.20) can also be rewritten as

$$-\rho_0\left(\dot{\psi} + \eta\dot{\theta}\right) + tr\left(\mathbf{T}.\dot{\mathbf{F}}\right) - \theta^{-1}\mathbf{Q}.\nabla_R\theta \geq 0. \tag{10.22}$$

This means that both local equations (10.15) and (10.22) read in their usual form if we use energies and entropies per unit mass in spite of the growth equation (10.9). Had we considered some possible diffusion in the right-hand side of (10.7), we would have obtained more complicated equations for the first and second laws (see Epstein and Maugin, 2000b).

It remains to establish the equation governing the canonical momentum (here a purely mechanical one). With

$$K = \frac{1}{2}\rho_0 \mathbf{v}^2 = \frac{1}{2}\rho_0 \mathbf{V}.\mathbf{C}.\mathbf{V}, \tag{10.23}$$

where $\mathbf{V} = -\mathbf{F}^{-1}.\mathbf{v}$ is the material velocity and $\mathbf{C} = \mathbf{F}^T.\mathbf{F}$, we have

$$\mathbf{p}_R = \frac{\partial K}{\partial \mathbf{v}} = \rho_0 \mathbf{v}, \quad \mathbf{P} = \frac{\partial K}{\partial \mathbf{V}} = \rho_0 \mathbf{C}.\mathbf{V} = -\mathbf{p}_R.\mathbf{F}. \tag{10.24}$$

We let the reader check by way of exercise that the material momentum $\mathbf{P}$ satisfies the following fully material balance law at any regular material point $\mathbf{X}$ in the body $B_R$ (see previous chapters and Epstein and Maugin, 2000b):

$$\left.\frac{\partial}{\partial t}\mathbf{P}\right|_{\mathbf{X}} - \mathrm{div}_R \mathbf{b} = \mathbf{f}^{\mathrm{int}} + \mathbf{f}^{\mathrm{ext}} + \mathbf{f}^{\mathrm{inh}} + \mathbf{f}^{g}, \tag{10.25}$$

where we have defined the following *material forces*:

$$\mathbf{f}^{\mathrm{int}} = tr\left(\mathbf{T}.\left(\nabla_R \mathbf{F}\right)^T\right) - \left.\frac{\partial W}{\partial \mathbf{X}}\right|_{\mathrm{impl}}, \quad \mathbf{f}^{\mathrm{ext}} = -\mathbf{f}^0.\mathbf{F}, \quad \mathbf{f}^{\mathrm{inh}} = \left.\frac{\partial L^{\mathrm{th}}}{\partial \mathbf{X}}\right|_{\mathrm{expl}}, \quad \mathbf{f}^{g} = \Pi \mathbf{V}, \tag{10.26}$$

together with

$$\mathbf{b} = -\left(L^{\mathrm{th}}\mathbf{1}_R + \mathbf{T}.\mathbf{F}\right), \quad L^{\mathrm{th}} = K - W\left(\ldots;\mathbf{X},t\right). \tag{10.27}$$

For a thermoelastic material we would take

$$W = \bar{W}\left(\mathbf{F},\theta;\mathbf{X},t\right) = \rho_0\left(\mathbf{X},t\right)\bar{\psi}\left(\mathbf{F},\theta;\mathbf{X}\right). \tag{10.28}$$

and a now-classical reasoning applied to (10.22) would deliver the constitutive equations

$$\mathbf{T} = \rho_0 \frac{\partial \bar{\psi}}{\partial \mathbf{F}}, \quad \eta = -\frac{\partial \bar{\psi}}{\partial \theta}. \tag{10.29}$$

And computing $\mathbf{f}^{\text{int}}$ we find that (10.25) takes on the following form:

$$\left.\frac{\partial \mathbf{P}}{\partial t}\right|_{\mathbf{x}} - \operatorname{div}_R \mathbf{b} = \mathbf{f}^{\text{th}} + \mathbf{f}^{\text{ext}} + \mathbf{f}^{\text{inh}} + \mathbf{f}^{g}, \quad \mathbf{f}^{\text{th}} := S\nabla_R \theta. \tag{10.30}$$

## 10.3 First-Order Constitutive Theory of Growth

We develop the theory within the context of an underlying thermoelastic model although the behavior may include rather general anelastic effects. Since growth is considered here as a local rearrangement of matter, although a special one, we can exploit the notions introduced in Chapter 6, in particular that of the *reference crystal* with respect to which the material behaves elastically. More precisely, this is a fixed reference in space with supposedly undistorted stress-free configuration, that is, what is usually called a natural state. This is *not* the reference configuration of the body, noted $K_R$, but just an undistorted spatial configuration of a material point. Constitutive equations for so-called simple materials (involving only the first gradient of the direct motion, hence the terminology of first-order constitutive theory) are always given in this way, namely, locally. This provides a hint for our formulation. Indeed, we shall note $E_c$, $W_c$, and $S_c$ the internal energy, free energy, and entropy per unit volume of the reference crystal (local configuration noted $K_c$). A heat-conducting thermoelastic material point abides by constitutive laws of the general type

$$\begin{aligned} \mathbf{T}_c &= \bar{\mathbf{T}}_c\left(\mathbf{F}_c, \theta, \mathbf{H}_c\right), \quad \mathbf{Q}_c = \bar{\mathbf{Q}}_c\left(\mathbf{F}_c, \theta, \mathbf{H}_c\right), \\ W_c &= \bar{W}_c\left(\mathbf{F}_c, \theta, \mathbf{H}_c\right), \quad S_c = \bar{S}_c\left(\mathbf{F}_c, \theta, \mathbf{H}_c\right), \end{aligned} \tag{10.31}$$

and thus

$$E_c = W_c + \theta S_c = \bar{E}_c\left(\mathbf{F}_c, \theta, \mathbf{H}_c\right). \tag{10.32}$$

Here $\mathbf{F}_c$ represents the deformation gradient with respect to $K_c$, and $\mathbf{H}_c$ is the gradient of temperature with respect to $K_c$, that is, the pull back to that local configuration of the spatial temperature gradient $\nabla\theta$. The reference crystal is at a fixed density $\rho_c$ corresponding to some reference temperature $\theta_c$. There is no growth phenomenon in the reference crystal as the infinitesimal die called the reference crystal behaves as a perfectly thermoelastic material. In contrast, the role of the global reference configuration $K_R$ is just to keep track of the moving body points throughout the motion $\mathbf{x} = \chi(\mathbf{X}, t)$, giving rise to

the (integrable) motion gradient **F.** To formulate the behavior translated in (10.31) we must, at each material point **X**, apply a linear **transplant**, noted **K**(**X**), from the reference crystal to the tangent neighborhood of **X** such that we have the composition

$$\mathbf{F}_c = \mathbf{F}\mathbf{K}, \tag{10.33}$$

is the appropriate entity to be used in Equations 10.31 and 10.32. Of course, we are just doing the same as in Section 6.3 using a more "surgical" wording. Furthermore, if we follow the notion of pseudo-inhomogeneitiy and pseudo-plastic effects (cf. Maugin, 2003), we can introduce a growth gradient (not a true gradient) $\mathbf{F}_g$ such that $\mathbf{K} = \mathbf{F}_g^{-1}$ and (10.33) is none other than a standard multiplicative decomposition of an *anelastic* total deformation since, $\mathbf{F}_c$ being elastic,

$$\mathbf{F} = \mathbf{F}_e\,\mathbf{F}_g\,. \tag{10.34}$$

Of course, $\mathbf{F}_g$ or its inverse **K** must have specific properties to be strictly associated with the growth phenomenon. First we note the inhomogeneity velocity gradient in the reference configuration $K_R$ by

$$\mathbf{L}_K := \dot{\mathbf{K}}.\mathbf{K}^{-1} = \frac{\partial}{\partial t}\left(\mathbf{F}_g^{-1}\right)\Big|_{\mathbf{X}}.\mathbf{F}_g\,. \tag{10.35}$$

Because $\rho_c$ is fixed, computing the time derivative of the reference density $\rho_0$, we obtain

$$\frac{\partial}{\partial t}\rho_0\Big|_{\mathbf{X}} = \rho_c\left(\frac{\partial}{\partial t}J_K^{-1}\right) = -\rho_0 tr\mathbf{L}_K\,, \tag{10.36}$$

since

$$\rho_0 = \rho_c J_K^{-1}\,. \tag{10.37}$$

On comparing (10.9) and (10.36), we deduce that in the present theory

$$\Pi = -\rho_0 tr\mathbf{L}_K. \tag{10.38}$$

This means that no separate time evolution needs to be given for the volumetric source $\prod$ if we know the time evolution of the transplant **K**. Furthermore, the time evolution of the determinant of **K**, $J_K = \det \mathbf{K}$, tells us whether there is actually growth (negative time derivative) or resorption (positive time

derivative). Accordingly, growth occurs at time $t$ for negative $\mathrm{tr}\mathbf{L}_K$, while $J_K$ itself is a measure of accumulated growth from the time origin. If $\mathbf{K}$ is non-spherical, then there is a rotation and/or a distortion in addition to growth or resorption.

Finally, the phenomenon of growth is associated with dissipation. This is shown as follows while uncovering the driving force behind growth. With (10.31) as the starting point and exploiting the Clausius–Duhem inequality in the usual manner, we obtain that

$$\frac{\partial W}{\partial \mathbf{H}} = \mathbf{0}, \quad S = -\frac{\partial W}{\partial \theta}, \quad \mathbf{T} = \frac{\partial W}{\partial \mathbf{F}}, \quad W = \bar{W}\left(\mathbf{F}, \theta, \mathbf{K}; \mathbf{X}, t\right), \tag{10.39}$$

or

$$\bar{W}\left(\mathbf{F}, \theta, \mathbf{K}; \mathbf{X}, t\right) = J_K^{-1} W_c \left(\mathbf{F}\mathbf{K}\left(\mathbf{X}, t\right), \theta\right), \tag{10.40}$$

along with

$$\mathbf{Q}\left(\mathbf{F}, \theta, \mathbf{H}, \mathbf{K}; \mathbf{X}, t\right) = J_K^{-1} \mathbf{K}\mathbf{Q}_c \left(\mathbf{F}\mathbf{K}\left(\mathbf{X}, t\right), \theta, \mathbf{H}\mathbf{K}\left(\mathbf{X}, t\right)\right), \quad \mathbf{H} \equiv \nabla_R \theta. \tag{10.41}$$

The residual dissipation inequality reads

$$\Phi = tr\left(\mathbf{M}.\mathbf{L}_K\right) - \theta^{-1}\mathbf{Q}.\nabla_R \theta \geq 0, \tag{10.42}$$

where

$$\mathbf{M} = \mathbf{T}.\mathbf{F} = -\left(L^{\mathrm{th}}\mathbf{1}_R + \mathbf{b}\right) \tag{10.43}$$

is the so-called *Mandel stress tensor* and $\mathbf{b}$ is the *material Eshelby stress tensor*. We can say that the Mandel stress is the driving force behind growth as it is formally the driving force behind many bulk structural rearrangements. A complete constitutive theory includes the datum of the expressions (10.40) and (10.41) and the relationship between generalized forces and rates in the inequality (10.42). Leaving aside a conduction law of the Fourier type this yields a relationship between $\mathbf{M}$ and $\mathbf{L}_K$. If the latter involves one or several characteristic times, then the material finally behaves as a generally *nonlinear*, heat-conducting, *viscoelastic* material. This will be discussed later on.

Summarizing the contents of this section we can state that the present approach (i) belongs in a tradition started by various authors such as Takamizawa and Matsuda (1990), Rodriguez et al. (1994), Taber (1995), and

Klisch et al. (2001), who consider a multiplicative decomposition of the total deformation gradient in the line of Lee (1969); and (ii) follows a conducting thread that inevitably yields that growth may well be triggered by both strain and strain rate, hence has a viscoelastic character (cf. Cowin, 1996; and references therein).

**REMARK 10.1:** Explicit material gradient in quasi-quasistatics

If we introduce a material connection based on **K** as in (6.24), a short computation allows us to rewrite (10.30) as (cf. Epstein and Maugin, 2000b)

$$\left(\mathrm{div}_R \mathbf{b}_S + \mathbf{b}_S : \Gamma\right) + \mathbf{f}^{\mathrm{ext}} + \mathbf{f}^{\mathrm{th}} + \mathbf{f}^{g} = \mathbf{0}. \tag{10.44}$$

Show this directly by computing the explicit gradient of (10.40) when inertia is neglected and parodying the computation made in Section 6.3. Just as in that section, the quantity within parentheses in (10.44) has a deep geometric meaning in the theory of continuously distributed defects such as dislocations.

**REMARK 10.2:** General restrictions on the evolution equation for growth

Following the ideas of Cowin (1996), a possible a priori evolution law relating **M** and **K** reads in the following implicit form:

$$\varphi\left(\mathbf{K}, \dot{\mathbf{K}}, \mathbf{b}, \mathbf{F}, \dot{\mathbf{F}}\right) = 0. \tag{10.45}$$

What are the restrictions on this form? Uniformity is already implied in (10.45) since we did not put **X** explicitly. This **X** intervenes only through **K** according to the very meaning of this **K**. Also, the evolution law must in some sense be independent of the particular reference configuration chosen. To obtain a precise mathematical expression of this restriction, we should compare the evolutions around the same material point but in two different reference configurations. This is called the G-*covariance* (Epstein and Maugin, 1997), noting that $\mathbf{K}_1$ and $\mathbf{K}_2$, the same transplant in two such configurations, are related by

$$\mathbf{K}_2 = \nabla\lambda \circ \mathbf{K}_1, \tag{10.46}$$

where $\nabla\lambda$ is the local value of the gradient of the (necessarily) smooth change of reference configuration $\lambda$. The proof given by Epstein and Maugin (2000b) shows that the function $\varphi$ is necessarily of the following form:

$$\tilde{\varphi}\left(\tilde{\mathbf{L}}_K, \mathbf{b}_0, \mathbf{C}_e, \dot{\mathbf{C}}_e\right) = 0, \tag{10.47}$$

where

$$\mathbf{C}_e = \mathbf{F}_e^T.\mathbf{F}_e\,, \quad \tilde{\mathbf{L}}_K := \mathbf{K}^{-1}.\dot{\mathbf{K}}, \quad \mathbf{b}_0 = J_K\mathbf{K}^{-1}\mathbf{b}\mathbf{K}, \quad \dot{\mathbf{C}}_e = \frac{\partial}{\partial t}\mathbf{C}_e\bigg|_{\mathbf{x}}. \tag{10.48}$$

Of course, the second and third of these can also be written as

$$\tilde{\mathbf{L}}_K \equiv \tilde{\mathbf{L}}_g := \mathbf{F}_g.\dot{\mathbf{F}}_g^{-1}\,, \quad \mathbf{b}_0 = -\Big(L^{\text{th}}\mathbf{1}_c + J_{F_e}^{-1}\mathbf{F}_e\,\mathbf{T}.\mathbf{F}_e\Big). \tag{10.49}$$

The invariance under the *symmetry group of the crystal* must also be applied. A simple special case of (10.47) is

$$\tilde{\mathbf{L}}_g = \mathbf{F}\big(\mathbf{M}_0\big), \tag{10.50}$$

for a fully isotropic reference crystal, where $\mathbf{M}_0$ is the Mandel stress in the reference crystal. But, in applying the material symmetry invariance to (10.47) or the special form in (10.50), we must note that the Eshelby or Mandel stress itself is orthogonal to the Lie algebra of the isotropy group (Epstein and Maugin, 1990). In the present case, this means that the Eshelby stress here is symmetric, since the relevant Lie algebra is that of skewsymmetric matrices. For the evolution law to prescribe an actual evolution (and not just a symmetry restriction), $\mathbf{L}_g$ itself must not belong to this algebra since otherwise we would be staying within the same inhomogeneity pattern while we expect a true evolution. In conclusion, only the symmetric part $\tilde{\mathbf{L}}_{gS}$ of $\tilde{\mathbf{L}}_g$ here represents a true evolution. Accordingly, by a standard representation theorem (Cauchy) of a symmetric tensor-valued function of a symmetric tensor, we can write (10.50) as

$$\tilde{\mathbf{L}}_{gS} = \varphi_0\mathbf{1} + \varphi_1\mathbf{M}_0 + \varphi_2\,\mathbf{M}_0^2, \tag{10.51}$$

where the $\varphi_i$ are scalar functions of the three characteristic invariants of $\mathbf{M}_0$. Finally, we note that when pulled back to the reference crystal, the principal directions of $\tilde{\mathbf{L}}_{gS}$ coincide not only with those of $\mathbf{M}_0$ but also with those of $\mathbf{C}_e$ (cf. Epstein, 2000).

**REMARK 10.3:** Second-order theory of growth

Had we introduced a diffusion term such as $\nabla_R.\mathbf{M}$—this $\mathbf{M}$ bears no relationship to the Mandel stress—our thermodynamic-constitutive-geometric model would be much more complicated. This was originally proposed by Epstein and Maugin (2000b), but it was soon discovered that the modeling rapidly becomes unmanageable. Indeed, this would introduce additional

terms in both the first and second laws of thermodynamics, the most remarkable facts being that $\prod$ is no longer simply determined by the evolution of a mapping **K**, and an annoying term coupling the newly introduced **M** and the material gradient of internal energy shows up in the second law. It is shown that such a term that truly accounts for the diffusion phenomenon of interest is forbidden unless we consider second-order gradients (i.e., the gradient of **F**). This means that, as we surmised in the preceding, mass-diffusive effects are not admitted in a first-order constitutive theory of growth. The discussion sketched out in Section 6.8 has exhibited the inherent complexity of a second-order (gradient) theory. In the present context of growth, this supposes considering, along with **K**, a *second-order transplant* **Q** that will satisfy composition rules for second gradients, that is,

$$\mathbf{G}_e = \mathbf{K}^T\mathbf{G}\mathbf{K} + \mathbf{F}\mathbf{Q}, \tag{10.52}$$

complementing the now-classic $\mathbf{F}_e = \mathbf{F}\mathbf{K}$, where the dependence of **K** and **Q** on **X** is understood. An easier specialized modeling would restrict the second-gradient dependence to that of the gradient of the density. Geometrically, however, the second-order theory leads to considering two different linear connections. It is possible to subordinate the evolution of the second-order structure to that of the first-order underlying counterpart. This avoids introducing any driving force behind the evolution of the second-order inhomogeneities. As a matter of fact the evolution of **Q** may be generally written in components as

$$\dot{Q}^I_{.\alpha\beta} = K^I_{.\gamma} f^{\gamma}_{.\alpha\beta}(\mathbf{b}_0) + \left(\tilde{\mathbf{L}}_K\right)^{\gamma}_{.\alpha} Q^I_{\gamma\beta} + \left(\tilde{\mathbf{L}}_K\right)^{\gamma}_{.\beta} Q^I_{.\gamma\alpha}. \tag{10.53}$$

For vanishing $f^{\gamma}_{.\alpha\beta}$, this yields

$$\dot{Q}^I_{.\alpha\beta} - \left(\tilde{\mathbf{L}}_K\right)^{\gamma}_{.\alpha} Q^I_{\gamma\beta} - \left(\tilde{\mathbf{L}}_K\right)^{\gamma}_{.\beta} Q^I_{.\gamma\alpha} = 0, \tag{10.54}$$

where the quantity in the left-hand side defines a type of convective time derivative in following the first-order inhomogeneity evolution. The prescription (10.54) will (i) preserve its form under arbitrary changes of reference configuration, and (ii) dictate a zero-rate process at a reference configuration locally and instantaneously coinciding with the reference crystal. We do not pursue further this line of thought since problems involving only the first-order theory are already not simple.

**REMARK 10.4:** In spite of obvious complications in the relevant kinematics, a second-gradient theory allowing for mass transport during morphogenesis is being developed by some authors at the time of completion of this book.

## 10.4 Application: Anisotropic Growth and Self-Adaptation

We first note that the tensors $\mathbf{C}_e$ and $\mathbf{S}_0 = \mathbf{S}_e$ defined by

$$\mathbf{C}_e = \mathbf{F}_e^T.\mathbf{F}_e\,, \quad \mathbf{S}_e = J_{F_e}\,\mathbf{F}_e^{-1}.\sigma.\mathbf{F}_e^{-T}\,, \tag{10.55}$$

are conjugated strain and stress on the material manifold but in the reference crystal. As easily checked, the corresponding Mandel stress is given by $\mathbf{M}_0 = \mathbf{S}_e.\mathbf{C}_e$. For a hyperelastic behavior with respect to the reference crystal, we have the constitutive equation

$$\mathbf{S}_e = 2\partial W_c\,/\partial \mathbf{C}_e\,, \tag{10.56}$$

where $W_c$ is the strain energy function per unit volume of the reference crystal. A possible expression for $W_c$ is given by

$$W_c = C_1\left(I_1 I_3^{-1/3} - 3\right) + C_2\left(I_2 I_3^{-2/3} - 3\right) + \frac{1}{2}C_3\left(I_3^{1/2} - \mathbf{1}\right)^2\,, \tag{10.57}$$

where the $I_\alpha$'s are the invariants of $C_e$ and the $C_\alpha$'s are material constants. The last term in (10.57) may be thought of as a penalty term for practically incompressible elastic materials. With this, (10.56) results in

$$\mathbf{S}_e = \phi_0\mathbf{1} + \phi_1\mathbf{C}_e + \phi_2\mathbf{C}_e^2\,, \tag{10.58}$$

with coefficients depending on the $I_\alpha$'s. Remember that the evolution equation for the transplant tensor has a similar form to (10.51), that is,

$$\tilde{\mathbf{L}}_{gS} = \varphi_0\mathbf{1} + \varphi_1\mathbf{M}_0 + \varphi_2\mathbf{M}_0^2 = \mathbf{G}_0\left(\mathbf{M}_0\right). \tag{10.59}$$

For example,

$$\varphi_0 < 0, \quad \varphi_1 = \varphi_2 = 0 \tag{10.60}$$

yields growth. But, as observed in physiology, *anisotropy is an unavoidable feature of growth*. There are several ways to account for this basic property. Privileged directions cannot be given out of the blue, although they could be hinted at in a special structure. We prefer here to assume that the directional properties follow from the instantaneous mechanical solution itself. Let $\mathbf{w}$ ($\mathbf{w}_0$ in the reference crystal) be the unit vector field that characterizes this

anisotropy. This influences the strain–stress relation, and we do not need to specify an evolution equation for **w.** Introducing the associated skewsymmetric tensor **W** such that $\mathbf{Wa} = \mathbf{a} \times \mathbf{w}$, for any **a**, and using representation theorems, we can propose a generalization of (10.59) as

$$\tilde{\mathbf{L}}_{gS} = \mathbf{G}_W\left(\mathbf{M}_0, \mathbf{W}_0\right). \tag{10.61}$$

Note that we consider here pure growth and that $\mathbf{G}_W$ is symmetric (without any intervening of an intermediate rotation). Neglecting some of the terms from the full representation (see the appendices in Eringen and Maugin, 1990), we may consider the following simple expression:

$$\mathbf{G}_W\left(\mathbf{M}_0, \mathbf{N}_0\right) = \varphi_0\mathbf{1} + \varphi_1\mathbf{M}_0 + \varphi_3\mathbf{N}_0 + \frac{1}{2}\varphi_7\left(\mathbf{M}_0\mathbf{N}_0 + \mathbf{N}_0\mathbf{M}_0\right), \tag{10.62}$$

where $\mathbf{N}_0$ is such that $\mathbf{W}_0^2 = \mathbf{N}_0 - \mathbf{1}$. The advantage of using **N** instead of **W** is that the nonzero component in the out-of-plane direction disappears in this form, and that is useful to clarify the characteristics of the vector field **w**, especially in plane-strain problems. According to (10.62), the functions $\varphi_0$ and $\varphi_1$ are related to isotropic growth/remodeling, while $\varphi_3$ and $\varphi_7$ are related to anisotropic growth.

As to the time development of anisotropy, we may envisage two possibilities. One of these consists in considering that the vector **w** is embedded in the material just as in fiber-reinforced materials; it is oriented like a float. Since this anisotropy vector describes only the characteristic orientation, its evolution is given in a purely kinematic way, and no phenomenological parameter is involved in the equation. With an embedding in the reference crystal, we can therefore write the following evolution equation:

$$\dot{\mathbf{w}}_0 = \left(\mathbf{w}_0.\left(\mathbf{G}_0\mathbf{w}_0\right)\right)\mathbf{w}_0 - \mathbf{G}_0\mathbf{w}_0. \tag{10.63}$$

This equation satisfies frame-indifference since $\mathbf{G}_0$ is a sort of stretching.

Noting that the time rate in (10.63) is always perpendicular to the vector itself, and while it is understood that $\mathbf{G}_0$ could be replaced by any second-order tensor that satisfies the frame-indifference in the reference crystal (Epstein, 2000), we can then also propose that the Mandel stress itself be in the evolution equation, which we can write as

$$\dot{\mathbf{w}}_0 = \mathbf{M}_0\mathbf{w}_0 - \left(\mathbf{w}_0.\left(\mathbf{M}_0\mathbf{w}_0\right)\right)\mathbf{w}_0. \tag{10.64}$$

Since the rate of the vector is linearly related to the current state of stress, the vector behaves like a float. Figure 10.1 shows the variation of the vector subject to a certain load. From (10.64) it must be understood that the rate of

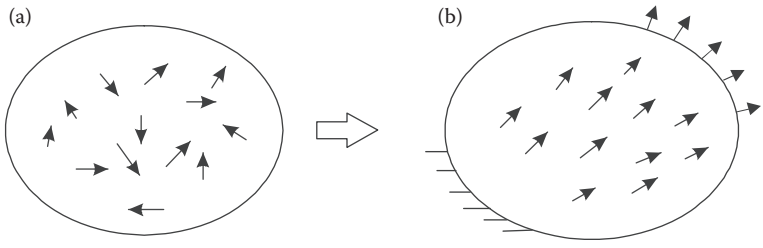


**FIGURE 10.1**
Variation of material symmetry: (a) Initial state, (b) after applied load. (Adapted from Imatani, S. and Maugin, G.A., *Mech. Res. Commun*., 29, 477–83, 2002.)

the vector approaches zero when the Mandel stress is free or when the direction of the vector coincides with the principal direction of this stress. This simply means that the vector varies asymptotically its direction so as to fit the principal direction of the Mandel stress. Even when the neighboring vectors take a different direction at the initial time, the vector will be pointing in the same direction during the loading process. In other words, growth takes place in a particular direction, which depends on the surrounding boundary conditions.

## 10.5 Illustrations: Finite-Element Implementation

The methodology used is as follows. The numerics are based on an incremental formulation in the reference configuration while the constitutive modeling was set in the local reference crystal. Mechanical variables need to be updated in a step-by-step procedure. The numerical formulation is documented in the works of Imatani and Maugin (2001a, 2001b, 2002) for two-dimensional problems. The starting point obviously is the principle of virtual work in the reference configuration:

$$\int_{B_R} \rho_0 \dot{\mathbf{v}}.\delta\mathbf{u}\,dV + \int_{B_R} \mathbf{S} : \delta\mathbf{E}\,dV = \int_{\partial B_R} \overline{\mathbf{T}}^d.\delta\mathbf{u}\,dA, \tag{10.65}$$

where $\mathbf{E}$ is the Green–Lagrange strain. For quasistatics, we write this in incremental form as

$$\int_{B_R} \mathbf{S}^\tau : \Delta(\delta\mathbf{E})dV + \int_{B_R} \Delta\mathbf{S} : \delta\mathbf{E}^\tau dV = \int_{\partial B_R} \Delta\overline{\mathbf{T}}^d.\delta\mathbf{u}\,dA \tag{10.66}$$

where $\Delta$ denotes the variation from time $\tau$ to time $\tau + \Delta\tau$, while in full dynamics this takes the form

$$\int_{B_R} \rho_0 \dot{\mathbf{v}}^{\tau+\Delta\tau}.\delta\mathbf{u}\,dV + \int_{B_R} \mathbf{S}^{\tau} : \delta\mathbf{E}^{\tau}\,dV + \int_{B_R} \mathbf{S}^{\tau} : \Delta(\delta\mathbf{E})dV + \int_{B_R} \Delta\mathbf{S} : \delta\mathbf{E}^{\tau}dV = \int_{\partial B_R} \overline{\mathbf{T}}^{d\tau+\Delta\tau}.\delta\mathbf{u}\,dA, \tag{10.67}$$

where one can implement Newmark's method, according to which quantities are evaluated at the next time $\tau + \Delta\tau$ and then the results are unconditionally stable. The following examples have been treated in this way.

### 10.5.1 Monotonic Growth and Adaptation

We consider a quarter part (fragment) of a ring that is analyzed under surface-force-free conditions and serves to illustrate isotropic growth. A circumferential growth is revealed under the conditions ($\varphi_0 = 0.0$, $\varphi_3 = 0.1$; $C_1 = 3.0$, $C_2 = 1.0$, $C_3 = 100.0$) and with the anisotropy vector also lying circumferentially (cf. Figure 10.2). Under the action of constant inner pressure, the mean radius varies as indicated in Figure 10.3 for different constitutive

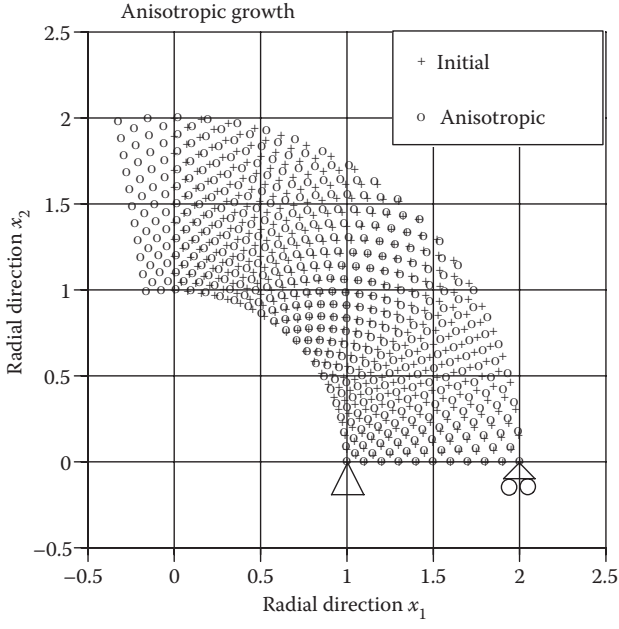


**FIGURE 10.2**
Growth of a fragment of ring. (Adapted from Maugin, G.A., and Imatani, S., *J. Phys. IV Coll.*, Figure 1, 105, 365–72, 2003.)

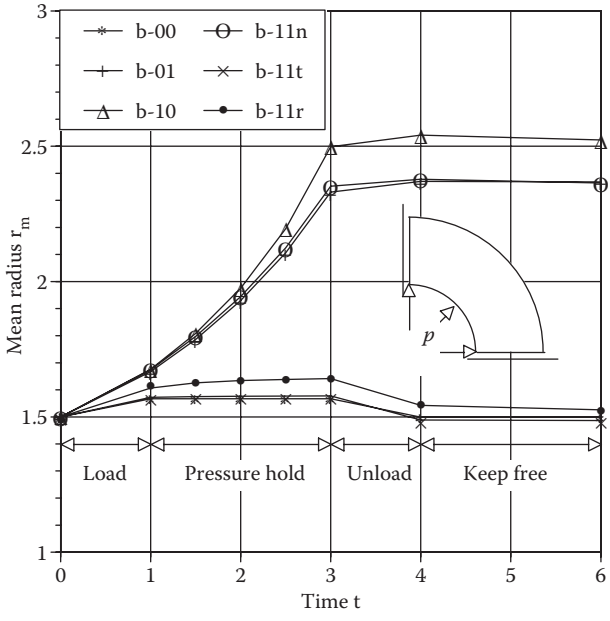


**FIGURE 10.3**
Variation of mean radius in the ring under pressure followed by unloading. The path b-00 means the result with the parameters set to zero corresponding to pure hyperelasticity. The recovery effect appears in the path b-11r where the anisotropy vector is randomly distributed in the domain. (Adapted from, Maugin, G.A., and Imatani, S., *J. Phys. IV Coll*. Figure 2, p. 371, 105, 365–72, 2003.)

assumptions regarding the coefficients. The case noted b-11r shows an *adaptive behavior*. The Cauchy stress distribution in a growing material in the form of a ring is illustrated in Figure 10.4, where the nodal displacement at the inner surface is prescribed, moving radially during 1 second. The pure hyperelastic case corresponds to path B. For other cases, competition between growth in the radial and circumferential directions creates completely different distributions.

### 10.5.2 Anisotropic Growth in the Float Model

We consider a quarter part of a cylinder (Figure 10.5) with anisotropy unit vector **w** randomly distributed in direction over the domain in the initial state, which implies quasi-isotropy, but **w** is supposed to evolve according to (10.64). Figure 10.5 shows the evolution in orientation of this vector during the course of deformation. When the internal pressure is imposed, the vectors **w** are activated, and some are going to be oriented in the circumferential direction, which is none other than the principal direction of the Mandel stress. The rate of variation depends on the initial configuration; the closer

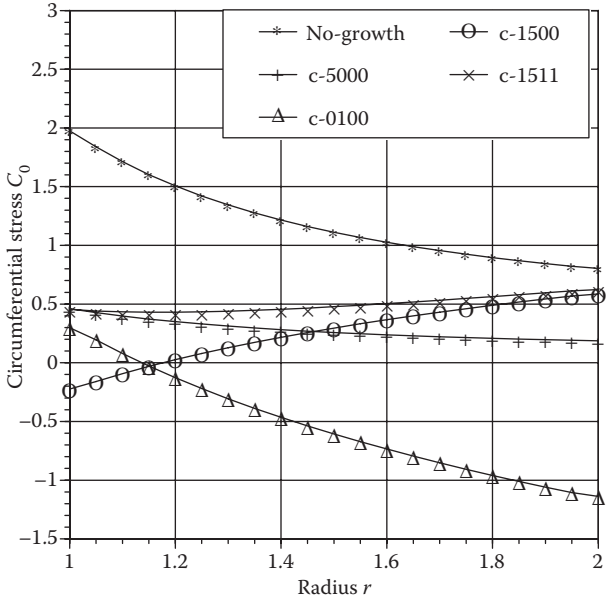


**FIGURE 10.4**
Circumferential (Cauchy) stress distribution under various patterns of material parameters. (Adapted from, Maugin, G.A., and Imatani, S., *J. Phys. IV Coll*. Figure 2, p. 371, 105, 365–72, 2003.)

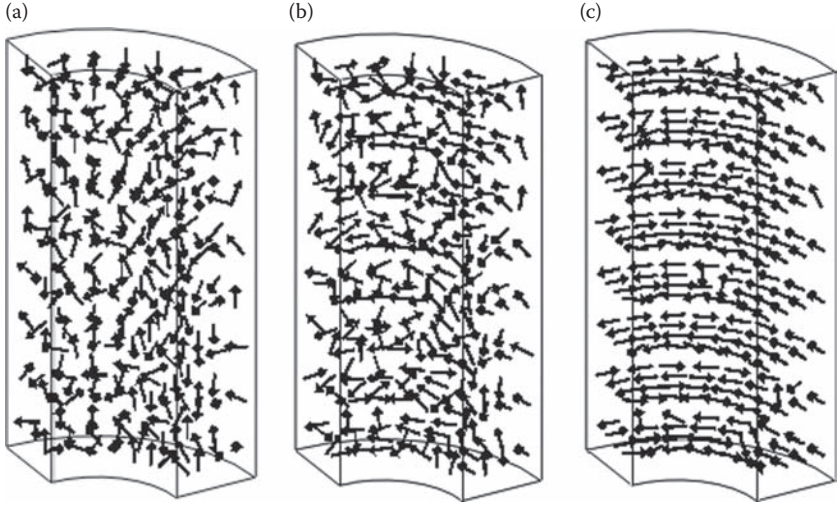


**FIGURE 10.5**
Variation in orientation of the anisotropy vector in the cylinder subjected to internal pressure with float model (10.64): (a) Initial state, (b) intermediate state, (c) final state. (Adapted from, Imatani, S., and Maugin, G.A., *Mech. Res. Commun*., Figure 3, p. 482, 29, 477–83, 2002.)

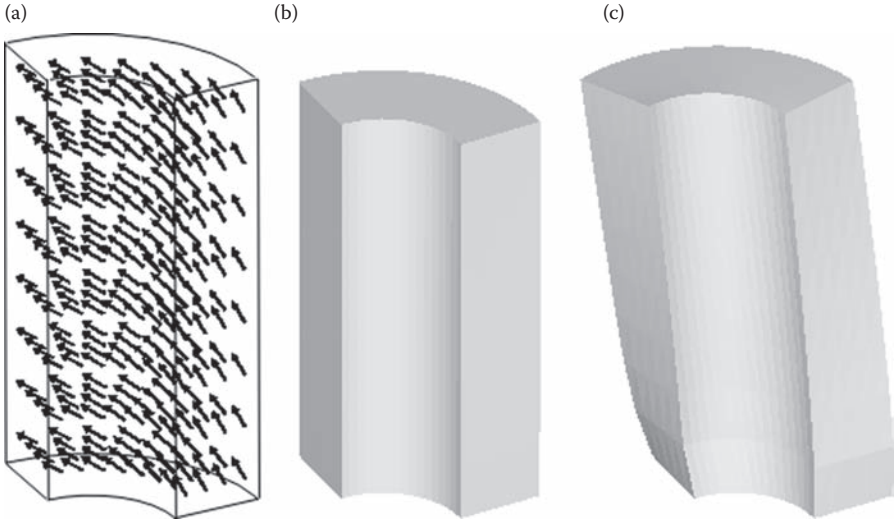


**FIGURE 10.6**
Helical flow pattern with evolution equation (10.63): (a) Vector orientation, (b) initial domain, (c) final domain at $t = 30$ s. (Adapted from, Imatani, S., and Maugin, G.A., *Mech. Res. Commun.*, Figure 4, p. 482, 29, 477–83, 2002.)

the initial orientation is to the circumferential direction, the more rapidly the vectors will approach that direction. In general, the vector is forward of the maximal principal direction of the Mandel stress. At the final stage in Figure 10.5, most of the vectors are oriented toward the circumferential direction. Although this simulation merely examines the variation of **w** subjected to the float model, we can conclude that the present model has a potential performance for describing the adaptation behavior.

We can revisit the problem of *monotonic growth under the stress-free state* for the same cylinder but with the evolution equation (10.63) for **w**. The same eight-node isoparametric brick element as in the previous case is used in the Finite Element (FE) scheme, but the bottom surface is fixed while the outer surfaces are kept free. The analyzed domain is shown in Figure 10.6a and b with the simulated deformation result in Figure 10.6c. The initial vector distribution **w** is set to be helicoidal, and we used a coefficient $\varphi_3 = -0.005$. The analyzed domain is extensible toward the vector direction without any stress. In fact, this model covers various growth patterns of not only a monotonic growth but also stress-induced growth, which have been reported elsewhere (e.g., Rodriguez et al., 1994; Hart et al., 1984) .

### 10.5.3 Growth Behavior under Cyclic Loading

Here we consider cyclic dynamic effects in a cantilever beam (2D problem; cf. Figures 10.7 through 10.9). A time triangular loading A is applied

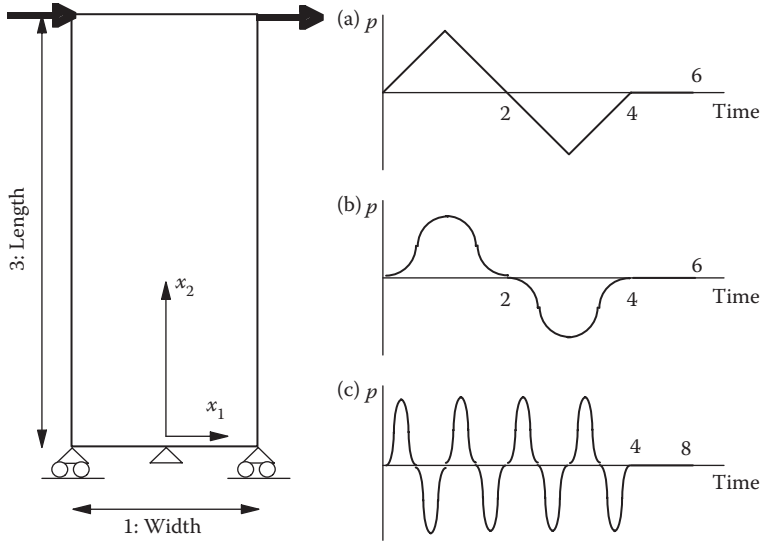


**FIGURE 10.7**
Schematic illustration of the boundary conditions for the cantilever beam problem. The surface force is imposed at the edge of the side walls as a normal force. The wave profile A is used in the quasistatic analysis while the B and C profiles are used in the dynamic analysis. (Adapted from Maugin, G.A., and Imatani, S., *J Phys. IV Coll.*, Figure 4, p.371, 105, 365–72, 2003.)

in quasistatics and combined wave forms such as in B or C are applied in the fully dynamical analysis. The input is composed of normal forces at the upper edge of the side walls as indicated by arrows in the left scheme of the settings in Figure 10.7. The anisotropy vector field **w** is vertically embedded in the material specimen resulting in some resistance to the ending stress. Figure 10.8 shows the trajectories of the neutral (central) axis of the beam. The dynamic result exhibits an asymmetry in time due to inertial effects that become important as the eigenfrequency of the beam is of the same order as the time scale of the forcing. Then the damping due to growth (here a type of viscoelasticity) takes place after release of the applied force. Finally, Figure 10.9 shows the volumetric growth ($\det\mathbf{K}^{-1} = \det\mathbf{F}_g$) during the course of cyclic loading. It is remarked that the quasistatic analysis clearly overestimates the growth. This example illustrates how a redistribution of mass takes place as a consequence of a purely mechanical applied field. Remodeling of some bones is a phenomenon of this type.

In the preceding we have privileged our own amateurish numerical simulations. However, we must also cite the beautiful colored illustrations obtained in 3D in a more professional way by Kuhl (2004) and also Kuhl et al. (2003) and Kuhl and Steinmann (2003a, 2003b) on the basis of an elastic potential different from (10.57) but in the absence of the induced anisotropy.

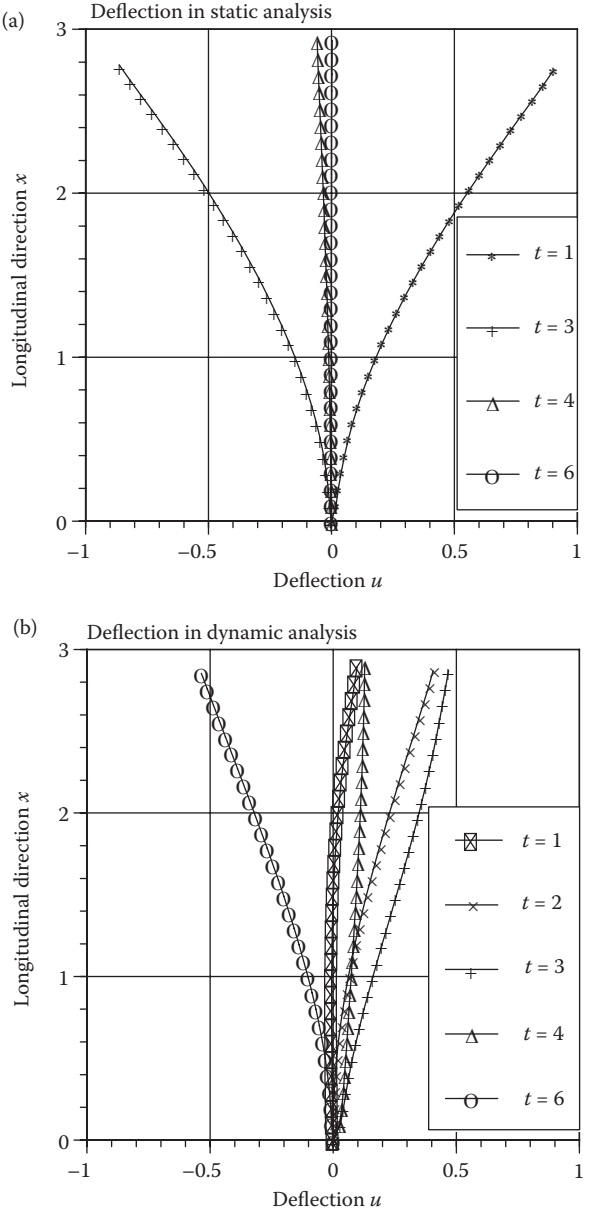


**FIGURE 10.8**
Deflection of the cantilever beam under (a) static and (b) dynamic load. (Adapted from Maugin, G.A., and Imatani, S., *J. Phys. IV Coll.*, Figure 5, p.372, 105, 365–72, 2003.)

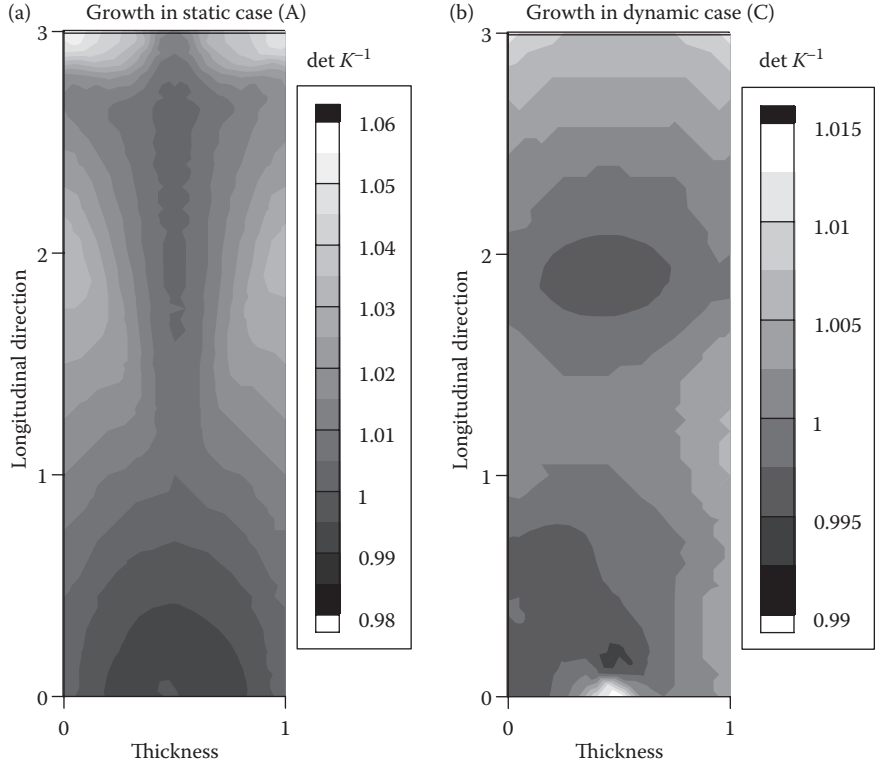


**FIGURE 10.9**
Growth behavior in the course of cyclic loading: (left) Quasistatic loading, (right) dynamic loading. (Adapted from Maugin, G.A., and Imatani, S., *J. Phys. IV Coll.,* Figure 6, p.372, 105, 365–72, 2003.)

## 10.6 Intervention of Nutriments

The theory presented in the preceding is one of stress-induced growth and adaptation or remodeling. Little progress has been made, at the time of writing, toward a theory accounting for the effects of nutriments, that is, a true mixed physiological–mechanical theory of growth and not only a pure mechanical theory. What must be retained from the preceding developments is that the driving force behind growth viewed as a local but special structural rearrangement of matter is necessarily of the Mandel or Eshelby stress type. In the same way as the interactions of electromagnetic fields and deformable matter may be accounted for by introducing *external forces* in the form of a stress (compared to the Cauchy stress conceived as an "internal" tensorial force) of the tensorial type (Maxwell stress) in a formulation of the principle of virtual power (cf. Maugin, 1980), an approach of the same type

could be envisaged for growth with an "external" Mandel stress acting as a source that will combine with the field thermomechanical Mandel stress **M** or Eshelby stress **b**. Such an additional term should come as a contribution of the type

$$\left(p_g^{\text{ext}}\right)^* = \mathbf{M}^{\text{ext}} : \left(\nabla_R \mathbf{V}^*\right)^T, \tag{10.68}$$

where **V** is a material velocity field and an asterisk indicates a virtual motion or the value taken by an expression in such a field. Pursuing thus the idea of such external terms, we propose to formulate the principle of virtual power in the following form in quasistatics for the material body occupying the material volume $B_R$:

$$\left(P^{\text{int}}\right)^* + \left(P^{\text{ext}}\right)^* = 0, \tag{10.69}$$

with

$$\left(P^{\text{int}}\right)^* = \int_{B_R} \left(\left(p_T^{\text{int}}\right)^* + \left(p_b^{\text{int}}\right)^*\right) dV, \tag{10.70}$$

$$\left(p_T^{\text{int}}\right)^* = -\mathbf{T} : \left(\nabla_R \mathbf{v}^*\right)^T, \quad \left(p_b^{\text{int}}\right)^* = -\mathbf{b} : \left(\nabla_R \mathbf{V}^*\right), \tag{10.71}$$

and

$$\left(P^{\text{ext}}\right)^* = \int_{B_R} \left(\mathbf{f}^{\text{ext}}.\mathbf{v}^* - \mathbf{M}^{\text{ext}} : \left(\nabla_R \mathbf{V}^*\right)^T\right) dV + \int_{\partial B_R} \bar{\mathbf{T}}^d.\mathbf{v}^* dA. \tag{10.72}$$

The local equations resulting from this for any $\mathbf{v}^*$ and $\nabla_R \mathbf{V}^*$ read

$$\text{div}_R \mathbf{T} + \mathbf{f}^{\text{ext}} = \mathbf{0} \quad \text{in} \quad B_R, \quad \mathbf{N}.\mathbf{T} = \bar{\mathbf{T}}^d \quad \text{at} \quad \partial B_R, \tag{10.73}$$

and the "material tensorial balance"

$$\mathbf{b} + \mathbf{M}^{\text{ext}} = \mathbf{0}. \tag{10.74}$$

As for the constitutive equations, in the absence of heat conduction and bulk heat source, they follow from an exploitation of the Clausius–Duhem inequality. In the present case the total dissipation is given by the difference between the power of external forces and the time rate of change of the energy, that is (without asterisks),

$$\Phi\left(B_R\right) = P^{\text{ext}} - \frac{d}{dt} \int_{B_R} W dV \geq 0. \tag{10.75}$$

On using (10.69) for real fields and localizing, this yields

$$\mathbf{T} : \left(\nabla_R \mathbf{v}\right)^T + \mathbf{b} : \left(\nabla_R \mathbf{V}\right)^T \geq \dot{W}. \tag{10.76}$$

Now $W$ is taken as in (10.40), that is,

$$W = J_K^{-1} W_c \left(\mathbf{FK}\right) = J_{F_e} W_c \left(\mathbf{F}_e\right) = \tilde{W}\left(\mathbf{F}, \mathbf{K} = \mathbf{F}_g^{-1}\right). \tag{10.77}$$

On substituting from this into the inequality (10.76) and computing the time derivative of $\tilde{W}$ just as in Section 5.8, we obtain the following constitutive equations:

$$\mathbf{T} = \mathbf{T}^{\text{rev}} + \mathbf{T}^{\text{irr}}, \quad \mathbf{T}^{\text{rev}} \equiv \mathbf{T}^e = \frac{\partial W}{\partial \mathbf{F}_e}, \tag{10.78}$$

$$\mathbf{b} = \mathbf{b}^{\text{rev}} + \mathbf{b}^{\text{irr}}, \quad \mathbf{b}^{\text{rev}} = W\mathbf{1}_R - \mathbf{T}^e.\mathbf{F}, \tag{10.79}$$

while there remains the dissipation inequality

$$D = \mathbf{T}^{\text{irr}} : \left(\nabla_R \mathbf{v}\right)^T + \mathbf{b}^{\text{irr}} : \left(\nabla_R \mathbf{V}\right)^T \geq 0. \tag{10.80}$$

From this, in particular, we deduce that the material balance (10.74) reads

$$\left(W\mathbf{1}_R - \mathbf{T}^e.\mathbf{F}\right) + \mathbf{b}^{\text{irr}} + \mathbf{M}^{\text{ext}} = \mathbf{0}, \tag{10.81}$$

in which we clearly see the contribution of the standard Eshelby stress tensor. This equation can also be written as

$$W\mathbf{1}_R + \mathbf{b}^{\text{irr}} + \mathbf{M}^{\text{ext}} = \mathbf{M}, \tag{10.82}$$

where $\mathbf{M} = \mathbf{T}^e.\mathbf{F}$ is the standard Mandel stress, $\mathbf{b}^{\text{irr}}$ is a dissipative stress having the same nature as the Mandel stress, and $\mathbf{M}^{\text{ext}}$ has to be prescribed in order to represent an input of nutriments. In particular, the latter may be spherical, that is, $\mathbf{M}^{\text{ext}} = W^{\text{ext}}\,\mathbf{1}_R$, so that it does represent an input of energy, as (10.82) then transforms to

$$\left(W + W^{\text{ext}}\right)\mathbf{1}_R + \mathbf{b}^{\text{irr}} = \mathbf{M}. \tag{10.83}$$

The originality of the present approach stems from the consideration of terms involving $\nabla_R \mathbf{V}$ in (10.69) and that of the expression (10.77) for the free energy.

This is the essence of a reasoning due to Di Carlo and Quiligotti (2002), as well as Di Carlo (2004)—in a different notation—who followed some of the arguments of Gurtin (1999) in considering simultaneously the physical and material velocity fields in a formulation of the principle of virtual power. We shall not pursue this line since little, if not nothing, is known about the expression of $\mathbf{M}^{\text{ext}}$. A more useful modeling may be the one that considers the growing medium of interest as a solid–fluid mixture following the works of Quiligotti (2002), Quiligotti, dell'Isola, et al. (2002), Quiligotti, Maugin, et al. (2002), and Quiligotti and Maugin (2003a, 2003b, 2004), of which we now examine the main lines.

## 10.7 Eshelbian Approach to Solid–Fluid Mixtures

### 10.7.1 Kinematics

This is the most questionable point in a continuum theory of mixtures since particles of different species—here the solid and the fluid—may occupy the *same* physical placement at time *t*. Quantities related to the solid are labeled with a subscript *S* and those related to the fluid with a subscript *F*. For the solid constituent, we have the direct motion

$$\mathbf{x} = \chi_S(\mathbf{X}, t) = \mathbf{X} + \varepsilon \mathbf{u}_S, \tag{10.84}$$

with direct gradient and physical velocity given by

$$\mathbf{F}_S = \mathbf{1} + \varepsilon(\nabla_R \mathbf{u}_S)^T, \quad \mathbf{v}_S = \left.\frac{\partial \chi_S(\mathbf{X}, \tau)}{\partial \tau}\right|_{\tau=t}. \tag{10.85}$$

The ε scaling parameter is introduced just to remind the reader that elastic displacements of the solid constituent will always remain small. We suppose that there exists a smooth inverse mapping $\chi_S^{-1}$ providing the inverse motion of the solid constituent in the same way as in the classical theory (Chapter 2). Thus,

$$\mathbf{X} = \chi_S^{-1}(\chi_S(\mathbf{X}, t), t), \tag{10.86}$$

so that the material velocity $\mathbf{V}_S$ is well defined:

$$\mathbf{V}_S = \left.\frac{\partial \chi_S^{-1}}{\partial t}\right|_{x=\chi_S} \quad \text{with} \quad \mathbf{F}_S \mathbf{V}_S + \mathbf{v}_S = \mathbf{0}. \tag{10.87}$$

Now let us turn to the fluid constituent. Any fluid "point" that belongs to the mixture at time $t$ interacts with a one-parameter family of solid "points," moving along the curve

$$\chi_S^{-1}\left(\chi_F\left(\mathbf{X}_F,.\right),.\right):t\to\mathbf{X}, \tag{10.88}$$

at the material velocity $\mathbf{W}_F(\mathbf{X}, t)$ such that

$$\mathbf{v}_F\left(\mathbf{x},t\right)=\mathbf{F}_S\left(\mathbf{X},t\right)\mathbf{W}_F\left(\mathbf{X},t\right)+\mathbf{v}_S\left(\mathbf{x},t\right)$$

since $\mathbf{x}=\chi_F=\chi_S$. The true material velocity of the fluid constituent is then given by

$$\mathbf{V}_F\left(\mathbf{X},t\right)=-\mathbf{F}_S^{-1}\left(\mathbf{X},t\right)\mathbf{v}_F\left(\mathbf{x},t\right), \tag{10.89}$$

so that

$$\mathbf{W}_F=\mathbf{V}_S-\mathbf{V}_F, \tag{10.90}$$

is none other than the relative velocity of the fluid component with respect to the solid one but described on the reference configuration of the solid component, although fluid and solid "particles" belong a priori to two different sets (manifolds). This is rather clearly illustrated by Figure 10.10. Because of the choice made concerning the special role of the solid material configuration, many quantities will be pulled back or pushed forward with the help of the "solid" gradient $\mathbf{F}_S$ or its inverse.

**Migrating surface and transport theorem**

Let a surface envelop at time $t$ a smooth region $\gamma(t)$ of the current shape of our mixture. Consider that such a surface moves independently of the solid component of the mixture. Then the time derivative of the integral of a smooth Eulerian field $\varphi$ over this migrating surface is given by (transport theorem)

$$\frac{d}{dt}\int_{\gamma(\tau)}\varphi dv\bigg|_{\tau=t}=\frac{d}{dt}\int_{V_S(\tau)}\varphi dv\bigg|_{\tau=t}+\int_{\partial\gamma(t)}\varphi\mathbf{n}.\left(\mathbf{v}-\mathbf{v}_S\right)da, \tag{10.91}$$

where $\mathbf{v}$ is the independent velocity of the boundary of outward unit normal $\mathbf{n}$ and $V_S(\tau)$ is the shape at time $\tau$ of the solid subbody associated with the smooth fixed region of the reference shape $V^*=\chi_S^{-1}\left(V_t,t\right)$. Since the inverse motion $\chi_S^{-1}$ carries $\gamma(\tau)$ onto $\gamma^*(\tau)$, denoting by $\mathbf{W}$ the velocity at which

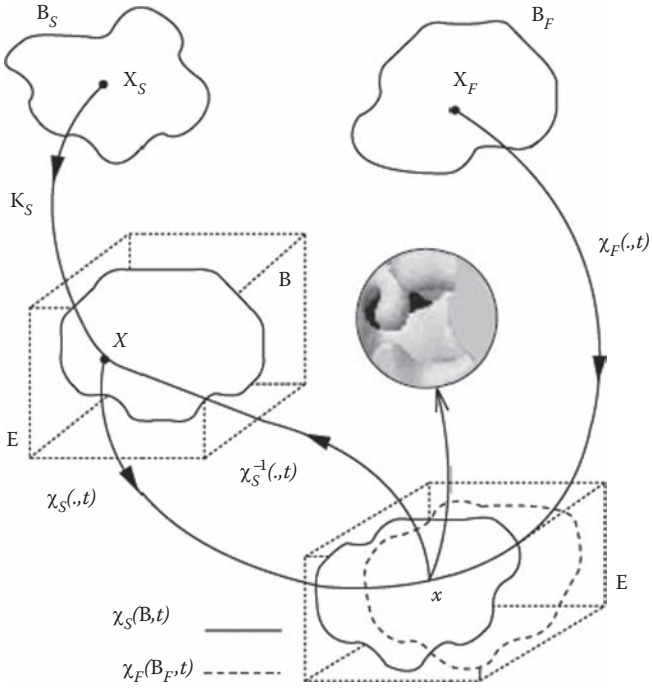


**FIGURE 10.10**
Kinematics of a binary solid-fluid mixture with solid and fluid particle- manifolds (top), material configuration for the solid constituent (center left), and actual configuration (common to the two species) at bottom. (Adapted from, Quiligotti, S., dell'Isola, F., and Maugin, G.A., *Proc. 2nd Biot Conference on Porous Media (Grenoble, August 2002), Poromechanics II*, Figure 1, p. 289, Rotterdam, the Netherlands: Balkema, 287–92, 2002.)

the boundary $\partial\gamma^*$ moves through the reference shape of the body, we can write the relationship

$$\mathbf{W}(\mathbf{X},t) = \mathbf{F}_S^{-1}(\mathbf{X},t)\big(\mathbf{v}(\mathbf{x},t) - \mathbf{v}_S(\mathbf{x},t)\big), \tag{10.92}$$

while we can associate with φ the referential field

$$\varphi^*(\mathbf{X},t) = \big(\det \mathbf{F}_S\big)\varphi. \tag{10.93}$$

Thus, instead of (10.91) we can as well consider the expression:

$$\frac{d}{dt}\int_{\gamma^*(\tau)} \varphi^* dV\Big|_{\tau=t} = \frac{d}{dt}\int_{V_S^*} \varphi^* dV\Big|_{\tau=t} + \int_{\partial V_t{}^*} \varphi^* \mathbf{N}.\mathbf{W} da. \tag{10.94}$$

We may also introduce the material velocity related to **v** by

$$\mathbf{v}(\mathbf{x},t) + \mathbf{F}_S(\mathbf{X},t)\mathbf{V}(\mathbf{X},t) = \mathbf{0}. \tag{10.95}$$

As a consequence of (10.92) and (10.95), we have thus

$$\int_{\partial V_t} \varphi \mathbf{n}.\left(\mathbf{v}-\mathbf{v}_S\right)da = -\int_{\partial V_t{}^*} \varphi^* \mathbf{N}.\left(\mathbf{V}-\mathbf{V}_S\right)dA = \int_{\partial V_t{}^*} \varphi^* \mathbf{N}.\mathbf{W}dA. \tag{10.96}$$

On account of this we have the following useful *transport theorems*:

$$\int_{V_t} \frac{\partial \varphi}{\partial \tau}\bigg|_{\tau=t} dv = \frac{d}{dt}\int_{\gamma(\tau)} \varphi dv\bigg|_{\tau=t} - \int_{\partial V_t} \varphi \mathbf{n}.\mathbf{v}da = \frac{d}{dt}\int_{\gamma^*(\tau)} \varphi^* dV\bigg|_{\tau=t} + \int_{\partial V_t{}^*} \varphi^* \mathbf{N}.\mathbf{V}dA. \tag{10.97}$$

This is useful in establishing global balance laws for our mixtures.

The following remark belongs to this section. If we think of a *fixed* Eulerian surface $\partial V$ in the material body, and if the material solid surface currently overlapped with $\partial V$ expands, then the migrating surface associated with $\partial V$ by the inverse solid motion $\chi_S^{-1}$ shrinks. Conversely, if the former shrinks, then the latter expands, since we can write

$$\int_{\partial V} \mathbf{n}.\mathbf{v}_S da = -\int_{\partial V_t{}^*} \left(\det \mathbf{F}_S\right)\mathbf{N}.\mathbf{V}_S dA, \tag{10.98}$$

for $V_t{}^* = \chi_S^{-1}\left(V,t\right)$.

### 10.7.2 Balance of Mass

Here we consider solid and fluid constituents that do not exchange mass. Accordingly, the local Eulerian equations of mass for these constituents have a classical form with fields indexed *S* or *F*, that is, in the actual configuration of the mixture:

$$\frac{\partial \rho_S}{\partial t} + \operatorname{div}\left(\rho_S \mathbf{v}_S\right) = 0, \tag{10.99}$$

and

$$\frac{\partial \rho_F}{\partial t} + \operatorname{div}\left(\rho_F \mathbf{v}_F\right) = 0, \tag{10.100}$$

for the solid and fluid constituents, respectively, at any point of the actual volume $V_S(t)$. Now we have (cf. (10.93))

$$\rho_S{}^*\left(\mathbf{X},t\right) = J_S\left(\mathbf{x},t\right)\rho_S\left(\mathbf{x},t\right), \quad \rho_F{}^*\left(\mathbf{X},t\right) = J_S\left(\mathbf{X},t\right)\rho_F\left(\mathbf{x},t\right), \tag{10.101}$$

where $J_S = \det \mathbf{F}_S \equiv J_{F_S}$. In the notation of Chapter 2, $\rho_S^*$ would have been noted $(\rho_0)_S$. Of course, the second of (10.101) is peculiar. With a homogeneous solid constituent, we clearly have

$$\frac{\partial \rho_S^*}{\partial t} = 0. \tag{10.102}$$

This is not the case of $\rho_F^*$, for which we check with the help of (10.94) that

$$\frac{\partial \rho_F^*}{\partial t} + \nabla_R . \left( \rho_F^* \mathbf{W}_F \right) = 0. \tag{10.103}$$

But we can look at the question of mass conservation in a slightly different light. We can refer to the motion of the mixture as a single body with physical velocity field

$$\mathbf{v} = \xi_S \mathbf{v}_S + \xi_F \mathbf{v}_F, \tag{10.104}$$

where the $\xi_\alpha$, $\alpha = S, F$ are the *mass fractions* associated with the solid and fluid constituent, that is, such that

$$\xi_\alpha := \rho_\alpha / \rho, \quad \rho = \rho_S + \rho_F, \quad \xi_S + \xi_F = 1. \tag{10.105}$$

Then we let the reader check the following two forms of the continuity equation:

$$\frac{\partial \rho}{\partial t} + \operatorname{div}(\rho \mathbf{v}) = 0, \tag{10.106}$$

and

$$\frac{\partial \rho^*}{\partial t} + \nabla_R . \left( \rho^* \mathbf{W} \right) = 0, \tag{10.107}$$

where $\rho^* = J_S \rho$ and $\mathbf{W} = \xi_F \mathbf{W}_F$.

Finally, we note the quantity

$$\frac{d}{dt} \int_{V_t} \rho_\alpha dv = - \int_{\partial V_t} \mathbf{n} . \left( \mathbf{v}_\alpha - \mathbf{v} \right) da \tag{10.108}$$

may not vanish. Here $\mathbf{d}_\alpha = \mathbf{v}_\alpha - \mathbf{v}$ is the (physical) velocity of diffusion of the $\alpha$th constituent. In particular, we can write

$$\mathbf{d}_S = \mathbf{v}_S - \mathbf{v} = \xi_F(\mathbf{v}_S - \mathbf{v}_F), \quad \mathbf{d}_F = \mathbf{v}_F - \mathbf{v} = \xi_S(\mathbf{v}_F - \mathbf{v}_S). \tag{10.109}$$

### 10.7.3 Stress Power, Kinetic Energy, and Acceleration

Considering a first-order gradient theory (cf. Maugin, 1980) for both velocity fields $\mathbf{v}_S$ and $\mathbf{v}_F$, we assume that the corresponding *stress power* is given by the following standard expression:

$$-p^{\text{int}} = \sum_{\alpha=S,F} \left( \pi_\alpha . \mathbf{v}_\alpha + \sigma_\alpha : (\nabla \mathbf{v}_\alpha)^T \right). \tag{10.110}$$

According to the principle of material frame-indifference, the stress power or power of "internal forces" in (10.110) must vanish in any rigid-body motion given by

$$\mathbf{v}_S = \mathbf{v}_F = \mathbf{w}_0(t) + \Omega(t).(\mathbf{x} - \mathbf{x}_0), \quad \Omega = -\Omega^T. \tag{10.111}$$

Where both $\mathbf{w}_0$ and $\Omega$ are spatially uniform, the following conditions follow from this requirement:

$$\pi_S + \pi_F = 0, \quad \sigma_S + \sigma_F = (\sigma_S + \sigma_F)^T. \tag{10.112}$$

Next we consider the *kinetic energy* of the mixture as a whole per unit actual volume:

$$K = \frac{1}{2}\rho \mathbf{v}^2. \tag{10.113}$$

We let the reader show by way of exercise that this is nothing but

$$K = \sum_{\alpha=S,F} \frac{1}{2}\rho_\alpha \mathbf{v}_\alpha . \mathbf{v}_\alpha + \frac{1}{2}\rho(\mathbf{d}_S . \mathbf{d}_F). \tag{10.114}$$

If the *acceleration* of the mixture as a single continuum is defined as usual by

$$\mathbf{a}(\mathbf{x}, t) := \left. \frac{d\mathbf{v}(\mathbf{x}, \tau)}{d\tau} \right|_{\tau = t}, \tag{10.115}$$

then the following results are easily established:

$$\mathbf{v}.(\rho\mathbf{a}) = \sum_{\alpha} \mathbf{v}_{\alpha}.(\rho_{\alpha}\mathbf{a}_{\alpha}) \tag{10.116}$$

and

$$\mathbf{a} = \sum_{\alpha} (\xi_{\alpha}\mathbf{a}_{\alpha}) - \rho^{-1}\operatorname{div}\bar{\sigma}, \tag{10.117}$$

where

$$\mathbf{a}_{\alpha} := \left.\frac{d\mathbf{v}_{\alpha}}{d\tau}\right|_{\tau=t}, \quad \bar{\sigma} := \sum_{\alpha} \rho_{\alpha}\mathbf{d}_{\alpha} \otimes \mathbf{d}_{\alpha}, \tag{10.118}$$

are, respectively, the time derivative in following the motion of the $\alpha$th constituent, and the *apparent stress* due to diffusive motions. Then we can establish from (10.117) the following two expressions:

$$\rho_S\mathbf{a} = \rho_S\mathbf{a}_S - \operatorname{div}(\xi_S\bar{\sigma}) + \frac{\rho_S\rho_F}{\rho_S+\rho_F}(\mathbf{a}_F - \mathbf{a}_S) + \bar{\sigma}.\nabla\xi_S, \tag{10.119}_1$$

$$\rho_F\mathbf{a} = \rho_F\mathbf{a}_F - \operatorname{div}(\xi_F\bar{\sigma}) + \frac{\rho_S\rho_F}{\rho_S+\rho_F}(\mathbf{a}_S - \mathbf{a}_F) + \bar{\sigma}.\nabla\xi_F. \tag{10.119}_2$$

### 10.7.4 The Principle of Virtual Power

Let $\hat{\mathbf{v}}_{\alpha}$ denote here a virtual (physical) velocity field. Then in the presence of body and surface forces, we express the principle of virtual power for the solid–fluid mixture occupying the regular region $B_t$ bounded by the regular surface $\partial B_t$ with unit outward normal $\mathbf{n}$ by

$$\begin{aligned}\sum_{\alpha}\int_{B_t} \rho_{\alpha}\mathbf{a}.\hat{\mathbf{v}}_{\alpha}dv = &\sum_{\alpha}\left(\int_{B_t}\rho_{\alpha}\mathbf{f}.\hat{\mathbf{v}}_{\alpha}dv + \int_{\partial B_t}\xi_{\alpha}\mathbf{t}.\hat{\mathbf{v}}_{\alpha}da\right)\\ &-\sum_{\alpha}\int_{B_t}\left(\pi_{\alpha}.\hat{\mathbf{v}}_{\alpha} + \sigma_{\alpha:}:(\nabla\hat{\mathbf{v}}_{\alpha})^T\right)dv,\end{aligned} \tag{10.120}$$

in which we recognize the standard statement of the balance between the power expended by the inertial forces and the total power of both external

and internal forces (cf. Chapter 2). For any $\hat{\mathbf{v}}_\alpha$ and any volume and surface elements, (10.120) yields the local equations

$$\rho_\alpha \mathbf{a} = \operatorname{div}\sigma_\alpha + \rho_\alpha \mathbf{f} - \pi_\alpha \quad \text{in} \quad B_t\,, \tag{10.121}$$

$$\mathbf{n}.\sigma_\alpha = \xi_\alpha \mathbf{t} \quad \text{at} \quad \partial B_t\,. \tag{10.122}$$

On summing these equations over α and taking account of (10.112), we also have the equations of linear (physical) momentum relating to a single body in a first-order gradient theory as

$$\rho\mathbf{a} = \operatorname{div}\sigma + \rho\mathbf{f} \quad \text{in} \quad B_t\,, \quad \mathbf{n}.\sigma = \mathbf{t} \quad \text{at} \quad \partial B_t\,, \tag{10.123}$$

wherein

$$\rho\mathbf{f} = \sum_\alpha \rho_\alpha \mathbf{f}, \quad \sigma := \sum_\alpha \sigma_\alpha = \sigma^T. \tag{10.124}$$

**NOTE 10.7.1:** Here, in the spirit of weak (or variational) formulations, the individual boundary conditions (10.122) follow in a straightforward manner, while in other approaches splitting the overall boundary condition in $(10.123)_2$ among the various constituents remains a tricky question (cf. Rajagopal and Tao, 1995).

**NOTE 10.7.2:** All conclusions drawn here might be consistently extended to higher-order gradient theories, provided that meaningful physical interpretation of additional boundary conditions can be taken for granted (cf. dell'Isola et al., 2000).

**NOTE 10.7.3:** If we further set

$$\bar{\sigma}_\alpha := \sigma_\alpha + \xi_\alpha \bar{\sigma}, \tag{10.125}$$

and

$$\rho_\alpha \bar{\mathbf{f}}_\alpha := \rho_\alpha \mathbf{f} + \rho_\alpha (\mathbf{a}_\alpha - \mathbf{a}) - \pi_\alpha - \operatorname{div}(\xi_\alpha \bar{\sigma}), \tag{10.126}$$

we can rewrite (10.121) and the total Cauchy stress as

$$\rho_\alpha \mathbf{a}_\alpha = \operatorname{div}\bar{\sigma}_\alpha + \rho_\alpha \bar{\mathbf{f}}_\alpha \tag{10.127}$$

and

$$\sigma = \sum_\alpha (\bar{\sigma}_\alpha - \xi_\alpha \bar{\sigma}). \tag{10.128}$$

### 10.7.5 Energy Equation in the Absence of Dissipation

In this case the total time derivative of the internal (or free) energy is balanced by the stress power, so that we can write

$$\frac{d}{dt}\int_{B_\tau} W dv\Big|_{\tau=t} = \sum_\alpha \int_{B_t} \left(\pi_\alpha . \mathbf{v}_\alpha + \sigma_{\alpha:} : \left(\nabla \mathbf{v}_\alpha\right)^T\right) dv. \tag{10.129}$$

This yields locally

$$\frac{dW}{dt} + W\left(\nabla . \mathbf{v}\right) = \sum_{\alpha=S,F} \left(\pi_\alpha . \mathbf{v}_\alpha + \sigma_\alpha : \left(\nabla \mathbf{v}_\alpha\right)^T\right). \tag{10.130}$$

We introduce the *partial* first Piola–Kirchhoff stresses $\mathbf{T}_\alpha$ by

$$\mathbf{T}_\alpha := J_S \mathbf{F}_S^{-1} . \sigma_\alpha . \tag{10.131}$$

That is, both are defined by means of the "solid" pull back. A consequence of this is that we can also rewrite (10.129) in the following form:

$$\frac{d}{dt}\int_{B_\tau *} J_S W dV\Big|_{\tau=t} = \sum_\alpha \int_{B_t *} \left(J_S \pi_\alpha . \mathbf{v}_\alpha + \mathbf{T}_\alpha : \left(\nabla_R \mathbf{v}_\alpha\right)^T\right) dV. \tag{10.132}$$

Bearing in mind the identity (10.97), we can define additionally the fields $\tau_\alpha$ and $\mathbf{b}_\alpha$ in such a way that we have the following identity for virtual velocity fields:

$$\begin{aligned} &\sum_\alpha \int_{B_t *} \left(J_S \pi_\alpha . \hat{\mathbf{v}}_\alpha + \mathbf{T}_\alpha : \left(\nabla_R \hat{\mathbf{v}}_\alpha\right)^T\right) dV + \int_{\partial B_t *} J_S W\left(\hat{\mathbf{V}} . \mathbf{N}\right) dV \\ &= \sum_\alpha \int_{B_t *} \left(\tau_\alpha . \hat{\mathbf{V}}_\alpha + \mathbf{b}_\alpha : \left(\nabla_R \hat{\mathbf{V}}_\alpha\right)^T\right) dV. \end{aligned} \tag{10.133}$$

Here, of course,

$$\hat{\mathbf{v}}_\alpha + \mathbf{F}_S . \hat{\mathbf{V}}_\alpha = \mathbf{0}, \qquad \hat{\mathbf{V}} = \xi_S \hat{\mathbf{V}}_S + \xi_F \hat{\mathbf{V}}_F . \tag{10.134}$$

From this we deduce the expression of the *peculiar Eshelby* (static) *stress tensors* as

$$\mathbf{b}_\alpha = \xi_\alpha J_S W \mathbf{1}_R - \mathbf{T}_\alpha . \mathbf{F}_S , \tag{10.135}$$

while the $\tau^{\alpha\prime}$s are given by

$$\tau_\alpha = \nabla_R\left(\xi_\alpha J_S W\right) - \mathbf{T}_\alpha : \left(\nabla_R \mathbf{F}_S\right)^T - J_S \mathbf{F}_S^T . \pi_\alpha . \tag{10.136}$$

It is again remarked that both solid and fluid Eshelby stresses are built uniquely with the "solid" pull back and an energy density in proportion to the relevant constituent (factor $\xi_\alpha$). Finally, to meet the symmetry requirement $(10.112)_2$, these Eshelby stresses have to respect the following symmetry:

$$\mathbf{C}_S . \left(\mathbf{b}_S + \mathbf{b}_F\right) = \left(\mathbf{b}_S + \mathbf{b}_F\right)^T . \mathbf{C}_S , \quad \mathbf{C}_S := \mathbf{F}_S^T . \mathbf{F}_S . \tag{10.137}$$

### 10.7.6 Constitutive Equations for Unconstrained Solid–Fluid Mixtures

To proceed toward a set of useful constitutive equations we must specify the functional dependency of the energy $W$. Let us assume for the sake of example that we are interested in a binary mixture made of a *materially inhomogeneous poroelastic solid* and a *compressible inviscid fluid*. It is natural, therefore, to consider an energy that depends on the elastic strain defined in $(10.137)_2$, on the fluid density $\rho_F$, and also explicitly on $\mathbf{X}$ because of the inhomogeneity property. Thus,

$$W = \bar{W}\left(\mathbf{F}_S(\mathbf{X},t), \rho_F(\mathbf{x},t), \mathbf{X}\right), \quad \mathbf{X} = \chi_S^{-1}(\mathbf{x},t). \tag{10.138}$$

Then we obtain from (10.132) the following constitutive prescriptions for the $\pi$-interaction forces:

$$\pi_S = \left(\xi_S - 1\right)\left(\nabla \mathbf{F}_S\right)^{T\cdot} . \frac{\partial \bar{W}}{\partial \mathbf{F}_S} + W \nabla \xi_S + \xi_S \frac{\partial \bar{W}}{\partial \rho_F} \nabla \rho_F + \left(\xi_S - 1\right) \mathbf{F}_S^{-T} . \left.\frac{\partial \bar{W}}{\partial \mathbf{X}}\right|_{\text{expl}}, \tag{10.139}$$

$$\pi_F = \xi_F \left(\nabla \mathbf{F}_S\right)^T \frac{\partial \bar{W}}{\partial \mathbf{F}_S} + W \nabla \xi_F + \left(\xi_F - 1\right) \frac{\partial \bar{W}}{\partial \rho_F} \nabla \rho_F + \xi_F \mathbf{F}_S^{-T} \left.\frac{\partial \bar{W}}{\partial \mathbf{X}}\right|_{\text{expl}}, \tag{10.140}$$

while for the $\sigma_\alpha$'s we have

$$\sigma_S = \xi_S W \mathbf{1} + \frac{\partial \bar{W}}{\partial \mathbf{F}_S} \mathbf{F}_S^T , \quad \sigma_F = -\left(\rho_F \frac{\partial \bar{W}}{\partial \rho_F} - \xi_F W\right)\mathbf{1}. \tag{10.141}$$

The symmetry of the total $\sigma$ results in

$$\sigma_S + \sigma_F = \frac{\partial \bar{W}}{\partial \mathbf{F}_S} \mathbf{F}_S^T + \rho_F \left(\frac{W}{\rho_F} - \frac{\partial \bar{W}}{\partial \rho_F}\right)\mathbf{1}_R. \tag{10.142}$$

Then (10.135) leads to the following straightforward expressions for the peculiar Eshelby stress tensors:

$$\mathbf{b}_S = -J_S \mathbf{F}_S^T \frac{\partial \bar{W}}{\partial \mathbf{F}_S}, \quad \mathbf{b}_F = J_S \rho_F \frac{\partial \bar{W}}{\partial \rho_F} \mathbf{1}_R. \tag{10.143}$$

Simultaneously, the π-interaction forces take on the following form:

$$\tau_S = J_S \frac{\partial \bar{W}}{\partial \mathbf{X}}\bigg|_{\text{expl}}, \quad \tau_F = \frac{\partial \bar{W}}{\partial \rho_F} \nabla_R \left( J_S \rho_F \right). \tag{10.144}$$

The expression (10.143) are of great interest, for they show that in the present formulation the partial Eshelby stresses take, up to a sign, the canonical form of stresses for an elastic solid and an inviscid fluid, respectively. This corroborates the importance of the role played by partial chemical potentials within the context of solid–fluid mixture theories (see Bowen, 1976, 1982).

### 10.7.7 Constitutive Equations for Saturated Porolastic Media

This case is mentioned for the sake of completeness. In this case, like other authors, we introduce the concept of *volume fractions* defined by the ratios

$$\nu_\alpha = \rho_\alpha / \hat{\rho}_\alpha, \tag{10.145}$$

where, in contrast to the constituent density $\rho_\alpha$, which may be considered *macroscopic*, $\hat{\rho}_\alpha$ may be called *microscopic* and assumed itself to depend on the usual state variables already introduced in (10.138), that is,

$$\hat{\rho}_\alpha \left( \mathbf{F}_S \left( \mathbf{X}, t \right), \rho_F \left( \mathbf{x}, t \right), \mathbf{X} \right), \ \mathbf{X} = \chi_S^{-1} \left( \mathbf{x}, t \right). \tag{10.146}$$

DEFINITION: A poroelastic solid infused by a compressible fluid is said to be *saturated* if the solid skeleton is perfectly permeated by the fluid. The corresponding constraint reads

$$\nu_S + \nu_F - 1 = 0. \tag{10.147}$$

Let $p$, the *saturation pressure*, be the Lagrange multiplier that will account for the mathematical constraint (10.147) so that we will augment $W$ to $W + p(\nu_S + \nu_F - 1)$. To proceed further one therefore needs to evaluate the various derivatives

of the $\nu_\alpha$ and $\hat{\rho}_\alpha$ functions mentioned in (10.146). In the absence of justified precise functions $\hat{\rho}_\alpha$, we refer the reader to the general results enunciated in Quiligotti, dell'Isola, et al. (2002). What must be retained from this is that the saturation pressure is the reactive action needed to maintain each constituent in contact with the other one, and it is distributed among the constituents proportionally to their volume fractions only if the latter are "microscopically" incompressible, that is, whenever the $\hat{\rho}_\alpha$ are independent of the macroscopic fluid density $\rho_F$ and of the gradient of the solid motion, $\mathbf{F}_S$. The reader will find in Quiligotti, Maugin, et al. (2002) a rather general treatment of bulk waves that can propagate in both unconstrained and saturated solid–fluid binary mixtures. Some of the Biot features are recovered and/or generalized. This is outside the scope of the present work, which intended rather to highlight any relationship to Eshelbian mechanics. What is clear in the preceding treatment is that the need to refer the active mechanical processes to a unique reference configuration imposes the choice of one configuration for the job. For this, it is more than natural to select that of the solid constituent in the binary mixtures of interest.

## 10.8 Single-Phase Transforming Crystal and Diffusion

### 10.8.1 Introductory Remark

As mentioned by Wu (2001), it may happen in metallurgy that when an inhomogeneous single-phase alloy is annealed, then matter flows in a manner that will decrease the concentration gradient $\nabla c$. The net flow will cease when the annealed specimen becomes homogeneous. In a somewhat standard small-strain description of this phenomenon, this should couple, although weakly, the conservation of mass written on account of *Fick's law* of diffusion with elasticity. It appears that while concentration contributes to the mechanical equilibrium equation via an *eigenstrain* linearly related to the concentration deviation from uniformity, the diffusion equation is practically independent of strains. This is a one-way coupling between composition $c$ and the elastic displacement $\mathbf{u}$ (see the introduction in Wu, 2001). An approximation of the same type often prevails in thermoelasticity, with temperature deviation replacing the concentration deviation. The present subject matter is revisited here in the finite-strain framework and in the light of the notion of configurational forces. We follow the works of a prominent contributor to this line (Wu, 2001, 2002).

### 10.8.2 Eigenstrains and Molar Concentrations

Remember that the configurational deformation of a single-phase mixture from a uniform reference state to a nonuniform state is characterized by

a so-called *eigentransformation* $\boldsymbol{F}_t$ that belongs to the general view of local structural rearrangements exposed in Chapter 6. This transformation brings an element of the global reference to a locally defined stress-free element according to $d\mathbf{X}^{SF} = \mathbf{F}_t.\ dX$. This is generally *incompatible* (see this concept in previous chapters). But $\mathbf{F}^e$, the elastic gradient (no longer compatible by itself), ties the stress-free (or "elastically released") element $dX^{SF}$ to the spatial differential element $d\mathbf{x}$ by $d\mathbf{X}^{SF} = \mathbf{F}_t\ \mathbf{F}^{-1}.d\mathbf{x}$, or by inversion

$$d\mathbf{x} = \mathbf{F}^e d\mathbf{X}^{SF}, \quad \mathbf{F}^e = \mathbf{F}\mathbf{F}_t^{-1} \quad \text{or} \quad \mathbf{F} = \mathbf{F}^e\mathbf{F}_t\ . \tag{10.148}$$

This is but one example of the multiplicative decomposition of finite strains mentioned in Chapter 6. But here the eigentransformation, which we already know to be related to the notion of the Eshelby stress tensor according to the general reasoning of Chapter 6, may be defined in terms of the underlying crystal structure and the experimentally measured molar volume of the mixture. Accordingly, we have to introduce some terminology of thermochemistry. Let the examined single-phase mixture of $N$ components be defined by $N$ molar concentrations noted $C_\alpha$ (in physical units of kmol/m$^3$) so that the total molar concentration (also called molar density) $C$ and the associated mole fractions $y_\alpha = C_\alpha/C$ satisfy the relations

$$C = \sum_{\alpha=1}^{N} C_\alpha, \quad \sum_{\alpha=1}^{N} y_\alpha = 1. \tag{10.149}$$

**REMARK:** The mole fractions $y_\alpha$ are noted $x_i$ in treatises on thermochemistry.

Only the first $N - 1$ molar fractions are independent according to the second of (10.149). They are globally referred to by the symbol $\underline{y}$. Let $\underline{V}\left(p,\theta,\underline{y}\right)$ be the molar volume (in m$^3$/kmol) of the mixture at pressure $p$ (in the reference configuration) and temperature $\theta$. This, according to specialists, is an important property that may be experimentally determined. The molar fraction $\underline{V}\left(0,\theta_0,\underline{y}_0\right)$ corresponds to a uniform state for the solid mixture occupying the material region $V$ in the reference configuration $K_R$ using coordinates X. As $\theta$ and/or $\underline{y}$ becomes non uniform in terms of X and time $t$, the molar fraction $\underline{V}\left(0,\theta,\underline{y}\right)$ may be used to compute the Jacobian $J_t$ of the eigentransformation $\mathbf{F}_t$ by

$$\begin{aligned} J_t\left(\mathbf{X},t\right) &= \underline{V}\left(0,\theta\left(\mathbf{X},t\right),\quad \underline{y}\left(\mathbf{X},t\right)\right)/\underline{V}\left(0,\theta_0,\underline{y}_0\right), \\ \mathbf{F}_t &= \left(J_t\right)^{1/3}\mathbf{F}_0\ , \quad \det\mathbf{F}_0 = 1, \end{aligned} \tag{10.150}$$

where $\mathbf{F}_0$ is a constant transformation that may be related to the underlying crystal structure of our mixture. Of course we accept the relation $dV^{SF} = J_t dV$,

and we can write the mixture property $\underline{V}$ in terms of the *partial molar volumes* $\bar{V}_\alpha\left(p,\theta,\underline{y}\right)$ by

$$\underline{V}\left(p,\theta,\underline{y}\right)=\sum_{\alpha=}^{N} y_\alpha \bar{V}_\alpha\left(p,\theta,\underline{y}\right),\quad \bar{V}_\alpha\left(p,\theta,\underline{y}\right)=\left.\frac{\partial\left(C\underline{V}\left(p,\theta,\underline{y}\right)\right)}{\partial C_\alpha}\right|_{p,\theta,C_{\beta\neq\alpha}}. \tag{10.151}$$

This relation can also be written down for $p = 0$.
This is complemented by setting

$$C=1/\underline{V}\left(0,\theta_0,\underline{y}_0\right),$$

so that $C$ is the constant number of moles per unit reference volume (this is the fixed number of substitutional sites per unit volume of the crystal structure). On account of this, molar densities can also be defined per unit volume of the actual configuration and of the elastically released *SF* configuration. Therefore, we can write

$$C=\sum_{\alpha=1}^{N} C_\alpha\left(\mathbf{X},t\right),\quad C^{SF}=\sum_{\alpha=1}^{N} C_\alpha^{SF}\left(\mathbf{X},t\right),\quad c=\sum_{\alpha=1}^{N} c_\alpha\left(\mathbf{x},t\right)=J_F^{-1}C. \tag{10.152}$$

The following relationships are easily established:

$$\begin{aligned} J_t &= dV^{SF}/dV = C/C^{SF}\left(\mathbf{X},t\right)=C_\alpha\left(\mathbf{X},t\right)/\,C_\alpha^{SF}\left(\mathbf{X},t\right),\\ J_F &= dv/dV = C/c\left(\mathbf{x},t\right)=C_\alpha\left(\mathbf{X},t\right)/c_\alpha\left(\mathbf{x},t\right),\\ J^e &= dv/dV^{SF} = C^{SF}\left(\mathbf{X},t\right)/c\left(\mathbf{x},t\right),\\ y_\alpha &= c_\alpha/c = C_\alpha/C = C_\alpha^{SF}\left(\mathbf{X},t\right)/c\left(\mathbf{x},t\right). \end{aligned} \tag{10.153}$$

### 10.8.3 Thermodynamic Equations

We write directly the local equations using material fields with the appropriate addition of terms due to diffusion (for details see Wu, 2001, 2002):

- Balance of species:

$$\left.\frac{\partial C_\alpha}{\partial t}\right|_{\mathbf{x}}+\nabla_R.\mathbf{J}_\alpha=0,\quad \alpha=1,\ldots,N \tag{10.154}$$

or globally

$$\left.\frac{\partial C}{\partial t}\right|_{\mathbf{x}} = 0 = -\sum_{\alpha=1}^{N} \nabla_R \cdot \mathbf{J}_\alpha \tag{10.155}$$

- Energy balance (theorem of "internal energy"):

$$\dot{E} = tr\left(\mathbf{T}.\dot{\mathbf{F}}\right) - \nabla_R.\mathbf{Q} - \sum_{\alpha=1}^{N} \nabla_R.\left(\bar{H}_\alpha \mathbf{J}_\alpha\right) \tag{10.156}$$

- Second law of thermodynamics:

$$\theta\dot{S} + \nabla_R.\mathbf{Q} - \theta^{-1}\mathbf{Q}.\nabla_R\theta + \sum_{\alpha=1}^{N} \theta\nabla_R.\left(\bar{S}_\alpha \mathbf{J}_\alpha\right) \geq 0 \tag{10.157}$$

Here $\bar{S}_\alpha$ is the partial molar entropy and $\bar{H}_\alpha$ is the partial molar internal energy. It is supposed that equilibrium $\mathrm{div}_R\mathbf{T} = \mathbf{0}$ is realized in the absence of body force and in the quasistatic approximation.

Introducing the Helmholtz free energy per unit reference volume by $W = E - \theta S$ and accounting for (10.156), we obtain the following expression for the *Clausius–Duhem inequality*:

$$\begin{aligned} &-\left(\dot{W} + S\dot{\theta}\right) + \mathrm{tr}\left(\mathbf{T}.\dot{\mathbf{F}}\right) + \sum_{\alpha=1}^{N} \bar{G}_\alpha \dot{C}_\alpha \\ &-\sum_{\alpha=1}^{N} \mathbf{J}_\alpha.\nabla_R\bar{G}_\alpha - \left(\theta^{-1}\mathbf{Q} + \sum_{\alpha=1}^{N} \bar{S}_\alpha \mathbf{J}_\alpha\right).\nabla_R\theta \geq 0, \end{aligned} \tag{10.158}$$

where $\bar{G}_\alpha = \bar{H}_\alpha - \theta\bar{S}_\alpha$ is the *partial molar Gibbs free energy* that satisfies the molar property (10.151). To exploit the inequality in (10.158) in the usual manner we may consider free energies $W$ depending on $\mathbf{F}$, $\theta$, and the $C_\alpha$'s. From this we deduce the constitutive equations

$$S = -\frac{\partial W}{\partial \theta}, \quad \mathbf{T} = \frac{\partial W}{\partial \mathbf{F}}, \quad \bar{G}_\alpha = \left.\frac{\partial\left(C\underline{G}\right)}{\partial C_\alpha}\right|_{\mathbf{T},\theta,C_{\beta\neq\alpha}} = \left.\frac{\partial W}{\partial C_\alpha}\right|_{\mathbf{F},\theta,C_{\beta\neq\alpha}}, \tag{10.159}$$

while there remains the following *dissipation inequality*:

$$-\sum_{\alpha=1}^{N}\mathbf{J}_\alpha.\nabla_R\bar{G}_\alpha-\theta^{-1}\left(\mathbf{Q}+\sum_{\alpha=1}^{N}\theta\bar{S}_\alpha\mathbf{J}_\alpha\right).\nabla_R\theta\geq 0. \tag{10.160}$$

This shows first that the real entropy flux (factor of $\nabla_R\theta$ up to a sign) in this diffusive mixture is not only the ratio of heat flux by temperature but it contains an additional contribution (extra entropy-flux; cf. Chapter 5) due to diffusion; second, heat conduction and diffusion are generally coupled effects. But here, for the sake of example, we consider isothermal conditions. Accordingly, a simple diffusion flux may be envisaged in the form

$$\mathbf{J}_\alpha=-M_\alpha C_\alpha\nabla_R\bar{G}_\alpha,\quad \alpha=1,2,...,N,\quad M_\alpha\geq 0, \tag{10.161}$$

where the nonnegative $M_\alpha$ is the molar mobility of component $\alpha$. Then the equations (10.154) yield

$$\frac{\partial C_\alpha}{\partial t}=\nabla_R.\left(M_\alpha C_\alpha\nabla_R\bar{G}_\alpha\right),\quad \alpha=1,2,...,N. \tag{10.162}$$

It remains to express diffusion in terms of the mole fractions. This is obtained by taking the time derivative of the second in the last line of (10.153) and then accounting for (10.162). This is not so much of interest for us here. Rather, we prefer to examine the following question.

### 10.8.4 Chemical Potential and Eshelby Stress

What we called *molar Gibbs energy* in the preceding is historically called *chemical potential*. That is, we indeed have with a more standard notation (cf. (10.159))

$$\mu_\alpha=\left.\frac{\partial W}{\partial C_\alpha}\right|_{\mathbf{F},\theta,C_{\beta\neq\alpha}}=\left.\frac{\partial\left(C\underline{G}\right)}{\partial C_\alpha}\right|_{\mathbf{T},\theta,C_{\beta\neq\alpha}}. \tag{10.163}$$

Thus we need to pay more attention to the expression of the free energy $W$. We can write it as

$$W\left(\mathbf{F},\theta,\underline{y}\right)=C\underline{W}\left(\mathbf{F},\theta,\underline{y}\right),\quad \mathbf{F}=\mathbf{F}^e\mathbf{F}_t, \tag{10.164}$$

where $\underline{W}$ is the molar Helmholtz free energy related to $\underline{G}$ by

$$\underline{W}\left(\mathbf{F},\theta,\underline{y}\right)=\underline{G}\left(\mathbf{T},\theta,\underline{y}\right)+tr\left(\mathbf{T}.\mathbf{F}\right). \tag{10.165}$$

This enjoys the following properties:

$$\underline{W}\left(\mathbf{0},\theta_0,\underline{y}_0\right)=0, \tag{10.166}$$

$$\underline{W}\left(\mathbf{F}_t,\theta,\underline{y}\right)=\underline{G}^{SF}\left(\theta,\underline{y}\right)=\underline{G}\left(\mathbf{T},\theta,\underline{y}\right)\Big|_{\mathbf{T}=\mathbf{0}}, \tag{10.167}$$

$$\underline{W}\left(\mathbf{F}^e\mathbf{F}_t,\theta,\underline{y}\right)=\underline{W}\left(\mathbf{F}_t,\theta,\underline{y}\right)+\underline{W}^{SF}\left(\mathbf{F}^e,\theta,\underline{y}\right). \tag{10.168}$$

The first of these fixes the uniform state as a reference. The second reflects the fact that $\mathbf{F}_t$ is the stress-free eigentransformation at temperature $\theta$ and composition $\underline{y}$. The last requires that

$$\underline{W}^{SF}\left(\mathbf{1},\theta,\underline{y}\right)=0.$$

Now (10.164) yields

$$W=CG^{SF}\left(\theta,\underline{y}\right)+J_tW^{SF}\left(\mathbf{F}^e,\theta,C_1^{SF},...,C_N^{SF}\right). \tag{10.169}$$

We can evaluate (10.163) by use of this. We obtain thus

$$\mu_\alpha=\mu_\alpha^{SF}+\frac{\partial}{\partial C_\alpha}\left(J_tW^{SF}\right),\quad \mu_\alpha^{SF}\equiv\bar{G}_\alpha^{SF},$$

or

$$\mu_\alpha=\mu_\alpha^{SF}+\frac{\partial J_t}{\partial C_\alpha}W^{SF}+\left(1-\frac{C_\alpha}{J_t}\frac{\partial J_t}{\partial C_\alpha}\right)\frac{\partial W^{SF}}{\partial C_\alpha^{SF}}+J_t\frac{\partial W^{SF}}{\partial\mathbf{F}_t}\frac{\partial\mathbf{F}_t}{\partial C_\alpha}. \tag{10.170}$$

But we can show that

$$J_t\frac{\partial W^{SF}}{\partial\mathbf{F}_t}\cdot\frac{\partial\mathbf{F}_t}{\partial C_\alpha}=J_t\,tr\left(\mathbf{F}_t^{-1}.\mathbf{b}_e.\frac{\partial\mathbf{F}_t}{\partial C_\alpha}\right)=tr\left(\mathbf{b}.\mathbf{F}_t^{-1}.\frac{\partial\mathbf{F}_t}{\partial C_\alpha}\right), \tag{10.171}$$

where we have introduced the following (quasistatic) Eshelby stresses:

$$\mathbf{b}_e := W^{SF}\mathbf{1} - \mathbf{T}^e.\mathbf{F}^e, \quad \mathbf{T}^e = \partial W^{SF}/\partial \mathbf{F}^e \tag{10.172}$$

and

$$\mathbf{b} := W\mathbf{1}_R - \mathbf{T}.\mathbf{F}, \quad \mathbf{T} = \partial\left(J_t W^{SF}\right)/\partial \mathbf{F}. \tag{10.173}$$

This establishes the relationship between the notions of chemical potential and Eshelby stress in the present setting. The results (10.170) through (10.173) are due to Wu (2002) in the perspective of treating bicrystal interfaces. This appears to open a path where finite deformation and atomic diffusion seem to merge in a unified theory (Wu, 2004). At this point we close our brief excursion in a difficult but promising field.

# 11

# *Electromagnetic Materials*

## Object of the Chapter

Where we see why Eshelby used the name "Maxwell elasticity stress" for what we now call Eshelby stress, and where a multifield theory exhibits in its splendor both the usefulness and ambiguity of the canonical formulation of momentum and energy, along with a rich field of applications in complex materials.

## 11.1 Maxwell Could Not Know Noether's Theorem but ...

### 11.1.1 The Notions of Maxwell Stress and Electromagnetic Momentum

Maxwell's equations in vacuum (in their *Heaviside* outfit) are composed of two groups, first the two equations

$$\nabla \times \mathbf{E} + \frac{1}{c}\frac{\partial \mathbf{B}}{\partial t} = \mathbf{0}, \quad \nabla.\mathbf{B} = 0, \tag{11.1}$$

which govern the electric field **E** and the magnetic induction **B**, and from which there exist the electromagnetic potentials (φ, A) such that

$$\mathbf{B} = \nabla \times \mathbf{A}, \quad \mathbf{E} = -\nabla\varphi - \frac{1}{c}\frac{\partial \mathbf{A}}{\partial t}, \tag{11.2}$$

where $c$ is the velocity of light in a vacuum. The second group of Maxwell's equations in a vacuum is given by

$$\nabla \times \mathbf{H} - \frac{1}{c}\frac{\partial \mathbf{D}}{\partial t} = \mathbf{0}, \quad \nabla.\mathbf{D} = 0, \tag{11.3}$$

where $\mathbf{H} = \mu_0^{-1}\mathbf{B}$ is the magnetic field and $\mathbf{D} = \varepsilon_0\mathbf{E}$ is the electric displacement. The vacuum magnetic permeability $\mu_0$ and the vacuum dielectric constant

$\varepsilon_0$ are such that $\mu_0\varepsilon_0 = c^{-2}$. In spite of the commonly used vocabulary, in the *field theory* of electromagnetism, the "fields" that appear, primarily in a Hamiltonian–Lagrangian formulation, are the potentials $(\varphi, \mathbf{A})$, so that the Lagrangian density per unit volume should read

$$L = \bar{L}\left(\varphi, \nabla\varphi, \frac{\partial\varphi}{\partial t}, \mathbf{A}, \nabla\mathbf{A}, \frac{\partial\mathbf{A}}{\partial t}\right) \tag{11.4}$$

for a "first-order gradient" theory. But electromagnetism is a gauge theory so that the zeroth-order gradients $(\varphi, \mathbf{A})$ themselves cannot appear as such, and the remaining space and time derivatives appear only in the form of the combinations (11.2) so that the true Lagrangian of electromagnetism in vacuum reads

$$L^{\text{emf}} = \frac{1}{2}\left(\mathbf{E}^2 - \mathbf{B}^2\right), \tag{11.5}$$

a form given—in appropriate electromagnetic units—by Waldemar Voigt (of crystal fame) and interpreted in mechanical terms as the difference between "kinetic" and "potential" energies. The remarkable results of Maxwell (obviously not written in the present formalism) are two *identities*, a *scalar* one and a *vectorial* one, respectively,

$$\frac{\partial}{\partial t}\frac{1}{2}\left(\mathbf{E}^2 + \mathbf{B}^2\right) - \nabla.\left(c\mathbf{E}\times\mathbf{H}\right) = 0 \tag{11.6}$$

and

$$\frac{\partial}{\partial t}\frac{\varepsilon_0}{c}(\mathbf{E}\times\mathbf{B}) - \nabla.\left(\mu_0^{-1}\mathbf{B}\otimes\mathbf{B} + \varepsilon_0\mathbf{E}\otimes\mathbf{E} - \frac{1}{2}(\mathbf{E}^2 + \mathbf{B}^2)\mathbf{1}\right) = \mathbf{0}, \tag{11.7}$$

which we nowadays identify as the local *conservation* of *energy* and a local *conservation of electromagnetic momentum*. We can rewrite (11.6) and (11.7) as

$$\frac{\partial H^{\text{emf}}}{\partial t} - \nabla.\mathbf{Q}^{\text{em}} = 0, \quad \frac{\partial\mathbf{P}^{\text{emf}}}{\partial t} - \operatorname{div}\mathbf{b}^{\text{emf}} = \mathbf{0}, \tag{11.8}$$

wherein

$$\begin{gathered} H^{\text{emf}} = \frac{1}{2}(\mathbf{E}^2 + \mathbf{B}^2), \quad \mathbf{Q}^{\text{em}} = c\mathbf{E}\times\mathbf{H}, \quad \mathbf{P}^{\text{emf}} = \frac{1}{c}\mathbf{D}\times\mathbf{B}, \\ \mathbf{b}^{\text{emf}} \equiv \mathbf{t}^{\text{emf}} = \mu_0^{-1}\mathbf{B}\otimes\mathbf{B} + \varepsilon_0\mathbf{E}\otimes\mathbf{E} - H^{\text{emf}}\mathbf{1}. \end{gathered} \tag{11.9}$$

Equations 11.6 and 11.7 are identities obtained by multiplying the basic equations (11.1) and (11.3) by appropriate factors and adding up the two results.

Nowadays, (11.6) is recognized as a degenerate form of the so-called *Poynting–Umov theorem* (in the absence of electricity conduction), and Equation 11.7 is a very special case of an identity that provides an expression for the so-called *ponderomotive force* (here in the absence of free charges, currents, magnetization, and electric polarization; see later on). Here $\mathbf{Q}^{\mathrm{em}} = c^2\mathbf{P}^{\mathrm{emf}}$. The tensor $\mathbf{t}^{\mathrm{emf}}$ is the so-called *Maxwell stress* tensor in a vacuum. But (11.6) and (11.7), in a modern view, express the invariance of the physical system of electromagnetic fields in a vacuum under time translation (parameter $t$ = Newtonian time) and space translations (parameters $\{x^i,\ i = 1,2,3\}$ = standard Euclidean coordinates). It is readily checked that (11.8) would follow from the application of Noether's theorem to the Lagrangian (11.5). Hence $(11.8)_2$ is the balance of *canonical momentum*, a concept that exists in all field theories. Now we unhesitatingly understand why Eshelby first referred to his tensor **b** as the *Maxwell stress tensor of elasticity*. Note that in the preceding there are no ambiguities between the fields (electromagnetic potentials) and the space-parametrization. The case of electromagnetic fields in matter is a much more complicated affair that, even until now, offers no unique solution because there exists in principle a multiplicity of generalizations of (11.7) with different nonzero right-hand sides (see, e.g., Trimarco and Maugin, 2001).

### 11.1.2 Lorentz Force on a Point Charge

Equation 11.7 or $11.8_2$ shows that a linear momentum may be attributed to the electromagnetic field in fact only when both electric and magnetic fields coexist, that is, in the framework of true *electrodynamics*. What about the interaction with more standard mechanics? The simplest relevant problem is that of a point electric charge $q$ of mass $m_0$ acted on by an electromagnetic field. According to H.A. Lorentz (1853–1928) the force exerted on this point particle is given by

$$\mathbf{f}^e(\mathbf{x},t;q) = q\bar{\mathbf{E}}, \quad \bar{\mathbf{E}}(\mathbf{x},t) = \mathbf{E}(\mathbf{x},t) + \frac{1}{c}\dot{\mathbf{x}} \times \mathbf{B}(\mathbf{x},t), \tag{11.10}$$

where $\bar{\mathbf{E}}$, called the *electromotive intensity*, is none other than the electric field in the frame of the moving point (at velocity $\dot{\mathbf{x}}$). Newton's motion equation for $m_0$ therefore reads

$$\frac{d}{dt}(m_0\mathbf{v}) = q\bar{\mathbf{E}}, \quad \mathbf{v} = \dot{\mathbf{x}}. \tag{11.11}$$

On substituting from $(11.10)_2$ and the representations (11.2) that are valid since the equations (11.1) are valid everywhere, we can rewrite (11.11) as

$$\frac{d}{dt}\mathbf{p}^t = -q\nabla\varphi + \frac{q}{c}(\nabla\mathbf{A}).\mathbf{v}, \tag{11.12}$$

an equation that is derivable as the Euler–Lagrange equation deduced from the Lagrangian

$$L = \bar{L}(\mathbf{v}, \varphi, \mathbf{A}) = \frac{1}{2} m_0 \mathbf{v}^2 - q\varphi(\mathbf{x}, t) + \frac{q}{c} \mathbf{v}.\mathbf{A}(\mathbf{x}, t), \tag{11.13}$$

such that the total linear momentum is given by

$$\mathbf{p}^t = \frac{\partial \bar{L}}{\partial \mathbf{v}} = m_0 \mathbf{v} + \frac{q}{c} \mathbf{A}, \tag{11.14}$$

thus combining both mechanical and electromagnetic parts. The same property, but in a much more complex form, will appear in an electromagnetic *continuum* with a possible distinction between material and spatial coordinates, so that *both* physical *and* material electromagnetic linear momenta may be present. As we shall see, the latter is not necessarily the pulled back of the former on the material manifold.

## 11.2 Electromagnetic Fields in Deformable Continuous Matter

While referring to specialized treatises such as Eringen and Nelson (1979), Maugin (1988), and Maugin (1990), we first emphasize the used notation. The fields noted **E**, **B**, **D**, **H**, **P**, and **M** are the usual electromagnetic fields (electric field, magnetic induction, electric displacement, magnetic field, electric polarization, and magnetization, the latter two per unit volume of the actual configuration $K_t$) as measured in a fixed laboratory frame $R_L$ at time $t$. The same quantities with a superimposed bar are measured in a frame $R_C(\mathbf{x},t)$ comoving with the element of matter, still in the actual configuration; the already introduced electromotive intensity is such a quantity. The same quantities with a superimposed hat (caret), for example, $\hat{\mathbf{E}}$, will be the corresponding properly defined *material* fields. Here there is a remarkable property: While physical space is neutral from that viewpoint (being equipped with a Euclidean metric always reducible to a diagonal one with units), the material manifold will automatically (if we may say so) make a distinction between vector and covectors, essentially according to whether, in vectorial analysis, we take their divergence or their curl, and this should be obvious from the very form of Maxwell's equations, which must remain form-invariant in the Piola–Kirchhoff transformation of the various geometric objects (fields). The presentation here is not relativistic, a

so-called Galilean formulation of electrodynamics being sufficient for our present purpose with engineering applications (aficionados and true amateurs may find a concise relativistic invariant formulation in Chapter 16 of Eringen and Maugin [1990] and in works by the present author, e.g., Maugin [1978a, 1978b]).

### 11.2.1 Maxwell's Equations in General Matter in $R_L$

In so-called Lorentz–Heaviside units (neither factor $4\pi$ nor $\mu_0$ and $\varepsilon_0$), with $\mathbf{D} = \mathbf{E} + \mathbf{P}$ and $\mathbf{H} = \mathbf{B} - \mathbf{M}$, Maxwell's equations at spatial point $(\mathbf{x},t)$ read

$$\nabla \times \mathbf{E} + \frac{1}{c}\frac{\partial \mathbf{B}}{\partial t}\bigg|_x = \mathbf{0}, \quad \nabla.\mathbf{B} = 0, \tag{11.15}$$

and

$$\nabla \times \mathbf{H} - \frac{1}{c}\frac{\partial \mathbf{D}}{\partial t}\bigg|_x = \frac{1}{c}\mathbf{J}, \quad \nabla.\mathbf{D} = q_f, \tag{11.16}$$

where $\mathbf{J}$ is the electric current vector and $qf$ is the density of free electric charges. By taking the divergence of the first of (11.16), we have the conservation of electric charges as

$$\frac{\partial q_f}{\partial t}\bigg|_x + \nabla.\mathbf{J} = 0, \tag{11.17}$$

while on taking the divergence of the first of (11.15), we find that if the second of (11.15) holds initially, then it holds in time. Note that the time derivatives involved in (11.15) through (11.17) are Eulerian time derivatives from the point of view of continuum mechanics.

### 11.2.2 Maxwell's Equations in Terms of Comoving Field in $R_C(\mathbf{x},t)$

We define the following fields in $R_C(\mathbf{x},t)$:

$$\bar{\mathbf{E}} = \mathbf{E} + \frac{1}{c}\mathbf{v} \times \mathbf{B}, \quad \bar{\mathbf{D}} = \bar{\mathbf{E}} + \bar{\mathbf{P}}, \quad \bar{\mathbf{P}} = \mathbf{P} \tag{11.18a}$$

and

$$\begin{aligned} &\bar{\mathbf{B}} = \mathbf{B} - \frac{1}{c}\mathbf{v} \times \mathbf{E}, \quad \bar{\mathbf{H}} = \mathbf{H} - \frac{1}{c}\mathbf{v} \times \mathbf{D} = \bar{\mathbf{B}} - \bar{\mathbf{M}}, \\ &\bar{\mathbf{M}} = \mathbf{M} + \frac{1}{c}\mathbf{v} \times \mathbf{P}, \quad \bar{\mathbf{J}} = \mathbf{J} - q_f \mathbf{v}. \end{aligned} \tag{11.18b}$$

These would be "Galilean" transformations if it weren't for the fact that **v** is *not* a uniform velocity. The lack of symmetry between the transformations for the fields **P** and **M** kindled research into special relativity (Lorentz invariance) early in the twentieth century. Here $\bar{\mathbf{J}}$ is the so-called *conduction current* since the convection current has been subtracted from **J**.

We let the reader check by way of exercise that (11.15) and (11.16) transform to the following set:

$$\nabla \times \bar{\mathbf{E}} + \frac{1}{c}\mathbf{B}^* = \mathbf{0}, \quad \nabla.\mathbf{B} = 0 \tag{11.19}$$

and

$$\nabla \times \bar{\mathbf{H}} - \frac{1}{c}\mathbf{D}^* = \bar{\mathbf{J}}, \quad \nabla.\mathbf{D} = q_f. \tag{11.20}$$

This somewhat strange formulation involves fields in **both** $R_L$ and $R_C(\mathbf{x},t)$. Here the asterisk indicates a so-called *convected time derivative* defined for any vector $\mathbf{M}(\mathbf{x},t)$ by

$$\mathbf{M}^* := \left.\frac{\partial \mathbf{M}}{\partial t}\right|_x + \nabla \times (\mathbf{M} \times \mathbf{v}) + \mathbf{v}(\nabla.\mathbf{M}) = \left.\frac{\partial \mathbf{M}}{\partial t}\right|_X - (\nabla \mathbf{v}).\mathbf{M} + \mathbf{M}(\nabla.\mathbf{v}). \tag{11.21}$$

The importance of this type of derivative (essentially a *Lie derivative*) will soon appear.

### 11.2.3 Maxwell's Equations in the Material Framework

We introduce the material electromagnetic fields by (cf. Maugin, 1988)

$$\hat{\mathbf{B}} = J_F \mathbf{F}^{-1}.\bar{\mathbf{B}}, \quad \hat{\mathbf{E}} = \mathbf{E}.\mathbf{F} - \frac{1}{c}\mathbf{V} \times \hat{\mathbf{B}}, \quad \hat{\mathbf{D}} = J_F \mathbf{F}^{-1}.\mathbf{D}, \quad \hat{\mathbf{H}} = \mathbf{H}.\mathbf{F} + \frac{1}{c}\mathbf{V} \times \hat{\mathbf{D}}, \tag{11.22}$$

and

$$\Pi \equiv \hat{\mathbf{P}} = J_F \mathbf{F}^{-1}.\mathbf{P}, \quad \hat{\mathbf{M}} = \bar{\mathbf{M}}.\mathbf{F}, \quad \bar{Q}_f = J_F q_f, \quad \hat{\mathbf{J}} = J_F \mathbf{F}^{-1}.\bar{\mathbf{J}}, \tag{11.23}$$

where **V** is the true material velocity (based on the inverse motion) introduced in Chapter 2. Of course, some of these, if not all, are in fact *Piola transformations* (compare to (2.29)). In such a transformation we ask the reader to check that the following holds true, for example,

$$\Pi = J_F \mathbf{F}^{-1}.\mathbf{P} \Rightarrow \left.\frac{\partial \Pi}{\partial t}\right|_X = J_F \mathbf{F}^{-1}.\mathbf{P}^*. \tag{11.24}$$

On account of the definitions (11.22) and (11.23) and the reciprocal of (11.24), the following form of Maxwell's equations is easily established:

$$\nabla_R \times \hat{\mathbf{E}} + \frac{1}{c}\frac{\partial \hat{\mathbf{B}}}{\partial t}\bigg|_X = \mathbf{0}, \quad \nabla_R . \hat{\mathbf{B}} = 0 \tag{11.25}$$

and

$$\nabla_R \times \hat{\mathbf{H}} - \frac{1}{c}\frac{\partial \hat{\mathbf{D}}}{\partial t}\bigg|_X = \frac{1}{c}\hat{\mathbf{J}}, \quad \nabla_R . \hat{\mathbf{D}} = \hat{Q}_f . \tag{11.26}$$

These are formally identical to (11.15) and (11.16) but written with purely material fields and the (**X**,*t*) space–time parametrization. The usual relations $\mathbf{D} = \mathbf{E} + \mathbf{P}$ and $\mathbf{H} = \mathbf{B} - \mathbf{M}$ translate to the material framework as

$$\hat{\mathbf{D}} = J_F \mathbf{C}^{-1} . \tilde{\mathbf{E}} + \hat{\mathbf{P}}, \quad \hat{\mathbf{H}} = J_F^{-1} \mathbf{C} . \hat{\mathbf{B}} - \hat{\mathbf{M}}, \quad \left(\tilde{\mathbf{E}} \equiv \mathbf{E} . \mathbf{F}\right).$$

To our knowledge the first formulation of the type of (11.25) and (11.26)—but in statics—was given by Walker et al. (1965); McCarthy (1968) also contributed, but the final results is due to Lax and Nelson (1976; also Nelson, 1979). In particular, (11.25), just like (11.15), suggests that there exist "material" electromagnetic potentials $\hat{\varphi}$ and $\hat{\mathbf{A}}$ such that

$$\hat{\varphi} = \varphi - \mathbf{v} . \mathbf{A}, \quad \hat{\mathbf{A}} = \mathbf{F}^T . \mathbf{A} \tag{11.27}$$

and reciprocally

$$\varphi = \hat{\varphi} - \mathbf{V} . \hat{\mathbf{A}}, \quad \mathbf{A} = \mathbf{F}^{-T} . \hat{\mathbf{A}} \tag{11.28}$$

while the two parts of (11.26) yield the conservation of charges in the form

$$\frac{\partial \hat{Q}_f}{\partial t}\bigg|_X + \nabla_R . \hat{\mathbf{J}} = 0. \tag{11.29}$$

### 11.2.4 Ponderomotive Force and Electromagnetic Stresses and Momentum

Now we should enunciate the generalization of (11.10) to the case of a general *continuum* that may present a density of free charges, may conduct

electricity, and may be both magnetized and electrically polarized. This is often referred to as evaluating the so-called *ponderomotive force*, and the concomitant *ponderomotive couple* and expense of energy. These much-looked-for expressions are sometimes postulated as materializing the result of macroscopic experimental results. A deeper physical approach consists in averaging over a volume, or more subtly in phase space, the action of Lorentz forces (11.10) acting on a stable cloud of electric particles in motion and defining during this procedure the macroscopic fields $q_f$, $\bar{\mathbf{J}}$, $\mathbf{P}$, and $\mathbf{M}$ in terms of microscopic entities. This was achieved within the framework of relativistic statistical physics by de Groot and Suttorp (1972), and in classical physics (using volume averages) by Dixon and Eringen (1965) and then Maugin and Eringen (1977) in its final form. The ponderomotive force thus obtained per unit volume of $K_t$ reads (in the absence of electric conduction)

$$\mathbf{f}^{\text{em}} = q_f \bar{\mathbf{E}} + \frac{1}{c}\mathbf{P}^* \times \mathbf{B} + (\mathbf{P}.\nabla)\bar{\mathbf{E}} + (\nabla \mathbf{B}).\bar{\mathbf{M}}, \tag{11.30}$$

which written entirely in terms of fields in $R_L$ yields the highly farfetched expression

$$\mathbf{f}^{\text{em}} = q_f \mathbf{E} + \frac{1}{c}(q_f \mathbf{v}) \times \mathbf{B} + (\nabla \mathbf{E}).\mathbf{P} + (\nabla \mathbf{B}).\mathbf{M} + \frac{\rho}{c}\frac{d}{dt}\left(\frac{\mathbf{P} \times \mathbf{B}}{\rho}\right). \tag{11.31}$$

These are entirely equivalent, but the former is more condensed, while the latter shows a greater symmetry in polarization and magnetization effects (electric conduction can be added by replacing $\mathbf{P}^*$ by $\mathbf{P}^* + \bar{\mathbf{J}}$ and $q_f\mathbf{v}$ by $\mathbf{J}$, respectively, in (11.30) and (11.31)), while the last contribution in (11.31) hints at the existence of an electromagnetic linear momentum. In this line of thought, however, we have the following results of Collet and Maugin (1974):

A nonsymmetric electromagnetic stress in matter $\mathbf{t}^{\text{em}}$, an electromagnetic linear momentum $\mathbf{p}^{\text{em}}$, a Maxwell free-field symmetric stress $\mathbf{t}^f$, and a nonsymmetric interaction stress $\mathbf{t}^{\text{inter}}$ can be introduced in such a way that from (11.30) or (11.31), there follow these identities:

$$\mathbf{f}^{\text{em}} = \text{div } \mathbf{t}^{\text{em}} - \frac{\partial}{\partial t}\mathbf{p}^{\text{em}} = \left(\text{div } \mathbf{t}^f - \frac{\partial}{\partial t}\mathbf{p}^f\right) + \text{div } \mathbf{t}^{\text{inter}},$$

$$(\mathbf{t}^{\text{inter}})_A = -\mathbf{c}^{\text{em}}, \quad \mathbf{p}^f = \mathbf{p}^{\text{em}}, \tag{11.32}$$

where $\mathbf{c}^{\text{em}}$ is the *torque* (skew tensor) exerted by the electromagnetic fields on matter, per unit volume, evaluated simultaneously with the force (11.30). We have defined the following quantities:

$$\mathbf{t}^f = \mathbf{E} \otimes \mathbf{E} + \mathbf{B} \otimes \mathbf{B} - \frac{1}{2}(\mathbf{E}^2 + \mathbf{B}^2)\mathbf{1}, \quad \mathbf{p}^f = \frac{1}{c}\mathbf{E} \times \mathbf{B}, \tag{11.33}$$

$$\mathbf{t}^{\text{inter}} = \mathbf{P} \otimes \bar{\mathbf{E}} - \mathbf{B} \otimes \bar{\mathbf{M}} + \left(\bar{\mathbf{M}}.\mathbf{B}\right)\mathbf{1}. \tag{11.34}$$

In a vacuum,

$$q_f = 0, \quad \mathbf{P} \equiv \mathbf{0}, \quad \mathbf{M} \equiv \mathbf{0}, \quad \mathbf{t}^{\text{inter}} \equiv \mathbf{0} \tag{11.35}$$

and the identity (11.32) reduces to (11.7) up to the system of electromagnetic units.

### 11.2.5 Equations of Motion in Cauchy Format

Classical continua responding to general electromagnetic effects such as those introduced in foregoing paragraphs are *generalized continua* in the sense that they are a priori endowed with a *nonsymmetric* Cauchy stress. The only changes compared to the local equations (2.81b) and (2.82) in the Cauchy format are that these are replaced by

$$\frac{\partial}{\partial t}\mathbf{p}\Big|_x + \nabla.\left(\mathbf{p} \otimes \mathbf{v} - \boldsymbol{\sigma}\right) = \rho\mathbf{f} + \mathbf{f}^{\text{em}}, \tag{11.36}$$

$$\boldsymbol{\sigma}_A \equiv \frac{1}{2}\left(\boldsymbol{\sigma} - \boldsymbol{\sigma}^T\right) = \mathbf{c}^{\text{em}}. \tag{11.37}$$

On account of the identities (11.32), we can also introduce a total linear physical momentum $\mathbf{P}^{\text{tot}}$ and a new (symmetric) stress tensor $\mathbf{t}^E$ such that

$$\mathbf{p}^{\text{tot}} = \mathbf{p} + \mathbf{p}^f, \quad \mathbf{t}^E = \boldsymbol{\sigma} + \mathbf{t}^{\text{inter}}. \tag{11.38}$$

Equations 11.36 and 11.37 are then rewritten as

$$\frac{\partial}{\partial t}\mathbf{p}^{\text{tot}}\Big|_x + \nabla.\left(\mathbf{p} \otimes \mathbf{v} - \left(\mathbf{t}^E + \mathbf{t}^f\right)\right) = \rho\mathbf{f}, \quad \left(\mathbf{t}^E\right)_A \equiv \mathbf{0}. \tag{11.39}$$

This is a most interesting formulation because only *symmetric* stresses are now involved just like in a classical continuum. Apparently, neither magnetization nor electric polarization is involved here. But this is only apparent, first of all because the accompanying boundary value problem still involves the initial Cauchy stress. Second, magnetization and electric polarization are hidden in the functional dependence of the strain energy function via $\mathbf{t}^E$, and this will yield the most interesting electro- and magneto-mechanical couplings such as piezoelectricity, electrostriction, and magnetostriction. Of course, energy arguments should be developed in parallel with the equations

of motion, in particular on account of an electromagnetic energy source that is evaluated together with the ponderomotive force and couple (cf. Maugin and Eringen, 1977). However, we do not need this for the moment.

### 11.2.6 Equations of Motion in Piola–Kirchhoff Format

We can introduce first Piola–Kirchhoff stresses associated with $\mathbf{t}^E$ and $\mathbf{t}^f$ and the Piola transform of $\mathbf{P}^f$ by

$$\mathbf{T}^E = J_F \mathbf{F}^{-1}.\mathbf{t}^E, \quad \mathbf{T}^f = J_F \mathbf{F}^{-1}.\mathbf{t}^f, \quad \hat{\mathbf{p}}^f = J_F \mathbf{F}^{-1}.\mathbf{p}^f, \tag{11.40}$$

so that just like in pure elasticity, by multiplying (11.39) by $J_F$ and doing some manipulations, we obtain the Piola–Kirchhoff form of the local balance of physical momentum at any regular material point $\mathbf{X}$ as

$$\left.\frac{\partial}{\partial t}\mathbf{p}_R^{\text{tot}}\right|_X - \text{div}_R\left(\mathbf{T}^E + \mathbf{T}^F + \hat{\mathbf{p}}^f \otimes \mathbf{v}\right) = \rho_0 \mathbf{f}, \tag{11.41}$$

while the symmetry of $\mathbf{T}^E$ with respect to $\mathbf{F}$ replaces the local balance of angular momentum, that is,

$$\mathbf{T}^E\mathbf{F} = \mathbf{F}^T\left(\mathbf{T}^E\right)^T, \tag{11.42}$$

and we have set

$$\mathbf{p}_R^{\text{tot}} = \rho_0\left(\mathbf{v} + \frac{1}{c}\frac{\mathbf{E}\times\mathbf{B}}{\rho}\right). \tag{11.43}$$

Maxwell's equations are already entirely written in the material framework, viz. (11.25) and (11.26). What about the canonical projection of (11.41) on the material manifold? If we were to pursue the same line of approach to canonical momentum as in Section 3.1, that is, through a straightforward but obviously now very cumbersome computation, we would apply $\mathbf{F}$ to the right of (11.41) and apply the possible commutations with space and time derivatives. We shall not do that and rather content ourselves with the nondissipative case by examining variational formulations of the electrodynamics of continua and their consequences insofar as canonical conservation laws are concerned. Of course, the cases of *quasielectrostatics* or *quasimagnetostatics*, the two most relevant cases for engineering applications (except for high-frequency waves) are much simpler in that (11.41) then reduces to

$$\text{div}_R\left(\mathbf{T}^E + \mathbf{T}^f\right) + \rho_0 \mathbf{f} = \mathbf{0}, \tag{11.44}$$

where, usually, either electric polarization or magnetization alone is present.

## 11.3 Variational Principle Based on the Direct Motion

### 11.3.1 Prerequisite

Before considering the case of full matter, let us consider the case where the Lagrangian is none other than the one usually considered in vacuum but now written per unit volume of matter, that is, a simple Lagrangian expressed on the basis of (11.5), which we write first as

$$L_0^{\text{emf}}\left(\mathbf{E},\mathbf{B}\right)=\frac{1}{2}\left(\mathbf{E}^2-\mathbf{B}^2\right), \tag{11.45}$$

per unit of actual volume in $K_t$. Per unit of undeformed volume this yields

$$L_R^{\text{emf}}\left(\mathbf{E},\mathbf{B};\mathbf{F}\right)=J_F L_0^{\text{emf}}. \tag{11.46}$$

Recalling that, or setting,

$$\tilde{\mathbf{E}}:=\mathbf{E}.\mathbf{F},\quad \tilde{\mathbf{B}}\equiv J_F\mathbf{F}^{-1}.\mathbf{B}, \tag{11.47}$$

this yields

$$L_R^{\text{emf}}=\frac{1}{2}J_F\tilde{\mathbf{E}}.\mathbf{C}^{-1}.\tilde{\mathbf{E}}-\frac{1}{2}J_F^{-1}\tilde{\mathbf{B}}.\mathbf{C}.\tilde{\mathbf{B}}, \tag{11.48}$$

an expression obtained by Nelson (1979) up to the notation. This expression tells us how $L_R^{\text{emf}}$ depends on the deformation gradient. Of course, this function cannot depend explicitly on $\mathbf{X}$. In particular, for *quasielectrostatics*, there remains only the first contribution in the right-hand side of (11.48), and Maugin and Epstein (1991) have proved that computing the material gradient of $L_R^{\text{emf}}$, one obtains the following identity:

$$\nabla_R L_R^{\text{emf}}-\text{div}_R\left(\frac{\partial L_R^{\text{emf}}}{\partial\mathbf{F}}.\mathbf{F}\right)=\text{div}_R\left(L_R^{\text{emf}}\mathbf{1}_R-\frac{\partial L_R^{\text{emf}}}{\partial\mathbf{F}}\mathbf{F}\right)\equiv\mathbf{0}. \tag{11.49}$$

This means that the material divergence of the Eshelby stress tensor of *free* electromagnetic fields is not balanced by any material force (inhomogeneity force). This is checked directly by computing the following two quantities:

$$\frac{\partial}{\partial X^K}\left(\frac{1}{2}J_F\mathbf{E}^2\right),\quad \frac{\partial}{\partial X^I}\left(\frac{\partial\left(J_F L_0^{\text{emf}}\right)}{\partial F_I^i}F_{.K}^i\right),$$

and subtracting the second result from the first. The following more general result can be checked (full dynamic electromagnetic case):

$$\frac{\partial}{\partial t}\mathbf{P}^{\mathrm{emf}}\Big|_{X} - \mathrm{div}_R\,\mathbf{b}^{\mathrm{emf}} \equiv \mathbf{0}, \tag{11.50}$$

where

$$\mathbf{P}^{\mathrm{emf}} := \frac{\partial L_R^{\mathrm{emf}}}{\partial \mathbf{V}}, \quad \mathbf{b}^{\mathrm{emf}} = -\left(L_R^{\mathrm{emf}}\mathbf{1}_R + \mathbf{T}^{\mathrm{emf}}\mathbf{F}\right), \quad \mathbf{T}^{\mathrm{emf}} := -\frac{\partial L_R^{\mathrm{emf}}}{\partial \mathbf{F}}. \tag{11.51}$$

In plain words, *free* electromagnetic fields do *not*, by themselves, develop any inhomogeneity force. This property encapsulates the essential difference in nature between the pervasive *pure field* contributions and those that pertain to true *material* fields (e.g., magnetization and electric polarization). Accordingly, the usual Maxwell stress tensor introduced in (11.9) cannot contribute to the balance of material momentum. Along the same line, the electromagnetic material momentum has to be different from the pull back of the electromagnetic momentum in vacuum.

Another prerequisite concerns the fact that the first group of Maxwell's equations—say (11.15) or (11.25)—is automatically taken care of by the introduction of the electromagnetic potentials. Thus a variational formulation will necessarily involve independent variations of $\hat{\varphi}$ and $\hat{\mathbf{A}}$ and either material or Eulerian variations of the motion. Accordingly, for the whole system consisting of matter *plus* electromagnetic fields, we may have to consider Lagrangian densities such as

$$L = L_R^{\mathrm{emf}}\left(\tilde{\mathbf{E}},\tilde{\mathbf{B}},\mathbf{F},\mathbf{V}\right) + L^{\mathrm{md}}\left(\mathbf{v},\mathbf{F},\tilde{\mathbf{E}},\tilde{\mathbf{B}};\mathbf{X}\right) \tag{11.52}$$

for a Lagrangian per unit volume in $K_R$ and a direct-motion description, and

$$\breve{L} = J_F^{-1}L = J_F^{-1}\left[L_R^{\mathrm{emf}} + L^{\mathrm{mi}}\left(\mathbf{V},\mathbf{F}^{-1},\tilde{\mathbf{E}},\tilde{\mathbf{B}};\mathbf{X}\right)\right] \tag{11.53}$$

for a Lagrangian per unit volume of $K_t$ and an inverse-motion description, where

$$L^{\mathrm{md}} = \frac{1}{2}\rho_0(\mathbf{X})\mathbf{v}^2 - W\left(\mathbf{F},\tilde{\mathbf{E}},\tilde{\mathbf{B}};\mathbf{X}\right) \tag{11.54}$$

and

$$L^{\mathrm{mi}} = \frac{1}{2}\rho_0(\mathbf{X})\mathbf{V}.\mathbf{C}.\mathbf{V} - \bar{W}\left(\mathbf{F}^{-1},\tilde{\mathbf{E}},\tilde{\mathbf{B}};\mathbf{X}\right). \tag{11.55}$$

It is understood that the local interactions of matter and electromagnetic fields, which give rise to magnetization and electric polarization, are contained in $W$ or $\bar{W}$, from which we shall derive these notions.

### 11.3.2 The Variational Principle Per Se

The Hamiltonian action considered reads

$$A\{\chi;\mathbf{E},\mathbf{B}\}=\int_t dt\int_{B_R}\left(L_R^{\text{emf}}+L^{\text{md}}\right)dV. \tag{11.56}$$

Then we have the following fundamental results (Maugin, 1990; Maugin, Epstein, et al., 1992b; Maugin, Epstein et al., 1992a, 1992b):

**THEOREM 11.1:** From a material variation accompanied by proper variations of the electromagnetic potentials of the action (11.56), there follows the second group of Maxwell's equations (11.26) in the absence of electricity conduction, the equation of motion (11.39) in the absence of body force, and the general constitutive equations

$$\mathbf{T}^E=\frac{\partial W}{\partial \mathbf{F}},\quad \Pi=-\frac{\partial W}{\partial \tilde{\mathbf{E}}},\quad \hat{\mathbf{M}}=-\frac{\partial W}{\partial \tilde{\mathbf{B}}} \tag{11.57}$$

with the

**COROLLARY 11.2:** By applying Noether's theorem to (11.56) for material space translations $\mathbf{X}$, we obtain the balance of material momentum for the system matter *plus* field in matter as

$$\left.\frac{\partial \mathbf{P}^{\text{tot}}}{\partial t}\right|_X-\text{div}_R\,\mathbf{b}^{\text{tot}}=\mathbf{f}^{\text{inh}}, \tag{11.58}$$

where we have defined the following entities:

$$\mathbf{P}^{\text{tot}}=\mathbf{P}^{\text{mech}}+\mathbf{P}^{\text{emm}},\quad \mathbf{P}^{\text{mech}}=\rho_0\mathbf{C}.\mathbf{V},\quad \mathbf{P}^{\text{emm}}=\frac{1}{c}\Pi\times\mathbf{B}, \tag{11.59}$$

$$\mathbf{b}^{\text{tot}}=-\left(L^{\text{md}}\mathbf{1}_R+\mathbf{S}.\mathbf{C}\right), \tag{11.60}$$

where

$$\mathbf{S}=\mathbf{S}^E-\left(\mathbf{C}^{-1}.\tilde{\mathbf{E}}\right)\otimes\Pi+\left(\mathbf{C}^{-1}.\hat{\mathbf{M}}\right)\otimes\tilde{\mathbf{B}}-\left(\hat{\mathbf{M}}.\tilde{\mathbf{B}}\right)\mathbf{1}_R, \tag{11.61}$$

and

$$\mathbf{S}^E=2\frac{\partial W}{\partial \mathbf{C}},\quad \Pi=-\frac{\partial W}{\partial \tilde{\mathbf{E}}},\quad \hat{\mathbf{M}}=-\frac{\partial W}{\partial \tilde{\mathbf{B}}},\quad W=W\left(\mathbf{C},\tilde{\mathbf{E}},\tilde{\mathbf{B}};\mathbf{X}\right), \tag{11.62}$$

$$\mathbf{f}^{\text{inh}} = \left.\frac{\partial L^{\text{md}}}{\partial \mathbf{X}}\right|_{\text{expl}}. \tag{11.63}$$

The last of (11.62) provides an *objective* (materially indifferent) form of the energy $W$. The *material* electromagnetic momentum defined by the last of (11.59) exists only in electrodynamics, but it in fact exists only if the material is electrically polarized and placed in a magnetic field. It is not the pull back, changed of sign, of the electromagnetic momentum defined by (11.43). Concerning the stress involved in the total Eshelby stress, the general form of the effective second Piola–Kirchhoff stress (11.61) is of great interest. Its electromagnetic contribution is essentially a second Piola–Kirchhoff stress built from the interaction "Cauchy-like" stress $\mathbf{t}^{\text{inter}}$ introduced (11.34). This again means, like in the prerequisite Section 11.3.1, that free fields are *filtered out* by the material manifold, the latter retaining only those terms that contain a true material quantity, such as magnetization or electric polarization (of course, in the presence of electromagnetic fields, **E** and **B**). Because of its length and technical aspect, the proof of Theorem 11.1 and Corollary 11.2 is reported in the Appendix to this chapter.

## 11.4 Variational Principle Based on the Inverse Motion

In this case we should start from the Hamiltonian action

$$A\{\chi^{-1}, \mathbf{E}, \mathbf{B}\} = \int_t dt \int_{B_t} \breve{L}\, dv, \tag{11.64}$$

where the Lagrangian density $\breve{L}$ is given by (11.53) and $B_t$ is the actual volume in $K_t$. Then we have the

**COROLLARY 11.3:** From a straightforward $\delta_x$ (at fixed actual placement **x**) variation accompanied by proper variation $\delta\hat{\varphi}$ and $\delta\hat{\mathbf{A}}$ of the Hamiltonian action (11.64), there follow (11.58) and (11.26)—without charge and current—together with the general constitutive equations. Then the application of Noether's theorem for **x**-translation in physical space (homogeneity of physical space) will yield (11.41)—in the absence of external body force (that is other than electromagnetic in nature).

We leave the proof of this to the reader. Of course, the second part of this corollary (Noether's theorem) can also be established by direct computation from the Euler–Lagrange variational equation of motion, which a priori reads

$$\left(\frac{\partial \breve{L}}{\partial \mathbf{X}}\right)_{\text{expl}} - \frac{\partial}{\partial t}\left(\frac{\partial \breve{L}}{\partial \mathbf{V}}\right)\Big|_{x} - \operatorname{div}\left(\frac{\partial \breve{L}}{\partial \mathbf{F}^{-1}}\right) = \mathbf{0}. \tag{11.65}$$

This is the primitive form of (11.58).

Here we do not deal with other invariances such as rotation and dilatation in material space, since this will not be exploited further. However, we note that the material law obtained by taking the inner product of the balance of material momentum by $\mathbf{X}$ plays a valuable role in the proof of uniqueness for certain boundary-value problems concerning electroelasticity (Knops and Trimarco, 2006). Also, we should note that the invariance of both of the previously recalled variational formulations under *time translation* will yield two equivalent forms of the *energy equation*.

But we can give elements of the *canonical Hamiltonian formulation* since this is typically based on the inverse-motion description (compare the pure elastic case in Section 4.3). We have to consider the motion $\chi^{-1}$ and the $\chi^{-1}$-dependent "fields":

$$\hat{\varphi} = \hat{\varphi}\left(\chi^{-1}(\mathbf{x},t),t\right), \quad \hat{\mathbf{A}} = \hat{\mathbf{A}}\left(\chi^{-1}(\mathbf{x},t),t\right). \tag{11.66}$$

The associated *generalized* velocities are

$$\mathbf{V} = \frac{\partial \chi^{-1}}{\partial t}\Big|_{x\,\text{fixed}}, \quad \hat{\varphi}^{*} := \frac{\partial \hat{\varphi}}{\partial t}\Big|_{x\,\text{fixed}}, \quad \hat{\mathbf{A}}^{*} := \frac{\partial \hat{\mathbf{A}}}{\partial t}\Big|_{x\,\text{fixed}}. \tag{11.67}$$

On account of (2.40), we note that

$$\hat{\varphi}^{*} = \frac{\partial \hat{\varphi}}{\partial t}\Big|_{X\,\text{fixed}} + \left(\mathbf{V}.\nabla_{R}\right)\hat{\varphi}, \quad \hat{\mathbf{A}}^{*} = \frac{\partial \hat{\mathbf{A}}}{\partial t}\Big|_{X\,\text{fixed}} + \left(\mathbf{V}.\nabla_{R}\right)\hat{\mathbf{A}}. \tag{11.68}$$

Then the *generalized momenta* are given by

$$\breve{\mathbf{P}} \equiv \frac{\partial \breve{L}}{\partial \mathbf{V}} = \breve{\mathbf{P}}^{\text{tot}}, \quad P_{\varphi} \equiv \frac{\partial \breve{L}}{\partial \hat{\varphi}^{*}} \equiv 0, \quad \mathbf{P}_{\mathbf{A}} \equiv \frac{\partial \breve{L}}{\partial \hat{\mathbf{A}}^{*}} = -\frac{1}{c} J_{F}^{-1} \hat{\mathbf{D}}. \tag{11.69}$$

The first set of Hamilton's canonical equations reads

$$\mathbf{V} = \frac{\delta \breve{H}}{\delta \breve{\mathbf{P}}}, \quad \hat{\varphi}^{*} = \frac{\delta \breve{H}}{\delta P_{\varphi}}, \quad \hat{\mathbf{A}}^{*} = \frac{\delta \breve{H}}{\delta \mathbf{P}_{\mathbf{A}}}, \tag{11.70}$$

with Hamiltonian

$$\breve{H} = J_F^{-1}\left\{\frac{1}{2}\rho_0(\mathbf{X})\mathbf{V}.\mathbf{C}.\mathbf{V} + \bar{W}\left(\mathbf{F}^{-1}, \tilde{\mathbf{E}}, \tilde{\mathbf{B}}; \mathbf{X}\right) + \frac{1}{2}J_F\tilde{\mathbf{E}}.\mathbf{C}^{-1}.\tilde{\mathbf{E}} + \frac{1}{2}J_F^{-1}\tilde{\mathbf{B}}.\mathbf{C}.\tilde{\mathbf{B}}\right\}. \quad (11.71)$$

Then we have to check the second set of Hamilton's canonical equations:

$$\left.\frac{\partial \breve{\mathbf{P}}^{\text{tot}}}{\partial t}\right|_x = -\frac{\delta \breve{H}}{\delta \mathbf{X}}, \quad 0 \equiv \frac{\delta \breve{H}}{\delta \hat{\varphi}}, \quad \left.\frac{\partial \mathbf{P}_{\mathbf{A}}}{\partial t}\right|_x = -\frac{\delta \breve{H}}{\delta \hat{\mathbf{A}}^*}. \quad (11.72)$$

The second of these is none other than

$$\text{div}\left(\frac{\partial \breve{H}}{\partial(\nabla\hat{\varphi})}\right) = J_F^{-1}\nabla_R.\hat{\mathbf{D}} = 0, \quad q.e.d. \quad (11.73)$$

The last of (11.72) is

$$\frac{\partial}{\partial t}\left(-\frac{1}{c}J_F^{-1}\hat{\mathbf{D}}\right)\Big|_x = \text{div}\left(\frac{\partial \breve{H}}{\partial(\nabla\hat{\mathbf{A}})}\right) = J_F^{-1}\text{div}_R\left(\frac{\partial H}{\partial(\nabla_R\hat{\mathbf{A}})}\right). \quad (11.74)$$

The computation of the right-hand side of this equation then yields

$$-\frac{1}{c}J_F^{-1}\left.\frac{\partial \hat{\mathbf{D}}}{\partial t}\right|_X = -\nabla_R \times \hat{\mathbf{H}}, \quad (11.75)$$

hence the first of (11.26) with vanishing conduction current. It remains to check that $J_F$ times the first of (11.72) is none other than (11.58). We leave this to the reader. An introduction to the formalism of Lie–Poison brackets is given in Maugin (1993, Chapter 8).

## 11.5 Geometric Aspects and Material Uniformity

Some of the considerations of Section 6.1 carry directly to the electromagnetic case, in particular to the case of *electroelastostatics* (Maugin and Epstein, 1991), in which case the Lagrangian density is reduced to

$$L = \frac{1}{2}\mathbf{E}^2 - \hat{W}\left(\mathbf{F}, \bar{\mathbf{E}}; \mathbf{X}\right). \quad (11.76)$$

The field $\bar{\mathbf{E}}$ is Eulerian and, therefore, not affected by a change in reference configuration. The "geometric" definition of the Eshelby stress holds good and yields

$$\mathbf{b}^{\text{tot}} = -\frac{\partial \bar{W}}{\partial \mathbf{K}}\mathbf{K}^T = \hat{W}\left(\mathbf{F}, \bar{\mathbf{E}}; \mathbf{X}\right)\mathbf{1}_R - \frac{\partial \hat{W}}{\partial \mathbf{F}}.\mathbf{F}, \tag{11.77}$$

where $\hat{W} = J_K^{-1}\bar{W}(\mathbf{FK}, \bar{\mathbf{E}})$. But on account of objectivity $\hat{W}$ becomes a function such as $\breve{W}(\mathbf{C} = \mathbf{F}^T\mathbf{F}, \tilde{\mathbf{E}} = \hat{\mathbf{E}} = \bar{\mathbf{E}}.\mathbf{F}; \mathbf{X})$ so that

$$\frac{\partial \hat{W}}{\partial \mathbf{F}} = \frac{\partial \breve{W}}{\partial \mathbf{C}} : \frac{\partial \mathbf{C}}{\partial \mathbf{F}} + \frac{\partial \breve{W}}{\partial \tilde{\mathbf{E}}}.\frac{\partial \tilde{\mathbf{E}}}{\partial \mathbf{F}} = \mathbf{S}^E : \mathbf{F}^T - \Pi.\tilde{\mathbf{E}}\mathbf{F}^{-1}, \tag{11.78}$$

and thus

$$\mathbf{b}^{\text{tot}} = \breve{W}\mathbf{1}_R - \mathbf{S}^E.\mathbf{F}^T.\mathbf{F} + \Pi.\tilde{\mathbf{E}}\mathbf{F}^{-1}.\mathbf{F} = \breve{W}\mathbf{1}_R - \left(\mathbf{S}^E - \Pi \otimes \left(\tilde{\mathbf{E}}.\mathbf{C}^{-1}\right)\right).\mathbf{C}. \tag{11.79}$$

In the equivalent case of *magnetoelastostatics* a similar reasoning would yield the following result:

$$\mathbf{b}^{\text{tot}} = \breve{W}\left(\mathbf{C}, \hat{\mathbf{M}}; \mathbf{X}\right)\mathbf{1}_R - \mathbf{S}^E.\mathbf{C} - \tilde{\mathbf{B}} \otimes \hat{\mathbf{M}}, \quad \tilde{\mathbf{B}} = \partial \breve{W}/\partial \hat{\mathbf{M}}. \tag{11.80}$$

Note that the case of electroelastostatics was studied from the variational point of view by Pak and Herrmann (1986a, 1986b) with a view to fracture studies, while the case of soft ferromagnets for which (11.80) holds good was established by Sabir and Maugin (1996). The expressions in (11.79) and (11.80) are but special cases of the general electrodynamic case (11.60) through (11.62). The typical contribution in $\prod \otimes \tilde{\mathbf{E}}$ in (11.79)—$\mathbf{P} \otimes \mathbf{E}$ in the actual framework of small strains—provides an electric correction to the electroelastic Peach–Koehler force, which, generalizing the classical formula (3.65), will read, according to Minagawa (1991):

$$\mathbf{f}^{(\text{PK}-E)} = \left(\tilde{\mathbf{b}}.\left(\sigma - \mathbf{E} \otimes \mathbf{P}\right)\right) \times \tau. \tag{11.81}$$

From (11.80) we deduce without computation that in magnetoelasticity we will have the result

$$\mathbf{f}^{(\text{PK}-M)} = \left(\tilde{\mathbf{b}}.\left(\sigma + \mathbf{M} \otimes \mathbf{B}\right)\right) \times \tau, \tag{11.82}$$

where we recall that $\tilde{\mathbf{b}}$ is the Burgers vector (not to be mistaken for the Eshelby stress).

## 11.6 Remark on Electromagnetic Momenta

Even written in a single frame (the actual one), the electromagnetic (physical) momentum $\mathbf{p}^f$ (cf. (11.33)) and the material electromagnetic momentum (cf. Equation 11.59) differ from one another since they then read

$$\mathbf{p}^f = \mathbf{p}^{\text{emf}} \equiv \frac{1}{c}\mathbf{E}\times\mathbf{B}, \quad \mathbf{P}^{\text{emm}} = \frac{1}{c}\mathbf{P}\times\mathbf{B}. \tag{11.83}$$

Of course we immediately have in our system of (Lorentz–Heaviside) units

$$\mathbf{p}^{\text{emf}} + \mathbf{P}^{\text{emm}} = \frac{1}{c}\mathbf{D}\times\mathbf{B}. \tag{11.84}$$

Early in the twentieth century various proposals were made for a possible expression of the electromagnetic linear momentum in matter (see the discussion in Eringen and Maugin, 1990), among them the so-called *Minkowski's* (1908) proposal,

$$\mathbf{p}^M = c\mathbf{D}\times\mathbf{B}, \tag{11.85}$$

and *Abraham's* (1909) proposal,

$$\mathbf{p}^A = \frac{1}{c}\mathbf{E}\times\mathbf{H}. \tag{11.86}$$

In a linear isotropic, nonmagnetized, dielectric of dielectric constant $\varepsilon$ we have

$$\mathbf{D} = \varepsilon_0\varepsilon\,\mathbf{E}, \quad \mathbf{B} = \mu_0\,\mathbf{H}, \quad c^2 = \left(\varepsilon_0\mu_0\right)^{-1}, \tag{11.87}$$

so that

$$\mathbf{p}^M = n^2\mathbf{p}^A, \quad n^2 \cong \varepsilon, \tag{11.88}$$

where the last relation, due to Maxwell, is only approximate with a refractive index $n$.

But in the preceding we have many candidates for the electromagnetic-field momentum. Basing on various arguments, some authors (Pauli in 1921; Jones and Richards, 1954; Brevik, 1970) favor Minkowski's proposal, while others (Pauli, 1921; Penfield and Haus, 1967; de Groot and Suttorp, 1972; Robinson, 1975) would prefer Abraham's. More modern authors including Livens (1962),

Maugin and Eringen (1977), Nelson (1990), and Tiersten (1990) recognize in the first of (11.83) what should a priori be a good candidate, recalling simultaneously that all depends on the decomposition considered in a result such as (11.32), which is not unique for a given electromagnetic body force $\mathbf{f}^{\text{em}}$. Blount (1971) seems to be the first to have proposed a distinction between the *true physical* linear momentum of electromagnetic fields and the *pseudomomentum* (here called the *material* momentum), relating these two concepts to the invariance of physical laws under translation of spatial and material coordinates, respectively. This is our point of view, shared by Nelson (1990). According to Blount (1971) Abraham's momentum corresponds to the true physical momentum and Minkowski's momentum is identified with the pseudomomentum. In our case, (11.83) yields

$$\mathbf{p}^{\text{emf}} + \mathbf{P}^{\text{emm}} = \frac{1}{c^2}\mathbf{p}^{M} \cong \frac{n^2}{c^2}\mathbf{p}^{A}, \tag{11.89}$$

and this ought to be compared to the purely mechanical analog given by (see (3.26))

$$\mathbf{p} + \mathbf{P} = \mathbf{P}^{f}, \tag{11.90}$$

where $\mathbf{P}^{f}$ is Brenig's field (or wave) momentum. According to this analogy, $\mathbf{P}^{\text{emf}}$ is the physical momentum of electromagnetic fields (in agreement with the way we introduced it), $\mathbf{P}^{\text{emm}}$ is the material momentum (in agreement with the manner we constructed it), and the Minskowski and Abraham momenta are to be related to the notion of field or wave momentum.

To conclude this point we note a series of works by a group from Zürich (Gurevich and Thellung, 1990, 1992; Schoeller and Thellung, 1992). These authors identify what they call the *quasimomentum* (our pseudomomentum or canonical momentum) of elasticity and electromagnetism by evaluating the quantities that appear jointly with the known quasimomentum of phonons (or crystal momentum in the quantum theory of solids), of which they know the expression, that is, a covector of components of the form

$$P_J^{(\text{phonons})} = \int d\xi_k N \hbar k_J,$$

where $k_J$ is the $J$th component of a wave vector, $N$ is the phonon distribution function, and $\int d\xi_k$ denotes integration over the phonon vectors $\boldsymbol{k}$ and summation over the various phonon branches. The canonical balances of momentum and energy are derived, as they should be, in parallel, presenting elastic, electromagnetic, and phonon contributions. The electromagnetic quasimomentum identified by these authors is none other than the Minkowski electromagnetic momentum (see our earlier discussion following (11.89) and (11.90)).

## 11.7 Balance of Canonical Momentum and Material Forces

Although the general framework is not so relevant from the applicative viewpoint, some general feeling can be gathered from some results in foregoing sections. This is the case of the material momentum equation (11.58). Integrated over a regular material volume $V$, this yields

$$\frac{d}{dt}\mathbf{P}(V) = \mathbf{B}_E(V) + \mathbf{F}^{\text{inh}}(V)\ , \tag{11.91}$$

with

$$\mathbf{P}(V) = \int_V \mathbf{P}^{\text{tot}} dV, \quad \mathbf{B}_E(V) = \int_{\partial V} \mathbf{N}.\mathbf{b}^{\text{tot}} dA, \quad \mathbf{F}^{\text{inh}}(V) = \int_V \mathbf{f}^{\text{inh}} dV \tag{11.92}$$

Of particular interest here is the surface contribution, which can be rewritten as

$$\mathbf{B}_E(V) = \int_{\partial V} \left\{ P\mathbf{N} - \tilde{\mathbf{T}}^E.\mathbf{C} + Q_P\tilde{\mathbf{E}} - \hat{\mathbf{M}}\left(\tilde{\mathbf{B}}.\mathbf{N}\right)\right\} dA, \tag{11.93}$$

where we have defined a pressure-like term $P$, a surface traction $\tilde{\mathbf{T}}^E$, and a surface electric charge density due to electric polarization, $Q_P$, by

$$P := -L^{\text{md}} + \hat{\mathbf{M}}.\tilde{\mathbf{B}}, \quad \tilde{\mathbf{T}}^E := \mathbf{N}.\mathbf{S}^E, \quad Q_P := \Pi.\mathbf{N}. \tag{11.94}$$

Several important cases are as follows. For a nonmagnetizable material (vanishing magnetization in a comoving frame), we obviously have $\hat{\mathbf{M}} = \mathbf{0}$, so that (11.93) reduces to a form relevant to the case of *electroelastic* materials:

$$\mathbf{B}_E(V) = \int_{\partial V} \left\{ -L\mathbf{N} - \tilde{\mathbf{T}}^E.\mathbf{C} + Q_P\tilde{\mathbf{E}}\right\} dA. \tag{11.95}$$

In quasistatics, but keeping both magnetization and electric polarization, we obtain an approximation valid for both *electroelasticity* and *magnetoelasticity*:

$$\mathbf{B}_E(V) = \int_{\partial V} \left\{ W\mathbf{N} - \tilde{\mathbf{T}}^E.\left(\mathbf{1}_R + 2\mathbf{E}\right) - Q_P\nabla_R\hat{\varphi} - \hat{\mathbf{M}}\left(\nabla_R \times \hat{\mathbf{A}}\right).\mathbf{N}\right\} dA, \tag{11.96}$$

where $\mathbf{E}$ is the finite strain expressible in terms of the displacement gradient, and $\hat{\varphi}$ and $\hat{\mathbf{A}}$ are the material electromagnetic potentials. The expression

(11.96) gives in advance an idea of what the *J*-integral generalized to electroelasticity or magnetoelasticity will be. This shows an essential difference between electric and magnetic processes because there is no magnetic equivalent here to the notion of polarization surface charge.

For a homogeneous material and for homogeneous boundary conditions or vanishing fields at infinity (in the case of an integration over the whole material space), (11.91) reduces to a pure conservation of the total material (canonical) momentum. This is what happens in certain problems of propagation dealing with solitons (see Chapter 12). More on the canonical Hamilton formalism associated with the general electrodynamic case is found in Maugin (1993, pp. 192–193). Instead of dealing with this mundane subject, we prefer to revisit the problem posed by electroelastic solids in finite strains (and its analog in magnetoelastic bodies) because of its many applications in electromechanical devices and in the industry of electronic components.

## 11.8 Electroelastic Bodies and Fracture

### 11.8.1 General Equations

For many applications it is sufficient to consider a quasistatic approximation to the general equations presented in Section 11.2. In particular, acceleration terms are discarded in the basic equation of motion, magnetization is ignored as well as couplings between electric and magnetic phenomena (although there exist magneto-electric materials of great interest), and most of the time the material is assumed to be a *dielectric*; that is, it does not conduct electricity and is free of charges. Under these conditions the basic field equations at any regular material point **X** are reduced to

- Balance of linear (physical) momentum in its equilibrium form (compare to (11.41)):

$$\mathrm{div}_R\left(\mathbf{T}^E + \mathbf{T}^F\right) = \mathbf{0} \tag{11.97}$$

- Reduced Faraday equation (compare to (11.25)):

$$\nabla_R \times \hat{\mathbf{E}} = \mathbf{0} \tag{11.98}$$

- Reduced Gauss equation (cf. ($11.26_2$)):

$$\nabla_R . \hat{\mathbf{D}} = 0 \tag{11.99}$$

where (11.97) introduces the first Piola–Kirchhoff stresses associated with elasticity and the "free" electromagnetic fields, while $\hat{\mathbf{E}}$ and $\hat{\mathbf{D}}$ are material electric fields. Because we are in quasielectrostatics, we have the relations (compare to (11.23) through (11.26))

$$\hat{\mathbf{E}} = \mathbf{E}.\mathbf{F}, \quad \hat{\mathbf{D}} = J_F \mathbf{F}^{-1}.\mathbf{D}, \quad \Pi = J_F \mathbf{F}^{-1}.\mathbf{P}, \quad \hat{\mathbf{D}} = J_F \mathbf{C}^{-1}.\hat{\mathbf{E}} + \Pi, \tag{11.100}$$

where $\mathbf{E}$, $\mathbf{D}$, and $\mathbf{P}$ are the standard fields in a laboratory frame. Equation 11.98 implies the existence of the material electrostatic potential $\hat{\varphi}$ such that

$$\hat{\mathbf{E}} = -\nabla_R \hat{\varphi}. \tag{11.101}$$

Because of our special interest in fracture and the evaluation of energy-release rates, the equation of energy associated with (11.97) through (11.99) is most relevant. To that purpose we note that

$$\mathbf{T}^F = \bar{\mathbf{E}} \otimes \mathbf{E} - \frac{1}{2}\mathbf{F}^{-1}\left(\hat{\mathbf{E}}.\bar{\mathbf{E}}\right), \quad \bar{\mathbf{E}} := J_F \mathbf{F}^{-1}.\mathbf{E}. \tag{11.102}$$

It is checked that

$$\mathrm{div}_R \mathbf{T}^F = -\left(\nabla_R.\Pi\right)\mathbf{E}, \tag{11.103}$$

where we recognize in the quantity within parentheses a so-called polarization charge density.

With an objective energy density for a homogeneous material, per unit reference volume,

$$W = \bar{W}\left(\mathbf{C}, \hat{\mathbf{E}}\right),$$

we have the mechanical and electric constitutive equations

$$\mathbf{S} = 2\frac{\partial \bar{W}}{\partial \mathbf{C}}, \quad \Pi = -\frac{\partial \bar{W}}{\partial \hat{\mathbf{E}}}, \tag{11.104}$$

corresponding to the energy equation (no dissipation of any kind)

$$\dot{W} = \frac{1}{2}\mathrm{tr}\left(\mathbf{S}.\dot{\mathbf{C}}\right) - \Pi.\dot{\hat{\mathbf{E}}}. \tag{11.105}$$

We can as well consider the so-called *electric enthalpy*:

$$\tilde{W} = \bar{W} - \frac{1}{2}\hat{\mathbf{E}}.\bar{\mathbf{E}}, \tag{11.106}$$

so that, on account of the last of (11.100), instead of (11.104), we have

$$\mathbf{S} = 2\frac{\partial \tilde{W}}{\partial \mathbf{C}}, \quad \hat{\mathbf{D}} = -\frac{\partial \tilde{W}}{\partial \hat{\mathbf{E}}}. \tag{11.107}$$

It is the multiplicity of possible electromechanical energies that causes some problems in the sequel. Indeed, starting from the field equations (11.97) through (11.99) and the energy equation (11.105), we can deduce some identities that will be useful for the evaluation of energy-release rates. All these are obtained at regular material points. For instance, (11.105) can first be rewritten as

$$\dot{W} = \mathrm{tr}\left(\mathbf{T}^E.\dot{\mathbf{F}}\right) - \Pi.\dot{\hat{\mathbf{E}}}. \tag{11.108}$$

But this can be transformed to

$$\frac{d}{dt}\tilde{W} + \hat{\mathbf{D}}.\dot{\hat{\mathbf{E}}} = \mathrm{tr}\left(\mathbf{T}^E.\left(\nabla_R \mathbf{v}\right)^T\right) + \frac{1}{2}\left(\bar{\mathbf{E}}.\dot{\hat{\mathbf{E}}} - \dot{\bar{\mathbf{E}}}.\hat{\mathbf{E}}\right). \tag{11.109}$$

But we can write

$$\mathrm{tr}\left(\mathbf{T}^E.\left(\nabla_R \mathbf{v}\right)^T\right) = \nabla_R.\left(\left(\mathbf{T}^E + \mathbf{T}^F\right).\mathbf{v}\right) - \mathrm{tr}\left(\mathbf{T}^F.\left(\nabla_R \mathbf{v}\right)^T\right), \tag{11.110}$$

and also prove that

$$\mathrm{tr}\left(\mathbf{T}^F.\left(\nabla_R \mathbf{v}\right)^T\right) = \frac{1}{2}\left(\bar{\mathbf{E}}.\dot{\hat{\mathbf{E}}} - \dot{\bar{\mathbf{E}}}.\hat{\mathbf{E}}\right). \tag{11.111}$$

The nontrivial proof of this is given in the Appendix to Dascalu and Maugin (1994). On combining (11.109) through (11.111), we obtain that, after introduction of the electric potential and enthalpy,

$$\frac{d}{dt}\tilde{W} = \nabla_R.\left(\left(\mathbf{T}^E + \mathbf{T}^F\right).\mathbf{v} + \hat{\mathbf{D}}\dot{\hat{\varphi}}\right). \tag{11.112}$$

This is a remarkable form of the energy equation because it is written as *a strict conservation law*. The dual material contravector to $\hat{\mathbf{D}}\dot{\hat{\varphi}}$, $-\hat{\varphi}\,\partial\hat{\mathbf{D}}/\partial t$, is the *Poynting vector* of quasielectrostatics (see Maugin, 1988, p. 238). In contrast, we can write it in another form, also totally admissible, by considering (11.111) and noting that

$$\frac{d}{dt}\left(\frac{1}{2}\hat{\mathbf{E}}.\bar{\mathbf{E}}\right) = \nabla_R.\left(\mathbf{T}^F.\mathbf{v} + \bar{\mathbf{E}}\dot{\hat{\varphi}}\right) + h^{\mathrm{elec}}, \tag{11.113}$$

where we have set

$$h^{\text{elec}} = \left(\text{div}_R \mathbf{T}^F\right).\mathbf{v} + \left(\nabla_R.\bar{\mathbf{E}}\right)\dot{\hat{\varphi}}. \tag{11.114}$$

From (11.112) takes on the form

$$\frac{d}{dt}\bar{W} = \nabla_R.\left(\mathbf{T}^E.\,\mathbf{v} + \Pi\dot{\hat{\varphi}}\right) + h^{\text{elec}}, \tag{11.115}$$

which is not in the form of a strict conservation law but emphasizes the consideration of the electric polarization as compared to that of the electric displacement. These two forms will necessarily have different consequences insofar as the evaluation of the corresponding energy-release rate of fracture is concerned.

### 11.8.2 Evaluation of the Energy-Release Rate in Electroelastic Fracture

The proofs will follow exactly those of the pure elastic case, and, therefore, details are not repeated, the reader being referred to the original research papers (here essentially Dascalu and Maugin, 1994). For instance, in the first case, where we start from the local energy equation (11.112), with the notation of Section 8.4, we obtain the following global energy balance in the presence of the straight-through crack:

$$\frac{d}{dt}\int_B \tilde{W}dA + G^{\text{crack}} = \int_S \left\{\mathbf{N}.\left(\mathbf{T}^E + \mathbf{T}^F\right).\mathbf{v} + \dot{\hat{\varphi}}\left(\hat{\mathbf{D}}.\mathbf{N}\right)\right\}dS, \tag{11.116}$$

where S is the boundary of $B - C$, $C$ is the crack, and we have defined the energy-release rate by

$$G^{\text{crack}} = \lim \int_\Gamma \left\{\tilde{W}\left(\bar{\mathbf{V}}.\mathbf{N}\right) + \mathbf{N}.\left(\mathbf{T}^E + \mathbf{T}^F\right).\mathbf{v} + \dot{\hat{\varphi}}\left(\hat{\mathbf{D}}.\,\mathbf{N}\right)\right\}d\Gamma \quad \text{as} \quad \Gamma \to 0. \tag{11.117}$$

Clearly, the latter involves not only the flux of electric enthalpy but also the full contributions of coupled and free electric fields. We can say that this is a "natural" formulation. If instead we start with the identity (11.115), we shall obtain the global energy balance as

$$\frac{d}{dt}\int_B \bar{W}dA + G_*^{\text{crack}} = \int_S \left\{\mathbf{N}.\mathbf{T}^E.\mathbf{v} + \dot{\hat{\varphi}}\left(\Pi.\mathbf{N}\right)\right\}dS + \int_B h^{\text{elec}}dA, \tag{11.118}$$

with an energy-release rate given by

$$G_*^{\text{crack}} = \lim \int_\Gamma \left\{\bar{W}\left(\bar{\mathbf{V}}.\mathbf{N}\right) + \mathbf{N}.\mathbf{T}^E.\mathbf{v} + \dot{\hat{\varphi}}\left(\Pi.\mathbf{N}\right)\right\}dS \quad \text{as} \quad \Gamma \to 0. \tag{11.119}$$

Notice that the stress contribution related to the free electric field is not involved in this formula. To obtain (11.118) we assumed that the integrals in this relation are convergent. For some linear piezoelectric materials (Pak, 1990; Sosa and Pak, 1990) or in the case of linearized electrostriction, as shown by Dascalu and Maugin (1994), the behavior of the solution at the tip shows that the term $h^{\text{elec}}$ is of order $r^{-2}$, so that the last integral in (11.118) generally diverges. However, if $h^{\text{elec}} = 0$, then the preceding computation holds good. If we examine the definition (11.114), we can show that this is nothing but

$$h^{\text{elec}} = -\left(\nabla_R . \Pi\right)\frac{\partial \varphi}{\partial t}, \tag{11.120}$$

where $\varphi$ is the electrostatic potential in the actual configuration. Thus, as $\partial\varphi/\partial t$ cannot be forced to vanish, the condition of vanishing $h^{\text{elec}}$ can be realized only if we impose the constraint

$$\nabla_R . \Pi = 0, \tag{11.121}$$

as a sufficient condition. This can be achieved in some concrete electroelastic problem (cf. Dascalu and Maugin, 1994).

### 11.8.3 Electroelastic Path-Independent Integrals

Now we express the energy-release rates obtained in the preceding in terms of contour integrals that do not depend on the integration path, an essential property for easy computation. These integrals were obtained first by Pak and Herrmann (1986a, 1986b) and Maugin and Epstein (1991). To do this we need an estimate of the degree of singularity of electromechanical fields in the neighborhood of the crack tip. Suppose that both the displacement $\mathbf{u}$ and the electric potential $\hat{\varphi}$ have a regular time behavior as observed from the crack tip. So, just as in pure elasticity (Gurtin, 1979; Nguyen Quoc Son, 1980), this assumption allows us to write

$$\dot{\mathbf{u}} = -\bar{\mathbf{V}} . \nabla_R \mathbf{u} + \mathbf{w}, \quad \dot{\hat{\varphi}} = -\bar{\mathbf{V}} . \nabla_R \hat{\varphi} + \psi, \tag{11.122}$$

where $\mathbf{w}$ and $\psi$ have no singular behavior at the crack tip. Then the terms in $G^{\text{crack}}$ containing these fields will vanish for $\Gamma \to 0$. This allows us to show that $G^{\text{crack}}$ takes on the form

$$G^{\text{crack}} = \lim \bar{\mathbf{V}} . \int_{\Gamma} \left\{ \tilde{W}\mathbf{N} - \nabla_R \mathbf{u} . (\mathbf{T}^E + \mathbf{T}^F)^T . \mathbf{N} - \nabla_R \hat{\varphi} \left( \hat{\mathbf{D}} . \mathbf{N} \right) \right\} dS$$

$$\text{as} \quad \Gamma \to 0. \tag{11.123}$$

The same technique applied to $G_*^{\text{crack}}$ yields

$$G_*^{\text{crack}} = \lim \bar{\mathbf{V}}.\int_{\Gamma}\left\{\bar{W}\mathbf{N} - \nabla_R \mathbf{u}.\left(\mathbf{T}^E\right)^T.\mathbf{N} - \nabla_R \varphi\left(\Pi.\mathbf{N}\right)\right\}dS \quad \text{as} \quad \Gamma \to 0. \tag{11.124}$$

In this relation we can replace $\nabla_R \mathbf{u}$ by $\mathbf{F}$ making the assumption that

$$\lim \int_{\Gamma} \mathbf{N}.\mathbf{T}^E dS = 0 \quad \text{as} \quad \Gamma \to 0, \tag{11.125}$$

an assumption that is verified when $\mathbf{T}^E$ behaves like $r^{-1/2}$ near the tip, just like in classical elasticity (cf. Pak, 1990; Sosa and Pak, 1990; Dascalu and Maugin, 1994). Then (11.124) reads

$$G^{\text{crack}} = \lim \bar{\mathbf{V}}.\int_{\Gamma}\left\{\tilde{W}\mathbf{N} - \mathbf{F}^T.\left(\mathbf{T}^E + \mathbf{T}^F\right)^T.\mathbf{N} - \nabla_R \hat{\varphi}\left(\hat{\mathbf{D}}.\mathbf{N}\right)\right\}dS \quad \text{as} \quad \Gamma \to 0. \tag{11.126}$$

But we restrict the analysis to the case of a straight-through crack along the $X_1$-axis and thus

$$\bar{\mathbf{V}} = \dot{l}(t)\mathbf{E}_1. \tag{11.127}$$

Now we formulate electroelastic *J*-integrals. For a piecewise smooth, nonintersecting path $\Gamma$ that begins and ends on the crack and surrounds the tip of the crack, we define

$$J(\Gamma) = \int_{\Gamma}\left\{\tilde{W}N_1 - \mathbf{N}.\left(\mathbf{T}^E + \mathbf{T}^F\right).\frac{\partial \mathbf{u}}{\partial X_1} - \left(\hat{\mathbf{D}}.\mathbf{N}\right)\frac{\partial \hat{\varphi}}{\partial X_1}\right\}dS. \tag{11.128}$$

If *J* does not depend on $\Gamma$, then (11.126) yields

$$G^{\text{crack}} = J\dot{l}, \tag{11.129}$$

the familiar dissipation form of the product of a "force" and a "velocity." The *J*-integral (11.128) was obtained by Pak and Herrmann (1986b) using the Eshelby theory of inhomogeneities. Their argument for the path independence stems from the relation

$$\operatorname{div}_R \mathbf{b} = \mathbf{0}, \tag{11.130}$$

with an electromechanical Eshelby stress given by

$$\mathbf{b} = \tilde{W}\mathbf{1}_R - \left(\mathbf{T}^E + \mathbf{T}^F\right).\left(\nabla_R \mathbf{u}\right)^T - \hat{\mathbf{D}} \otimes \nabla_R \hat{\varphi}. \tag{11.131}$$

Here also, the path independence requires that some conditions hold true along the faces of the crack. These conditions are

$$\mathbf{N}.\hat{\mathbf{D}}^{\pm} = 0, \quad \mathbf{N}.\left(\mathbf{T}^{E} + \mathbf{T}^{F}\right)^{\pm} = \mathbf{0}; \tag{11.132}$$

that is, neither electric charges nor tractions exist along the crack. If, however, we deal with paths that start and end at the same point along the crack, then only the jumps in (11.132) are required to vanish.

To deal with $G_{*}^{\text{crack}}$, we define another $J$-integral, $J^{*}$, by

$$J^{*} = \int_{\Gamma} \left\{ \bar{W} N_1 - \mathbf{N}.\mathbf{S}^{E}.\mathbf{C}.\mathbf{E}_1 - \left(\Pi.\mathbf{N}\right) \frac{\partial \hat{\varphi}}{\partial X_1} \right\} dS, \tag{11.133}$$

which was obtained by Maugin and Epstein (1991) using the same method as Eshelby but remarking that an identity verified by the free electric fields permits us to work with the following electroelastic Eshelby stress tensor (compare (11.79)):

$$\mathbf{b}^{*} = \bar{W}\mathbf{1}_R - \mathbf{S}^{E}.\mathbf{C} - \Pi \otimes \nabla_R \hat{\varphi}, \tag{11.134}$$

for which

$$\operatorname{div}_R \mathbf{b}^{*} = \mathbf{0}, \tag{11.135}$$

at all regular material points $\mathbf{X}$. For the path independence of $J^{*}$ we must have

$$\mathbf{N}.\left(\mathbf{T}^{E}\right)^{\pm} = \mathbf{0}, \quad \mathbf{N}.\Pi^{\pm} = 0, \tag{11.136}$$

on the faces of the crack. The same conditions, but for the jumps, are valid when the contour of $J^{*}$ starts and ends at the same point.

### 11.8.4 An Application: Antiplane Crack in a Dielectric with Induced Piezoelectricity

This problem was examined by Dascalu and Maugin (1995a, 1995b) with a view to determining whether the conditions (11.132) and (11.136) hold good in realistic situations. This concerns mode III fracture, for which the singular part of the solution, the only one of interest in the evaluation of the $J$-integrals, can be obtained in a closed form. We consider an electroelastic material with a center of symmetry (in fact an isotropic body), so that it cannot a priori exhibit piezoelectricity (cf. Maugin, 1988). The first electroelastic coupling of interest is *electrostriction*. But for small electric fields $\mathbf{E}$

superimposed on a bias electric field $\mathbf{E}_0 = (0, 0, E_{03})$ that breaks the symmetry of the material, we obtain a field *induced piezoelectricity* effect such that we have the constitutive equations (Ani and Maugin, 1989, p. 608; only one type of indices is used)

$$T_{ij}^{E} = C_{ijkl}u_{k,l} - \lambda_{mnij}E_{0n}E_m, \tag{11.137a}$$

$$T_{ij}^{F} = E_{0i}E_j + E_i E_{0j} - \left(\mathbf{E}_0.\mathbf{E}\right)\delta_{ij}, \tag{11.137b}$$

$$\Pi_m = \chi_{mn}E_n + \lambda_{mnij}E_{0n}u_{i,j}, \tag{11.137c}$$

$$\hat{E}_m = E_m + \left(\delta_{ij}\delta_{mn} - \delta_{mi}\delta_{nj} - \delta_{ni}\delta_{mj}\right)E_{0n}u_{i,j}, \tag{11.137d}$$

with material constitutive tensors (for isotropy) given by

$$\begin{aligned} C_{ijkl} &= \lambda\delta_{ij}\delta_{kl} + \mu\left(\delta_{jk}\delta_{il} + \delta_{jl}\delta_{ik}\right), \quad \chi_{mn} = \chi\delta_{mn}, \\ \lambda_{mnij} &= c\delta_{mn}\delta_{ij} + d\left(\delta_{ni}\delta_{mj} + \delta_{nj}\delta_{mi}\right), \end{aligned} \tag{11.137e}$$

where $\lambda$ and $\mu$ are Lamé coefficients, $\chi$ is the electric susceptibility, and $c$ and $d$ are the only two surviving electrostriction coefficients for an isotropic body (see Maugin, 1988).

The problem considered relates to out-of-plane displacements and in-plane electric fields such that

$$u_1 = u_2 = 0, \quad u = u_3\left(x_1, x_2\right); E_3 = 0, E_3 = 0, \; E_1 = E_1\left(x_1, x_2\right), E_2 = E_2\left(x_1, x_2\right).$$

Introducing the electrostatic potential $\hat{\varphi} = \varphi$, the field equations yield ($\Delta$ is the 2D Laplacian)

$$\mu\Delta u + e\,\Delta\varphi = 0, \quad e\Delta u - \varepsilon\,\Delta\varphi = 0, \tag{11.138}$$

where $e = (d-1)E_{03}$ and $\varepsilon = 1 + \chi$ are the effective piezoelectric coefficient and the electric permeability, respectively. These must be such that $e^2 + \mu\varepsilon \neq 0$, so that both $u$ and $\varphi$ are harmonic functions. We consider a straight-through crack with the origin of coordinates situated at the crack tip and the crack $C$ lies along the negative $x_1$-axis. The boundary conditions (11.132) read

$$\mu\, u_{,2} + e\varphi_{,2} = 0, \quad eu_{,2} - \varepsilon\varphi_{,2} = 0.$$

With $u$ and $\varphi$ harmonic functions, these are equivalent to vanishing Neumann conditions. The singular part of the electroelastic solution has a standard form ("singularity of the Laplacian"; cf. (8.1))

$$u = K^S\sqrt{\frac{2r}{\pi}}\sin\frac{\theta}{2}, \quad \varphi = K^E\sqrt{\frac{2r}{\pi}}\sin\frac{\theta}{2}, \tag{11.139}$$

where $(r, \theta)$ are polar coordinates, and the scalars $K^S$ and $K^E$ are the strain and electric field intensity factors. We let the reader evaluate the various electric and stress fields, as well as the $J$-integrals. It is found (Dascalu and Maugin, 1994) that

$$J = \frac{1}{2}\left\{\mu\left(K^S\right)^2 - \varepsilon\left(K^E\right)^2\right\} - eK^EK^S, \tag{11.140}$$

$$J^* = \frac{1}{2}\left\{\mu\left(K^S\right)^2 - \chi\left(K^E\right)^2\right\} - dE_{03}K^EK^S, \tag{11.141}$$

so that

$$J - J^* = -\frac{1}{2}\left(K^E\right)^2 + E_{03}K^EK^S. \tag{11.142}$$

This difference represents the contribution of the free electric field to crack propagation. With $E_{03} = 0$, this shows that the electric field may have a negative contribution to the energy-release rate. This agrees with Pak (1990) and Deeg (1980), whose results show that crack arrestment can be produced by the electric field effect on the propagation. Considering a similar problem for a transversely isotropic piezoelectric material of hexagonal class 6 mm, Pak found a similar form of the solution. The reason is that equations similar to Equation 11.138 hold true but with real electroelastic–piezoelectric coefficients for that symmetry:

$$\mu \to c_{44}^E, \quad e \to e_{15}, \quad \varepsilon \to \varepsilon_{11}^e, \tag{11.143}$$

with the standard notation of piezoelectricity (cf. Maugin, 1988, Chapter 4; Maugin, 1993, pp. 200–202). For PZT-5H ceramics, the critical crack extension force $J_{cr}$ was found to be of the order of 5 N/m (Deeg, 1980).

To be more complete we should cite McMeeking (1989, 1991) for a nice discussion about other problems such as the possible breakdown of a deformable dielectric through crack extension. Also, we recall the original work of Parton (1976) on the elliptic crack in a dielectric (see also Parton and Kudryavtsev, 1988), the thorough investigation of stress intensity factors in elastic dielectrics by Kurlandzka (1988), the work of Belokopitova and Filshtinski (1979),

and that of Park and Sun (1995) and Suo et al. (1992). A thorough mathematical discussion concerning the propagation of an electrically conducting crack in a dielectric was given by Dascalu and Maugin (1995c). There, the controversy concerning the choice of path-independent integrals is identified as a controversy between two different formulations of the electroelasticity equations. The obtained results actually represent an argument in favor of the theory that views the action of electromagnetic fields as occurring via contact forces rather than at-a-distance forces (an old discussion in electromagnetic continua; see Maugin, 1988). We cannot quote the multitude of analytical works dealing with cracks of different types in linear piezoelectricity. These, interesting as they are from the solution viewpoint and for technological applications, especially in electronic equipment, do not bring any new contributions from the conceptual viewpoint. Direct computational approaches are also numerous, and we cite only our own finite-element works (Benkaci and Maugin, 2001a, 2001b) for the consideration of energy-domain integrals, 3D computations, and evaluations of electroelastic *J*-integrals for various crack modes. Concerning the *dynamic fracture of piezoelectric materials*, there exist only a few works, one of which is that of Dascalu and Maugin (1995c), which generalizes to the piezoelectric case a purely elastic problem treated by Kostrov (1966), Eshelby (1969), and Brock (1974), that of the extension of the crack lips symmetrically in the direction of the crack line: Only the acceleration term is kept in the mechanical equation; for the antiplane fracture of a transversely isotropic piezoelectric solid, the stress and electric field intensity factors are obtained for short times of extension, and the use of a Griffith-type propagation criterion leads to a differential equation for the crack-tip trajectory that can be numerically solved only depending on the electric field applied at infinity. That paper also considers two different energy-release rates based on two different formulations of the balance of energy, but again these two rates are shown to be equivalent in the given circumstances.

### 11.8.5 Note on Linear Piezoelectricity

In this case all terms that are quadratic in the fields are disregarded in the fields and constitutive equations (cf. Chapter 5 in Maugin, 1988). The electromechanical couplings reduce to those of pure constitutive origin, that is, the linear dependence of the "elastic stress" on the small-amplitude electric field, and the reciprocal dependence of the electric displacement on the small strain, which we can express by the linear equations

$$\mathbf{T}^E \to \sigma_{ij} = C_{ijkl}u_{k,l} - e_{kij}E_k\,, \quad \hat{\mathbf{D}} \to D_i = \varepsilon_{ij}E_j + e_{ikl}u_{k,l} \tag{a}$$

with the field equations reduced to

$$\rho_0 \ddot{u}_i = \sigma_{ij,j}\,, \quad \nabla \times \mathbf{E} = 0 \to \mathbf{E} = -\nabla\varphi, \quad D_{i,i} = 0. \tag{b}$$

The tensorial coefficients $e_{kij} = e_{kji}$ are those of piezoelectricity—the only remaining electromechanical coupling of pure constitutive origin—and this exists, we remind the reader, only if the material does *not* possess a center of symmetry.

Accordingly, the *J*-integral of electroelastic quasistatic fracture reduces to the simple formula

$$J = \int_{\Gamma} \left( WN_1 - \mathbf{n}.\boldsymbol{\sigma}.\mathbf{u}_{,1} - \mathbf{n}.\mathbf{D}\varphi_{,1} \right) d\Gamma, \tag{c}$$

where $W$ is jointly quadratic in $(\nabla \mathbf{u})_S$ and $\mathbf{E}$, the parallel role of $\mathbf{u}$ and $\varphi$ is obvious, and the Eshelby stress plays well its role of capturing the gradients of these two fields, so that the form of (c) is *canonical* and was obviously given before the present developments were worked out.

## 11.9 Transition Fronts in Thermoelectroelastic Crystals

Here we consider a more general framework than in the preceding section by allowing the presence of thermal effects and of a density of electric charges. The last ingredient may have some importance in electroelastic bodies that may contain these charges, such as in piezoelectric semiconductors. Furthermore, they allow for interesting developments in the case of transition zones such as phase-transition fronts.

### 11.9.1 General Equations

Still in the framework of electrostatics we have

- Maxwell's electrostatic equations:

$$\nabla_R \times \hat{\mathbf{E}} = \mathbf{0}, \quad \nabla_R . \hat{\mathbf{D}} = \hat{Q}_f \tag{11.144}$$

- Conservation of mass:

$$\frac{\partial}{\partial t} \rho_0 \Big|_X = 0 \tag{11.145}$$

- Balance of linear (physical) momentum:

$$\frac{\partial}{\partial t} \mathbf{p} \Big|_X - \mathrm{div}_R \mathbf{T} = \mathbf{f}^{\mathrm{em}} \tag{11.146}$$

- Balance of energy:

$$\frac{\partial}{\partial t}\left(\frac{1}{2}\rho_0\mathbf{v}^2 + E - \hat{Q}_f\hat{\varphi}\right)\Big|_X - \nabla_R.\left(\mathbf{T}.\mathbf{v} + \mathbf{S}^e - \mathbf{Q}\right) = h^e \tag{11.147}$$

- Balance of entropy:

$$\theta\frac{\partial S}{\partial t}\Big|_X + \nabla_R.\mathbf{Q} = 0 \tag{11.148}$$

This presentation (Maugin, 1988) isolates the electric force $\mathbf{f}^{\text{em}}$, incorporates the action of the free charge in the total energy, and emphasizes the notions of Poynting vector $\mathbf{S}_e$ and electric energy source $h^e$ with

$$\mathbf{f}^{\text{em}} = \left(\hat{Q}_f + \Pi.\nabla_R\right)\mathbf{E}, \quad \mathbf{S}^e = -\hat{\varphi}\frac{\partial\hat{\mathbf{D}}}{\partial t}\Big|_X, \quad h^e = -\hat{Q}_f\frac{\partial\hat{\varphi}}{\partial t}\Big|_X, \tag{11.149}$$

together with

$$\hat{\mathbf{D}} = \bar{\mathbf{E}} + \Pi, \quad \hat{\mathbf{E}} = \mathbf{E}.\mathbf{F}, \quad \bar{\mathbf{E}} = J_F\mathbf{F}^{-1}.\mathbf{E} = J_F\mathbf{C}^{-1}.\hat{\mathbf{E}}, \quad \hat{\mathbf{E}} = -\nabla_R\hat{\varphi}. \tag{11.150}$$

The following identities can be proved (Maugin, 1988; Dascalu and Maugin, 1994):

$$\mathbf{f}^{\text{em}} = \text{div}_R\mathbf{T}^{\text{em}}, \quad \text{div}_R\mathbf{T}^F = \left(\hat{Q}_f - \nabla_R.\Pi\right)\mathbf{E}, \tag{11.151}$$

$$\mathbf{T}^{\text{em}} = \hat{\mathbf{D}}\otimes\mathbf{E} - \frac{1}{2}\left(\hat{\mathbf{E}}.\bar{\mathbf{E}}\right)\mathbf{F}^{-1}, \quad \mathbf{T}^F = \bar{\mathbf{E}}\otimes\mathbf{E} - \frac{1}{2}\left(\hat{\mathbf{E}}.\bar{\mathbf{E}}\right)\mathbf{F}^{-1}, \tag{11.152}$$

and

$$\text{tr}\left(\mathbf{T}^F.\left(\nabla_R\mathbf{v}\right)^F\right) = \frac{1}{2}\left(\bar{\mathbf{E}}.\frac{\partial\hat{\mathbf{E}}}{\partial t}\Big|_X - \frac{\partial\bar{\mathbf{E}}}{\partial t}\Big|_X.\hat{\mathbf{E}}\right), \tag{11.153}$$

$$\nabla_R.\bar{\mathbf{E}} = \hat{Q}_f - \nabla_R.\Pi, \tag{11.154}$$

$$\frac{d}{dt}\left(\frac{1}{2}\hat{\mathbf{E}}.\bar{\mathbf{E}}\right) = -\nabla_R.\left(\mathbf{T}^F.\mathbf{v} + \bar{\mathbf{E}}\frac{\partial\hat{\varphi}}{\partial t}\Big|_X\right) + H, \tag{11.155}$$

$$H = \mathbf{v}.\mathrm{div}_R\mathbf{T}^F + \left(\nabla_R.\bar{\mathbf{E}}\right)\frac{\partial\hat{\varphi}}{\partial t}\bigg|_X = \left(\hat{Q}_f - \nabla_R.\Pi\right)\frac{\partial\varphi}{\partial t}\bigg|_x. \tag{11.156}$$

Here $\varphi = \hat{\varphi}\left(\mathbf{X}\left(\mathbf{x},t\right),t\right) = \varphi\left(\mathbf{x},t\right)$ is the Eulerian electrostatic potential such that

$$\frac{\partial\varphi}{\partial t}\bigg|_x = \frac{\partial\hat{\varphi}}{\partial t}\bigg|_X + \mathbf{V}.\nabla_R.\hat{\varphi}.$$

Equation 11.146 can also be written as a strict conservation law in the form

$$\frac{\partial}{\partial t}\mathbf{p}\bigg|_X - \mathrm{div}_R\mathbf{T}^{\mathrm{tot}} = \mathbf{0}, \tag{11.157}$$

wherein

$$\mathbf{T}^{\mathrm{tot}} = \mathbf{T} + \mathbf{T}^{\mathrm{em}} = \mathbf{T}^E + \mathbf{T}^F. \tag{11.158}$$

### 11.9.2 Constitutive Relations

We recall that $\mathbf{S}^E$ is the second (material and symmetric) Piola–Kirchhoff stress associated with $\mathbf{T}^E$ and that $W$ denotes the free energy per unit reference volume, $W = E - S\theta$, so that the Clausius–Duhem inequality reads

$$-\left(\dot{W} + S\dot{\theta}\right) + \frac{1}{2}\mathrm{tr}\left(\mathbf{S}^E.\dot{\mathbf{C}}\right) + \hat{\mathbf{E}}.\dot{\Pi} - \theta^{-1}\mathbf{Q}.\nabla_R\theta \geq 0 \tag{11.159}$$

or

$$-\left(\dot{\bar{W}} + S\dot{\theta}\right) + \frac{1}{2}\mathrm{tr}\left(\bar{\mathbf{S}}^E.\dot{\mathbf{C}}\right) - \Pi.\dot{\hat{\mathbf{E}}} - \theta^{-1}\mathbf{Q}.\nabla_R\theta \geq 0, \tag{11.160}$$

with

$$\bar{W} = W - \hat{\mathbf{E}}.\Pi, \quad \bar{\mathbf{S}}^E = \mathbf{S}^E - \left(\hat{\mathbf{E}}.\Pi\right)\mathbf{C}^{-1}. \tag{11.161}$$

Still another possibility is provided with (Maugin and Trimarco, 1997)

$$-\left(\dot{\hat{W}} + S\dot{\theta}\right) + \frac{1}{2}\mathrm{tr}\left(\hat{\mathbf{S}}^E.\dot{\mathbf{C}}\right) - \hat{\mathbf{D}}.\dot{\hat{\mathbf{E}}} - \theta^{-1}\mathbf{Q}.\nabla_R\theta \geq 0, \tag{11.162}$$

wherein

$$\hat{W} = \bar{W} + \frac{1}{2}\hat{\mathbf{E}}.\bar{\mathbf{E}}, \quad \hat{\mathbf{S}}^E = \bar{\mathbf{S}}^E + \frac{1}{2}\left(\hat{\mathbf{E}}.\bar{\mathbf{E}}\right)\mathbf{C}^{-1} - J_F^{-1}\bar{\mathbf{E}}\otimes\bar{\mathbf{E}}. \tag{11.163}$$

With the choice of free energy

$$\hat{W} = \hat{W}\left(\mathbf{C}, \hat{\mathbf{E}}, \theta; \mathbf{X}\right), \tag{11.164}$$

the usual argument of thermodynamic admissibility yields the constitutive equations

$$\hat{\mathbf{S}}^E = 2\frac{\partial \hat{W}}{\partial \mathbf{C}}, \quad \hat{\mathbf{D}} = -\frac{\partial \hat{W}}{\partial \hat{\mathbf{E}}}, \quad S = -\frac{\partial \hat{W}}{\partial \theta}, \tag{11.165}$$

while there remains the residual dissipation inequality

$$\mathbf{Q}\left(\mathbf{C}, \hat{\mathbf{E}}, \theta, \nabla_R \theta; \mathbf{X}\right).\nabla_R \theta \leq 0. \tag{11.166}$$

### 11.9.3 Canonical Balance Laws

These are the balance laws of energy and momentum associated with the space–time parametrization $(\mathbf{X},t)$. Since there are already several equivalent forms of the local balance of energy, the most sensible one is that obtained via the equation of mechanical energy, obtained by the inner product of (11.157) with $\mathbf{v}$, and then combining with $(11.158)_2$ to yield

$$\frac{\partial}{\partial t}\left(\frac{1}{2}\rho_0 \mathbf{v}^2 + \bar{E}\right)\Big|_X - \nabla_R.\left\{\left(\mathbf{T}^E + \mathbf{T}^F\right).\mathbf{v} + \hat{\mathbf{D}}\frac{\partial \hat{\varphi}}{\partial t}\Big|_X - \mathbf{Q}\right\} = -\hat{Q}_f \frac{\partial \hat{\varphi}}{\partial t}\Big|_X, \tag{11.167}$$

where

$$\bar{E} = W + S\theta - \hat{\mathbf{D}}.\hat{\mathbf{E}}. \tag{11.168}$$

Equation 11.167 has the advantage that, although not in a strict conservative form, it emphasizes the analogy between the roles played by the "velocities" $\mathbf{v} = \partial\chi/\partial t|_X$ and $\partial\hat{\varphi}/\partial t|_X$, hence between the elastic displacement and the electrostatic potential (which we know may form a useful four-dimensional Euclidean vector in some computations; cf. Maugin, Pouget et al., 1992). It obviously takes the form of a strict conservation law in the absence of free charges. Equation 11.147 is immediately recovered from (11.167) by noting that

$$\nabla_R.\mathbf{S}^e = \frac{\partial}{\partial t}\left(\hat{\mathbf{E}}.\hat{\mathbf{D}} - \hat{Q}_f\hat{\varphi}\right) + \nabla_R.\left(\hat{\mathbf{D}}\frac{\partial \hat{\varphi}}{\partial t}\Big|_X\right), \quad E = \bar{E} + \hat{\mathbf{E}}.\hat{\mathbf{D}}. \tag{11.169}$$

The second canonical balance law, that of material momentum, is obtained in strict parallel with (11.167) now following a routine procedure. The result is

$$\left.\frac{\partial \mathbf{P}}{\partial t}\right|_X - \mathrm{div}_R \mathbf{b} = \mathbf{f}^{\mathrm{inh}} + \mathbf{f}^{\mathrm{th}} + \mathbf{f}^e, \tag{11.170}$$

where we have set

$$\mathbf{P} = -\mathbf{p}.\mathbf{F} = \rho_0 \mathbf{C}.\mathbf{V}, \quad \mathbf{b} = -\left(L^{\mathrm{th}}\mathbf{1}_R + (\mathbf{T}^E + \mathbf{T}^F).\mathbf{F} - \hat{\mathbf{D}} \otimes \hat{\mathbf{E}}\right), \tag{11.171}$$

$$L^{\mathrm{th}} = \frac{1}{2}\rho_0(\mathbf{X})\mathbf{v}^2 - W\left(\mathbf{C}, \hat{\mathbf{E}}, \theta; \mathbf{X}\right), \quad \mathbf{f}^{\mathrm{inh}} = \left(\partial L^{\mathrm{th}}/\partial \mathbf{X}\right)_{\mathrm{expl}}, \tag{11.172}$$

$$\mathbf{f}^{\mathrm{th}} = S\nabla_R \theta, \quad \mathbf{f}^e = -\hat{Q}_f \hat{\mathbf{E}}. \tag{11.173}$$

The really new quantity here is the last material force, $\mathbf{f}^e$, which is none other than the pull back of the original volume force due to free charges, changed of sign. It is of interest to evaluate its power in a material motion, that is, the quantity $\mathbf{f}^e.\mathbf{V}$. On account of (11.156) we have the following remarkable result (Maugin and Trimarco, 1997):

$$P_B^e := \mathbf{f}^e.\mathbf{V} = \hat{Q}_f \left( \left.\frac{\partial \varphi}{\partial t}\right|_x - \left.\frac{\partial \hat{\varphi}}{\partial t}\right|_X \right). \tag{11.174}$$

This really exemplifies the fictitious nature of some material forces such as $\mathbf{f}^e$, as their power vanishes identically when the distinction between actual and reference configurations is lost.

### 11.9.4 Jump Relations at a Front

We consider from the start a homothermal singular surface with no dislocations so that we have the following two conditions of continuity:

$$[\theta] = 0, \quad [\mathbf{V}] = \mathbf{0} \quad \text{at} \quad \Sigma. \tag{11.175}$$

Now, without further explanation (see Chapter 7), we can apply the thumb rule to replace the partial differential operators $\nabla_R$ and $\partial/\partial t|_X$ applied to functions $f(\mathbf{X}, t)$ by the jump operators $\mathbf{N}.[..]$ and $-\overline{V}_N[..]$ and to introduce unknown surface source terms for those equations that are not strict conservations

laws at regular material points. Thus we have the following roster of jump equations in the present case:

$$\mathbf{N}\times\left[\hat{\mathbf{E}}\right]=\mathbf{0},\quad \mathbf{N}.\left[\hat{\mathbf{D}}\right]=Q_{\Sigma}^{e}, \tag{11.176}$$

$$\bar{V}_{N}\left[\rho_{0}\right]=0, \tag{11.177}$$

$$\mathbf{N}.\left[\bar{\mathbf{V}}\otimes\mathbf{p}+\mathbf{T}^{E}+\mathbf{T}^{F}\right]=\mathbf{0}, \tag{11.178}$$

$$\mathbf{N}.\left[\bar{\mathbf{V}}\left(\frac{1}{2}\mathbf{v}^{2}+\bar{E}\right)+\left(\mathbf{T}^{E}+\mathbf{T}^{F}\right).\mathbf{v}+\hat{\mathbf{D}}\frac{\partial\hat{\varphi}}{\partial t}\Big|_{X}-\mathbf{Q}\right]=h_{\Sigma}^{e}, \tag{11.179}$$

$$\mathbf{N}.\left[\bar{\mathbf{V}}\otimes\mathbf{P}+\mathbf{b}\right]+\mathbf{f}_{\Sigma}=\mathbf{0}, \tag{11.180}$$

$$\mathbf{N}.\left[\bar{\mathbf{V}}S\theta-\mathbf{Q}\right]-q_{\Sigma}=0, \tag{11.181}$$

and

$$\mathbf{N}.\left[\bar{\mathbf{V}}S-\left(\mathbf{Q}/\theta\right)\right]=\sigma_{\Sigma}\geq 0, \tag{11.182}$$

where a set of unknown surface sources is present in (11.179) through (11.182). These must be all consistent in order to respect the second law of thermodynamics expressed by the inequality in (11.182). The consistency between (11.181) and (11.182) already requires that

$$q_{\Sigma}\geq 0\quad \text{at}\quad \Sigma(t). \tag{11.183}$$

We do not give all the details of the derivation, which follows the same pattern as in previous sections (see, e.g., Section 7.5). Accordingly, on one hand we compute

$$P_{\Sigma}:=\mathbf{f}_{\Sigma}.\bar{\mathbf{V}}=-\bar{V}_{N}\left[\mathbf{P}.\bar{\mathbf{V}}\right]-\left[\mathbf{N}.\mathbf{b}.\bar{\mathbf{V}}\right], \tag{11.184}$$

from which there follows that

$$q_{\Sigma}=-\bar{V}_{N}\mathrm{Hugo}_{\mathrm{PT}}+Q_{\Sigma}^{e}\left\langle\frac{\partial\varphi}{\partial t}\Big|_{x}-\frac{\partial\hat{\varphi}}{\partial t}\Big|_{X}\right\rangle-\left(h_{\Sigma}^{e}+\left[\left(\mathbf{N}.\hat{\mathbf{D}}\right]\frac{\partial\boldsymbol{\varphi}}{\partial t}\Big|_{x}\right)\geq 0 \tag{11.185}$$

or

$$q_\Sigma = -\bar{V}_N \mathrm{Hugo}_{\mathrm{PT}} - Q_\Sigma^e \left\langle \left. \frac{\partial \hat{\varphi}}{\partial t} \right|_X \right\rangle - \left( h_\Sigma^e + \left\langle \mathbf{N}.\hat{\mathbf{D}} \right\rangle \left[ \left. \frac{\partial \varphi}{\partial t} \right|_x \right] \right) \geq 0, \tag{11.186}$$

where we have introduced the Hugoniot–Gibbs functional (which depends on the value of fields on both "sides" of Σ):

$$\mathrm{Hugo}_{\mathrm{PT}} := \left[ W - \left\langle \mathbf{N}.\left( \mathbf{T}^E + \mathbf{T}^F \right) \right\rangle . \frac{\partial \chi}{\partial N} - \left\langle \mathbf{N}.\hat{\mathbf{D}} \right\rangle \frac{\partial \varphi}{\partial N} \right], \tag{11.187}$$

where $\partial/\partial N$ denotes the normal derivative. The expression (11.186) deserves the following comments. First, only the normal component of $\bar{\mathbf{V}}$ is involved, thus emphasizing the local normal growth of one phase with respect to the other. The other two contributions in (11.186) are peculiar. We notice that application of a gauge condition at $\Sigma(t)$ for quasielectrostatics processes requires that

$$\left[ \left. \frac{\partial \varphi}{\partial t} \right|_x \right] = 0. \tag{11.188}$$

This condition is formally analogous to the coherency condition $(11.175)_2$. Therefore, it could be referred to as the *electric coherency condition*. Then from (11.186) there remains

$$q_\Sigma = -\bar{V}_N \mathrm{Hugo}_{\mathrm{PT}} - Q_\Sigma^e \left\langle \left. \frac{\partial \hat{\varphi}}{\partial t} \right|_X \right\rangle - h_\Sigma^e \geq 0. \tag{11.189}$$

The formally introduced surface heat $h_\Sigma^e$ may be viewed as some kind of latent heat characteristic of the examined electroelastic crystal.

Had we considered a *dielectric* material to start with, we would have introduced neither $h_\Sigma^e$ nor $Q_\Sigma^e$, and so (11.186) would reduce to the "simple" expression

$$\theta_\Sigma \sigma_\Sigma = q_\Sigma = f_\Sigma \bar{V}_N \geq 0, \tag{11.190}$$

where the scalar *driving force* $f_\Sigma$ is introduced through the following *surface balance* of scalar material forces:

$$f_\Sigma + \mathrm{Hugo}_{\mathrm{PT}} = 0 \quad \text{at} \quad \Sigma(t). \tag{11.191}$$

This emphasizes the different ontological nature of the two scalar material forces as $\text{Hugo}_{\text{PT}}$ is a (functional) field quantity, while $f_\Sigma$ is a thermodynamic force determined by the application of the theory of irreversible thermodynamics to the pair of conjugate variables $(f_\Sigma, \bar{V}_N)$, yielding eventually a *kinetic relation* of the type

$$\bar{V}_N = \tilde{V}\left(f_\Sigma; \theta_\Sigma\right) \tag{11.192}$$

respecting the inequality (11.190).

Returning to the more general case in Equation 11.189, we note that the expression

$$P_\Sigma^e = -Q_\Sigma^e \left\langle \left. \frac{\partial \hat{\varphi}}{\partial t} \right|_X \right\rangle \tag{11.193}$$

has formally the same structure as the bulk power (11.174) because, if a gauge condition of the type $\partial\varphi/\partial t\big|_x = 0$ holds at all material points, the latter reduces to

$$P_B^e = -Q_f \left. \frac{\partial \hat{\varphi}}{\partial t} \right|_X, \tag{11.194}$$

whose the similarity with (11.193) is obvious. Quantities such as (11.193) will naturally appear if, at $\Sigma$, we have possible recombinations of charge, as this phenomenon occurs at junctions in electroelastic semiconductors (classical jump conditions for these are given in Daher and Maugin [1986b, 1988]).

**REMARK 11.1:** Concerning works in the line of the presentation in this chapter, we note Jiang Qing (1994), but he is **erroneous**. In the line of further generalization to the case of more complex electroelastic materials, we first note that the most promising way of expressing the electric constitutive equation was provided in the 1960s and 1970s by R.A. Toupin, H.F. Tiersten, and the present author, via a local bulk balance equation

$$\mathbf{E} + \mathbf{E}^L = \mathbf{0}, \tag{11.195}$$

where $\mathbf{E}$ is the Maxwellian electric field (i.e., the one appearing in Maxwell's equation) and $\mathbf{E}^L$ is a *local* electric that, in a crystal, represents phenomenologically the interactions between the crystal lattice and the electric polarization field and for which a constitutive equation is given. There is, therefore, some similarity between a balance equation such as (11.195) in the bulk and a surface balance equation such as (11.191). The latter will be more involved if the interface possesses its own energy and elasticity, and maybe some

inertia (mass) adding surface divergence and inertial terms. Similarly, in more complex electroelastic materials such as elastic ferroelectrics and elastic ionic crystals (see Chapter 7 in Maugin, 1988, and also Maugin, Pouget et al., 1992), Equation 11.195 is augmented by a divergence term related to the gradient of electric polarization and an inertia term, reading in a generic form as

$$\mathbf{E} + \mathbf{E}^L + \mathrm{div}\,\widehat{\mathbf{E}} = d\ddot{\mathbf{P}}, \tag{a}$$

where $\widehat{\mathbf{E}}$ basically accounts for the gradient of electric polarization (a term representative of ferroelectric ordering in the case of ferroelectrics, of the shell–shell interaction in ionic crystals), and the right-hand side is obviously related to some "acceleration" effect with an "inertia" $d$, $\mathbf{P}$ being considered as an additional *observable* field related to the electric microstructure. Equation (a) is the basis for dynamic studies such as that of polaritons and also electric solitons (Maugin and Pouget, 1980; Pouget and Maugin, 1984; Maugin, Pouget et al., 1992). With the appropriate energy considerations, the left-hand side of (a) can be shown to be nothing but the functional derivative of an electric enthalpy $H$ with respect to electric polarization, for example,

$$\mathbf{E}^{\mathrm{eff}} := \mathbf{E} + \mathbf{E}^L + \mathrm{div}\,\widehat{\mathbf{E}} \equiv -\frac{\delta H}{\delta \mathbf{P}} = -\left(\frac{\partial H}{\partial \mathbf{P}} - \nabla.\frac{\partial H}{\partial(\nabla \mathbf{P})}\right). \tag{b}$$

The corresponding canonical equations of energy and momentum that are useful in fracture and phase-transition front progress have been established by Maugin and Restuccia (2004). We do not report these since we shall deal at some length in the following with the magnetic analog in elastic ferromagnets. However, recent progress has been achieved in the study of ferroelectric domain walls and their interactions with defects in ferroelectrics. For this purpose, one does not need to consider polarization gradients (which play a prominent role in thin layers of strong gradients presenting no discontinuity per se). In this case, a ferroelectric domain wall separating two domains of spatially uniform electric polarization is acted on by a driving force that is the sum over the wall of a material force akin to a pressure, such as

$$T_N = \int_{\mathrm{wall}} \tau_N dA, \quad \tau_N = \mathbf{N}.\left[\mathbf{b}\right]_{\mathrm{wall}}.\mathbf{N}, \tag{c}$$

with, in the quasistatics of small strains (see (11.187) and (11.171))$_2$,

$$\mathbf{b} = H\mathbf{1} - \sigma.(\nabla \mathbf{u})^T - \mathbf{D} \otimes \nabla\varphi, \quad \sigma = \frac{\partial H}{\partial \varepsilon}, \quad \mathbf{D} = -\frac{\partial H}{\partial \mathbf{E}}. \tag{d}$$

Let $\bar{V}_N$ be the normal velocity of the wall. Thermodynamic admissibility (satisfaction of the second law at the wall) applies with a *kinetic relation* of the (over-)simplified form (Schrade et al., 2006):

$$\bar{V}_N = \mu_T (T_N - T_0) \text{ for } T_N \geq T_0, \quad = 0 \text{ for } |T_N| < T_0,$$
$$\text{and} \quad = \mu_T (T_N + T_0) \text{ for } T_N \leq -T_0, \tag{e}$$

where the parameters $\mu_T$ and $T_0$ are material parameters to be calibrated such that the material response is consistent with reported homogeneous defect-free cases. Such kinetics is exploited in the study of the interaction of domain walls with electrode defects at the surface of a sample or a polarization defect represented by a small region of frozen polarization (Schrade et al., 2006). Polarization gradients can also be reintroduced but with **P**, then the remanent polarization, considered as an *internal* variable of state (in fact, an order parameter for the electric behavior according to the Landau theory; see Maugin, 1999), in which case the dissipation inequality reduces to

$$\widehat{\mathbf{E}}.\dot{\mathbf{P}} \geq 0. \tag{f}$$

A simple relation à la Ginzburg–Landau in the form

$$\dot{\mathbf{P}} = \tau \widehat{\mathbf{E}} = -\tau \left( \frac{\partial H}{\partial \mathbf{P}} - \nabla . \frac{\partial H}{\partial (\nabla \mathbf{P})} \right) \tag{g}$$

will do, with a scalar coefficient $\tau$ playing the role of a relaxation time measuring the distance from thermodynamic equilibrium. This model was exploited by Schrade et al. (2007) to study numerically the domain evolution in ferroelectrics with domain walls of nonvanishing thickness.

## 11.10 The Case of Magnetized Elastic Materials

### 11.10.1 Introductory Remark

Various classes of magnetizable elastic materials exist, among which one identifies the paramagnetic and soft-ferromagnetic bodies, and the so-called hard ferromagnets (see Maugin, 1988). Within the working hypothesis of quasimagnetostatics in insulators, the first two classes are treated on the basis of Maxwell's magnetostatic equations (in the Laboratory frame):

$$\nabla . \mathbf{B} = 0, \quad \nabla \times \mathbf{H} = \mathbf{0}, \quad \mathbf{H} = \mathbf{B} - \mathbf{M}. \tag{11.196}$$

This translates into the material form as

$$\nabla_R.\hat{\mathbf{B}} = 0, \quad \nabla_R \times \hat{\mathbf{H}} = \mathbf{0}, \tag{11.197}$$

with

$$\hat{\mathbf{B}} = J_F\mathbf{F}^{-1}.\mathbf{B}, \quad \hat{\mathbf{H}} = \mathbf{H}.\mathbf{F}, \quad \hat{\mathbf{M}} = \mathbf{M}.\mathbf{F}, \quad \hat{\mathbf{H}} = J_F^{-1}\mathbf{C}.\hat{\mathbf{B}} - \hat{\mathbf{M}}. \tag{11.198}$$

The coupling between the crystal lattice and the magnetization field is represented by a local bulk balance equation, comparable to (11.195), that is,

$$\mathbf{B} + \mathbf{B}^L = \mathbf{0}, \tag{11.199}$$

where $\mathbf{B}$ is the Maxwellian field appearing in the first of Equation 11.196 and $\mathbf{B}^L$ is the local magnetic induction for which one needs a constitutive equation in terms of magneto-mechanical fields. Because of (11.197), there exists a quasistatic magnetic potential $\varphi$ in the actual configuration or $\hat{\varphi}$ in the material framework, so that

$$\mathbf{H} = -\nabla\varphi, \quad \hat{\mathbf{H}} = -\nabla_R\hat{\varphi}. \tag{11.200}$$

Then the perspicacious reader has already noticed that we can practically translate all that we did in the quasielectrostatic case to this magnetic case. This was indeed achieved by Sabir and Maugin (1996), who gave the canonical equations of energy and material momentum for this case and corresponding *J*-integrals for *magnetoelastic fracture*, noting that, just like in the electric case, there is a plurality of formulations of the energy conservation and, therefore, the possibility to construct different *J*-integrals. This applies in particular to materials with high *magnetostrictive coupling* (piezomagnetism being a rare event) such as TERFENOL-D. We refer the reader to these authors for such developments.

Much more interesting from the conceptual viewpoint is the case of elastic (hard) ferromagnets because such materials exemplify the problem of formulating canonical balance laws in media equipped with a microstructure, here a magnetic one, which is equivalent to considering additional internal degrees of freedom in a continuum (compare to Chapter 9). Here, this is materialized by the fact that Equation 11.199 is replaced by a true dynamic equation containing a flux. In addition, the new internal degree of freedom, represented by the precession of a *spin*, is peculiar in the sense that it has a gyroscopic nature, having no closed form for its kinetic energy in classical physics (the phenomenon is inherently quantum mechanical). It is a so-called *d'Alembertian inertia couple* that does not expend power (see Maugin, 1988, Chapter 6). This is an interesting challenge for the formulation of canonical

balance laws in the material framework. This was achieved by Fomethe and Maugin (1996) with applications to the propagation of ferromagnetic phase-transition fronts and ferromagnetic domain walls (Fomethe and Maugin, 1997b; Maugin and Fomethe, 1997).

### 11.10.2 The Equations Governing Elastic Ferromagnets

Working within the framework of the quasimagnetostatics of insulators for which (11.196) through (11.198) hold good, it is also assumed that the magnetization per unit mass, the vector $\mu$ in the actual configuration, has reached *saturation*, so that we have

$$\mu^2 = \mu.\mu = \mu_S^2, \quad \mu = \mu(\mathbf{X},t) = \mathbf{M}/\rho, \tag{11.201}$$

so that

$$\mu.\dot{\mu} = 0, \quad (\nabla_R \mu).\mu = 0, \tag{11.202}$$

wherein

$$\dot{\mu} = \left.\frac{\partial \mu(\mathbf{X},t)}{\partial t}\right|_X. \tag{11.203}$$

Then, in addition to (11.197), we have the following field equations in the Piola–Kirchhoff format:

$$\left.\frac{\partial}{\partial t}\rho_0\right|_X = 0, \tag{11.204}$$

$$\left.\frac{\partial \mathbf{p}}{\partial t}\right|_X - \mathrm{div}_R \mathbf{T} = \mathbf{f}^M, \tag{11.205}$$

$$\left.\frac{\partial}{\partial t}\left(\frac{1}{2}\rho_0 \mathbf{v}^2 + E - \rho_0 \mathbf{B}.\mu\right)\right|_X - \nabla_R.\left(\mathbf{T}.\mathbf{v} + \widehat{\mathbf{B}}.\dot{\mu} - \mathbf{Q}\right) = 0, \tag{11.206}$$

and

$$\left.\frac{\partial \mu}{\partial t}\right|_X - \omega \times \mu = \mathbf{0}, \quad \omega = -\gamma \mathbf{B}^{\mathrm{eff}}, \tag{11.207}$$

where (11.204) through (11.206) are traditional, and (11.207) is the *precession equation* of the magnetic spin density in which $\gamma$ is the so-called *gyromagnetic ratio* of the material, $\mathbf{T}$ is the standard first Piola–Kirchhoff stress (defined from the Cauchy stress), $\mathbf{f}^M$ is the magnetic force in the quasimagnetostatic approximation, $\mathbf{B}^{\text{eff}}$ is the effective magnetic induction felt by the magnetization field, and $\widehat{\mathbf{B}}$ is a two-point tensor field associated with spin–spin interactions (so-called ferromagnetic exchange effects), such that

$$\mathbf{T} = J_F \mathbf{F}^{-1}.\sigma, \quad \mathbf{T}^M = J_F \mathbf{F}^{-1}.\mathbf{t}^M, \tag{11.208}$$

$$\mathbf{f}^M = \mathrm{div}_R \mathbf{T}^M, \quad \mathbf{t}^M = \mathbf{B}\otimes\mathbf{B} - \mathbf{B}\otimes\mathbf{M} - \left(\frac{1}{2}\mathbf{B}^2 - \mathbf{M}.\mathbf{B}\right)\mathbf{1}, \tag{11.209}$$

$$\mathbf{B}^{\text{eff}} = \mathbf{B} + \mathbf{B}^L + \rho^{-1}\mathrm{div}\,\breve{\mathbf{B}} = \mathbf{B} + \mathbf{B}^L + \rho_0^{-1}\mathrm{div}_R\widehat{\mathbf{B}}, \quad \widehat{\mathbf{B}} = J_F^{-1}\mathbf{F}.\breve{\mathbf{B}}. \tag{11.210}$$

With a free energy per unit reference volume

$$W = E - S\theta = \bar{W}\left(\mathbf{F}, \theta, \mu, \nabla_R \mu; \mathbf{X}\right), \tag{11.211}$$

a thermodynamic study based on the exploitation of the relevant Clausius–Duhem inequality shows that the following constitutive equations are obtained:

$$\mathbf{T} = \frac{\partial \bar{W}}{\partial \mathbf{F}}, \quad S = -\frac{\partial \bar{W}}{\partial \theta}, \quad \mathbf{B}^L = -\rho_0^{-1}\frac{\partial \bar{W}}{\partial \mu}, \quad \widehat{\mathbf{B}} = \frac{\partial \bar{W}}{\partial\left(\nabla_R \mu\right)}, \tag{11.212}$$

while there remains heat conduction $\mathbf{Q}$ satisfying the second law in the form

$$\mathbf{Q}.\nabla_R\theta \le 0, \quad \mathbf{Q}\left(.,.,.,\nabla_R\theta \to 0; \mathbf{X}\right) = \mathbf{0}. \tag{11.213}$$

Heat conduction being the only dissipative process considered at this point, the balance of entropy has the now-traditional form

$$\theta \left.\frac{\partial S}{\partial t}\right|_X + \nabla_R.\mathbf{Q} = 0. \tag{11.214}$$

Note. Equation 11.207 obviously fulfills the constraint (11.201). It also justifies the naming of d'Alembertian inertia couple for the magnetic spin inertia, since in computing the power of the mechanical couple $(-\gamma^{-1}\dot{\mu})$ we obviously have

$$\left(\gamma^{-1}\dot{\mu}\right).\omega \equiv 0. \tag{11.215}$$

Accordingly, there is no kinetic energy in closed form for the spin inertia (at least in the framework of classical continuum mechanics), and this has consequences for the next point examined here.

### 11.10.3 Canonical Balance of Material Momentum

This has been established by Fomethe and Maugin (1996) in the following form using the same method as for other cases in previous sections and chapters:

$$\left.\frac{\partial \mathbf{P}}{\partial t}\right|_X - \mathrm{div}_R \mathbf{b} = \mathbf{f}^{\mathrm{inh}} + \mathbf{f}^{\mathrm{th}} + \mathbf{f}^{\mathrm{fer}}, \tag{11.216}$$

wherein

$$\mathbf{P} = -\mathbf{p}.\mathbf{F} = \rho_0 \mathbf{C}.\mathbf{V}, \tag{11.217}$$

$$\mathbf{b} = -\left(L^{\mathrm{th}}\mathbf{1}_R + \mathbf{T}.\mathbf{F} + \widehat{\mathbf{B}}.\left(\nabla_R \mu\right)^T\right), \tag{11.218}$$

$$L^{\mathrm{th}} = \frac{1}{2}\rho_0 \mathbf{v}^2 - W + \rho_0 \mathbf{B}.\mu, \quad \mathbf{f}^{\mathrm{inh}} = \left(\partial \overline{W}/\partial \mathbf{X}\right)_{\mathrm{expl}}, \tag{11.219}$$

$$\mathbf{f}^{\mathrm{th}} = S\nabla_R \theta, \quad \mathbf{f}^{\mathrm{fer}} = \rho_0 \mathbf{B}^{\mathrm{eff}}.\left(\nabla_R \mu\right)^T. \tag{11.220}$$

Here the originality of this case is most obvious. Although we are dealing with a material with an internal degree of freedom of rotation (precession to be more precise), the kinetic energy and the Lagrangian density do not contain a related inertial term. This latter, with its peculiar gyroscopic nature, materializes in the presence of an additional material force in the right-hand side of (11.216). This is the "force" $\mathbf{f}^{\mathrm{fer}}$. Fomethe and Maugin (1996, Appendix), via a somewhat tedious but definitive and clear-cut computation, have shown that the canonical balance covariant law (11.216) is exactly consistent with the canonical energy balance (11.206). They did this by computing the inner product of (11.216) with the material velocity and showing that the result is none other than (11.206), with the particular enlightening intermediate result

$$\mathbf{f}^{\mathrm{fer}}.\mathbf{V} = \rho_0 \mathbf{B}^{\mathrm{eff}}.\left.\frac{\partial \mu}{\partial t}\right|_X, \tag{11.221}$$

with the timelike component complementing the material force $\mathbf{f}^{\mathrm{fer}}$ in a four-dimensional formulation (the time derivative $\partial/\partial t|_X$ replacing the material

gradient $\nabla_R$). This consistency being checked, one can now establish the set of jump relations that will govern ferromagnetoelastic transition fronts.

### 11.10.4 Phase-Transition Fronts in Thermoelastic Ferromagnets

With the conditions (11.175) being fulfilled at the propagating discontinuity surface $\Sigma(t)$, the jump relations of the present theory are established following the same method as in previous sections for other cases, save for the complexity of some calculations. We report only the results as obtained by Fomethe and Maugin (1997a, 1997b):

$$\mathbf{N}.\left[\hat{\mathbf{B}}\right]=0,\quad \mathbf{N}\times\left[\hat{\mathbf{H}}\right]=\mathbf{0}, \tag{11.222}$$

$$\bar{V}_N\left[\rho_0\right]=0, \tag{11.223}$$

$$\mathbf{N}.\left[\bar{\mathbf{V}}\otimes\mathbf{p}+\mathbf{T}+\mathbf{T}^M\right]=\mathbf{0}, \tag{11.224}$$

$$\mathbf{N}.\left[\bar{\mathbf{V}}\left(\frac{1}{2}\rho_0\mathbf{v}^2+E-\rho_0\mathbf{B}.\mu\right)+\left(\mathbf{T}.\mathbf{v}+\hat{\mathbf{B}}.\dot{\mu}-\mathbf{Q}\right)\right]=0, \tag{11.225}$$

which exhibit no source terms, and the set

$$\mathbf{N}.\left[\bar{\mathbf{V}}\otimes\mathbf{P}+\mathbf{b}\right]+\mathbf{f}_\Sigma=\mathbf{0}, \tag{11.226}$$

$$\mathbf{N}.\left[\bar{\mathbf{V}}S\theta-\mathbf{Q}\right]-q_\Sigma=0, \tag{11.227}$$

$$\mathbf{N}.\left[\bar{\mathbf{V}}S-\left(\mathbf{Q}/\theta\right)\right]=\sigma_\Sigma\geq 0. \tag{11.228}$$

Furthermore, the jump relation associated with the precession equation (11.207) reads

$$\left[\left(\mathbf{N}.\hat{\mathbf{B}}\right)\times\mu+\gamma^{-1}\mu\,\bar{V}_N\right]=\mathbf{0}, \tag{11.229}$$

or the stronger conditions

$$\mathbf{N}.\left[\hat{\mathbf{B}}\right]+\lambda_\Sigma\left[\mu\right]=\mathbf{0}, \tag{11.230}$$

where $\lambda_\Sigma$ is an unknown multiplier.

The continuity conditions

$$[\theta] = 0, \quad [\mathbf{V}] = \mathbf{0} \tag{11.231}$$

are imposed. It follows from the first of these that $\sigma_\Sigma = \theta_\Sigma^{-1} q_\Sigma$. Finally, in the discrete vision, if the same lattice sites (particles) belong to the two lattices (no dislocations; this is here accounted for by the second of (11.231)), then the "particles" at $\Sigma(t)$ must have a magnetic spin that evolves in the same way as seen from each side of the interface. Thus an extra kinematic condition is needed that is necessarily of the form (note the analogy with the second of (11.231)) on account of the initial definition of $\mathbf{V}$):

$$\left[ \left. \frac{\partial \mu(\mathbf{x},t)}{\partial t} \right|_x \right] = \mathbf{0}. \tag{11.232}$$

On account of (11.222) through (11.232), Maugin and Fomethe (1997) have proved the following results:

$$P_\Sigma(\mathbf{f}_\Sigma) = \mathbf{f}_\Sigma . \bar{\mathbf{V}} = -\bar{V}_N \mathrm{Hugo}_{\mathrm{PT}}^{\mathrm{fer}} \tag{11.233}$$

and

$$q_\Sigma = P_\Sigma - [\mathbf{N}.\widehat{\mathbf{B}}] . \left\langle \left. \frac{\partial \mu}{\partial t} \right|_x \right\rangle = -\left( [\mathbf{N}.(\mathbf{b} + \mathbf{V} \otimes \mathbf{P})] . \left\langle \left. \frac{\partial \mathbf{X}}{\partial t} \right|_x \right\rangle + [\mathbf{N}.\widehat{\mathbf{B}}] . \left\langle \left. \frac{\partial \mu}{\partial t} \right|_x \right\rangle \right), \tag{11.234}$$

the latter exhibiting a symmetry between the effects of mechanics and ferromagnetism. The Hugoniot–Gibbs functional here is given by

$$\mathrm{Hugo}_{\mathrm{PT}}^{\mathrm{fer}} := \left[ W^{\mathrm{tot}} + \rho_0 \langle \tau \rangle \langle \mathbf{M} \rangle . \mathbf{B} - \langle \mathbf{N}.\mathbf{T} \rangle . \mathbf{F}.\mathbf{N} - \langle \mathbf{N}.\widehat{\mathbf{B}} \rangle . (\mathbf{N}.\nabla_R) \mu \right], \tag{11.235}$$

where $\tau = \rho^{-1}$.

In the case where the strong condition (11.230) applies, then on account of the saturation condition, we have the orthogonality relation

$$[\mu] \cdot \left\langle \frac{\partial \mu(\mathbf{x},t)}{\partial t} \right\rangle \equiv 0 \tag{11.236}$$

and the second term in $q_\Sigma$ vanishes, so that we are reduced to a more classical result (compare to other chapters):

$$\theta_\Sigma \sigma_\Sigma = q_\Sigma = f_\Sigma \bar{V}_N \geq 0, \quad f_\Sigma + \mathrm{Hugo}_{\mathrm{PT}}^{\mathrm{fer}} = 0 \quad \text{at} \quad \Sigma(t). \tag{11.237}$$

One is then led to construct a *kinetic relation* between $\bar{V}_N$ and $f_\Sigma$ that respects the second law of thermodynamics expressed by the inequality sign in (11.237).

**Soft Ferromagnets and Paramagnets**

The case of soft ferromagnets or paramagnets can be recovered from the present case by neglecting magnetic-spin inertia and magnetic ordering, which are characteristic of hard ferromagnets. Thus, we have to set $\dot{\mathbf{B}} = \mathbf{0}$, and the first of (11.207) will be reduced to the "equilibrium" form (11.199). Considering small strains, (11.235) now takes the reduced form

$$\mathrm{Hugo}^{\mathrm{s.fer}}_{\mathrm{PT}} = \left[W - \langle \mathbf{B} \rangle . \mathbf{M} - \langle \mathbf{N}.\mathbf{T} \rangle . \mathbf{F}.\mathbf{N}\right], \tag{11.238}$$

where

$$\mathbf{B} = \frac{\partial W}{\partial \mathbf{M}}, \quad \mathbf{T} = \frac{\partial W}{\partial \mathbf{F}}, \quad S = -\frac{\partial W}{\partial \theta}, \quad W = W(\mathbf{F}, \mathbf{M}, \theta). \tag{11.239}$$

The first two contributions in the jump in (11.238) can be transformed thus. Setting

$$\bar{W}(\mathbf{F}, \mathbf{H}, \theta) = W + \frac{1}{2}(\mathbf{H}^2 - \mathbf{B}^2) = W - \mathbf{M}.\mathbf{B} + \frac{1}{2}\mathbf{M}^2 = W - \left(\frac{1}{2}\mathbf{H}^2 + \mathbf{M}.\mathbf{H}\right), \tag{11.240}$$

and introducing the magnetic scalar potential $\varphi$, the strain $\varepsilon$, and the elastic displacement $\mathbf{u}$, we immediately show that (11.238) takes on the following form:

$$\mathrm{Hugo}^{\mathrm{s.fer}}_{\mathrm{PT}} = \left[\bar{W}(\varepsilon, \mathbf{H}, \theta) - \langle \mathbf{M} \rangle . \nabla\varphi - \langle \mathbf{N}.\mathbf{T} \rangle . (\nabla \mathbf{u})^T . \mathbf{N}\right], \tag{11.241}$$

with the constitutive equations

$$\mathbf{M} = \frac{\partial \bar{W}}{\partial \mathbf{H}}, \quad \mathbf{T} = \frac{\partial \bar{W}}{\partial \varepsilon}, \quad S = -\frac{\partial \bar{W}}{\partial \theta}. \tag{11.242}$$

An equivalent formulation is

$$\mathrm{Hugo}^{\mathrm{s.fer}}_{\mathrm{PT}} = \left[\tilde{W}(\varepsilon, \mathbf{H}, \theta) - \langle \mathbf{B} \rangle . \nabla\varphi - \langle \mathbf{N}.\mathbf{T} \rangle . (\nabla \mathbf{u})^T . \mathbf{N}\right], \tag{11.243}$$

with

$$\mathbf{B} = \frac{\partial \tilde{W}}{\partial \mathbf{H}}, \quad \mathbf{T} = \frac{\partial \tilde{W}}{\partial \varepsilon}, \quad S = -\frac{\partial \tilde{W}}{\partial \theta}. \tag{11.244}$$

We recognize in the formulas (11.241) and (11.243) the structure of the two possible Eshelby stresses and the two *J*-integrals introduced previously in the study of the fracture of elastic paramagnets and soft ferromagnets (Sabir and Maugin, 1996). The transformation (11.240) was originally introduced in Maugin (1971, p. 85c)—also in Abd-Alla and Maugin (1987).

### 11.10.5 Domain Walls in Ferromagnets

The remarkable feature about the results (11.233) is that, although they most often describe a kinematics on the material manifold, they also apply to the case of *rigid bodies*, where, then, $\Sigma(t)$ reduces to a transition in magnetic properties only. Indeed, for rigid bodies (11.233) reduces to

$$\text{Hugo}^{\text{fer}} = \left[ W(\mathbf{M},\theta) - \langle \mathbf{B} \rangle . \mathbf{M} - \langle \mathbf{N}.\widehat{\mathbf{B}} \rangle . (\mathbf{N}.\nabla\mu) \right]. \tag{11.245}$$

We can also use a free energy

$$\hat{W}(\mathbf{M},\theta) = W(\mathbf{M},\theta) - \frac{1}{2}\mathbf{M}^2, \tag{11.246}$$

so that (11.245) also reads

$$\text{Hugo}^{\text{fer}} = \left[ \hat{W}(\mathbf{M},\theta) - \langle \mathbf{H} \rangle . \mathbf{M} - \langle \mathbf{N}.\widehat{\mathbf{B}} \rangle . (\mathbf{N}.\nabla\mu) \right]. \tag{11.247}$$

In particular, this relation holds through a magnetic domain wall that separates two magnetic domains, when the wall is viewed as an interface of vanishingly small thickness, a magnetic domain being a region of the material where magnetization has reached a spatially uniform state. Then we may inquire about the possible propagation of a magnetic domain wall under the application of a magnetic field of sufficient strength. This, indeed, with an irreversible motion of the wall, is the basic mechanism of the irreversible magnetization of macroscopic ferromagnetic samples, which gives rise to *magnetic hysteresis*. Let us show that the basic ideas are contained in the phenomenological description given in the preceding. To that purpose we consider the case of a so-called 180° domain wall through which magnetization, of the same amplitude $M_S$ but in the opposite direction on both sides and parallel to the wall, rotates by 180° (but we do not see this rotation in the flattened wall and so just observe a jump from a distance—only a zoom on the wall would evidence this rotation—see Figure 11.1). Accordingly we do not pay attention to whether the wall is of the *Bloch type* (out-of-plane rotation) or of the *Néel type* (in-plane rotation) as this detail is irrelevant. Let us apply in thought a magnetic field $\mathbf{H}^{\text{appl}}$ parallel to the wall and in the direction of the magnetization on the minus side $V^-$ of the wall. Physical common

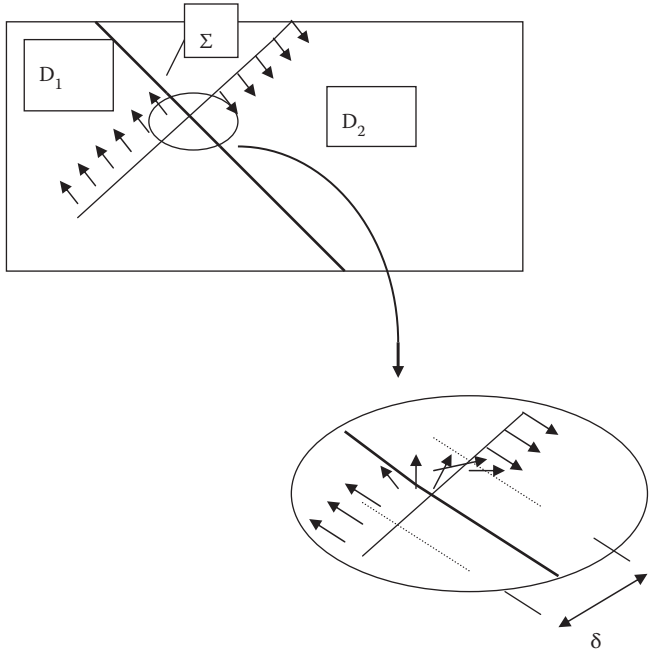


**FIGURE 11.1**
Domain wall seen as a sharp discontinuity surface and blowup showing the wall structure (in-plane rotation of a 180° Néel wall).

sense says that the domain on the minus side $V^-$, being already favorably oriented, should grow at the expense of the domain $V^+$. As the magnetization has reached saturation in both domains with the same magnitude $M_S$ and is spatially uniform in each domain, and both domains have, therefore, the same energy density, the Hugoniot–Gibbs driving force of interest in (11.247) reduces to the very simple expression

$$\text{Hugo}^{\text{fer}} = \left[-\langle \mathbf{H} \rangle . \mathbf{M}\right] = \mathbf{H}^{\text{appl}} . \left[-\mathbf{M}\right] = 2 M_S H^{\text{appl}}, \tag{11.248}$$

where $H^{\text{appl}}$ is the amplitude of the applied field. As $M_S$ is a characteristic property of the ferromagnet under examination and we consider a flat domain wall, we can as well replace the normal velocity $\bar{V}_N$ by the time rate of change of the residual magnetization $M^R$ and $\text{Hugo}^{\text{fer}}$ and its opposite $f_\Sigma$ by a quantity akin to a magnetic field. We simply have to divide the energies by $2M_S$ and note that, per unit area of $\Sigma(t)$ and unit time, $\bar{V}_N$ generates a magnetization equal to $M_S \times \bar{V}_N$. Thus the application of the formalism (11.248) and (11.233), and an analogy with the evolution equation in elastoplasticity (cf. Maugin, 1992b), provide an admissible evolution equation for irreversible magnetization due to the displacement of one wall (in a one-dimensional model) in the form

$$\dot{M}^R = -\dot{\lambda}\left.\frac{\partial F}{\partial H}\right|_{H=H^{\text{appl}}}, \quad \dot{\lambda} \geq 0, \tag{11.249}$$

where $F$ is a dissipation potential, $\dot{\lambda}$ is a multiplier, and the minus sign originates from the fact that we use directly $\text{Hugo}^{\text{fer}} / 2M_S$ as a *dissipative driving force* rather than $f_\Sigma$. As an example, we may consider Néel's (1942, 1943) celebrated process of irreversible magnetization, where magnetic domain walls move in a landscape of energy barriers, or a distribution of pinning magnetic field $H^A$, the latter providing the threshold that the applied field must reach to detach a wall from its anchoring and allowing for its subsequent motion (practically a jump being given the quasi-instantaneity of the process) to the next anchoring site. This argument yields for (11.249) the following elementary *evolution equation of* irreversible magnetization:

$$\dot{M}^R = \left(\text{sign}\, H^{\text{appl}}\right)\left|\dot{M}^R\right| \quad \text{for} \quad \left|H^{\text{appl}}\right| = H^A, \quad \text{and} \quad 0 \quad \text{otherwise.} \tag{11.250}$$

We have thus recovered the semimicroscopic magnetization model devised by Sabir and Maugin (1988) by analogy with elastoplasticity. Although they did not use the present Eshelbian concepts, these authors indeed had the volume energy $2M_S H^{\text{appl}}$ as the driving force of irreversible magnetization. At this point it must be recalled that the macroscopic irreversible magnetization for a multidomain sample is then obtained by statistical average over an ensemble of magnetic domains of various orientations. Furthermore, according to the preceding vision the motion of domain walls between obstacles is instantaneous. This is the so-called *Barkhausen effect*, which materializes in a magnetic-flux emission by the jerky motion of domain walls. A more realistic vision should grant a characteristic (but short) time to the transition of a magnetic domain wall between two anchoring sites, hence some kind of internal viscosity. This supports a view of magnetization processes that is closer in spirit to that of viscosplasticity (cf. Maugin, 1992b). This was indeed formulated by Sabir and Maugin (1988) and the analogy with the viscoplasticity of Bingham fluids is fully drawn in Maugin (1999).

## Appendix A11.1: Proof of Theorem 11.1 and Corollary 11.2

- First, we show that (11.26) follows from the action (11.56). There is no shame in using components when it proves more convenient than the intrinsic notation. The Euler–Lagrange equations generated by the fields $\hat{\varphi}$ and $\hat{\mathbf{A}}$ read

$$\left(\frac{\partial L}{\partial \hat{\varphi}}\right)_{\text{expl}} - \frac{\partial}{\partial t}\left(\frac{\partial L}{\partial\left(\partial\hat{\varphi}/\partial t\right)}\right)\Bigg|_X - \nabla_R \cdot \left(\frac{\partial L}{\partial\left(\nabla_R \hat{\varphi}\right)}\right) = 0 \tag{A11.1}$$

and

$$\left(\frac{\partial L}{\partial \hat{\mathbf{A}}}\right)_{\text{expl}} - \frac{\partial}{\partial t}\left(\frac{\partial L}{\partial\left(\partial\hat{\mathbf{A}}/\partial t\right)}\right)\Bigg|_X - \text{div}_R\left(\frac{\partial L}{\partial\left(\nabla_R \hat{\mathbf{A}}\right)}\right) = \mathbf{0}. \tag{A11.2}$$

In the present case

$$\left(\frac{\partial L}{\partial \hat{\varphi}}\right)_{\text{expl}} = 0, \quad \frac{\partial L}{\partial\left(\partial\hat{\varphi}/\partial t\right)} = 0, \tag{A11.3}$$

and

$$c\frac{\partial L}{\partial\left(\partial\hat{\mathbf{A}}/\partial t\right)} = -\frac{\partial L}{\partial \tilde{\mathbf{E}}} = -\frac{\partial L^{\text{emf}}}{\partial \tilde{\mathbf{E}}} + \frac{\partial W}{\partial \tilde{\mathbf{E}}} = -J_F \mathbf{C}^{-1}.\tilde{\mathbf{E}} + \left(\partial W/\partial \tilde{\mathbf{E}}\right) = -\hat{\mathbf{D}}, \tag{A11.4}$$

$$\frac{\partial L}{\partial\left(\nabla_R \hat{\varphi}\right)} = -\frac{\partial L}{\partial \hat{\mathbf{E}}} = -\frac{\partial L}{\partial \tilde{\mathbf{E}}} = -\hat{\mathbf{D}}, \tag{A11.5}$$

$$\frac{\partial L}{\partial\left(\nabla_R \hat{\mathbf{A}}\right)_{KL}} = -\varepsilon^{KLM}\frac{\partial L}{\partial \tilde{B}^M}, \tag{A11.6}$$

or

$$\begin{aligned}\frac{\partial L}{\partial\left(\nabla_R \hat{\mathbf{A}}\right)_{KL}} &= -\varepsilon^{KLQ}\left(\left(J_F/c\right)\varepsilon_{QNP}V^P\left(\mathbf{C}^{-1}\right)^{NJ}\tilde{E}_J - J_F^{-1}C_{QP}\hat{B}^P + \left(\partial W/\partial \hat{B}\right)^Q\right) \\ &= \varepsilon^{KLQ}\left(J_F^{-1}\left(\mathbf{C}.\hat{\mathbf{B}}\right)_Q - \frac{1}{c}\mathbf{V}\times\left(\mathbf{C}^{-1}.\tilde{\mathbf{E}}\right)_Q - \hat{M}_Q\right),\end{aligned} \tag{A11.7}$$

if we set

$$\hat{\mathbf{D}} = J_F\mathbf{C}^{-1}.\tilde{\mathbf{E}} + \Pi, \quad \Pi = -\partial W/\partial \tilde{\mathbf{E}}, \quad \hat{\mathbf{M}} = -\partial W/\partial \hat{\mathbf{B}}. \tag{A11.8}$$

Furthermore, with the definition

$$\hat{\mathbf{H}} = J_F^{-1}\mathbf{C}.\hat{\mathbf{B}} - \hat{\mathbf{M}}, \tag{A11.9}$$

and accounting for the results (A11.3) through (A.11.8), we obtain the equations (11.26).

- Next we consider the equation of motion that follows from the Euler–Lagrange equation:

$$\left(\frac{\partial L}{\partial \mathbf{x}}\right)_{\text{expl}} - \frac{\partial}{\partial t}\left(\frac{\partial L}{\partial \mathbf{v}}\right)\Big|_X - \text{div}_R\left(\frac{\partial L}{\partial \mathbf{F}}\right) = \mathbf{0}. \tag{A11.10}$$

Here we have

$$\left(\frac{\partial L}{\partial \mathbf{x}}\right)_{\text{expl}} = \mathbf{0}, \quad \frac{\partial L}{\partial \mathbf{v}} = \frac{\partial L^{\text{md}}}{\partial \mathbf{v}} + \frac{\partial L^{\text{emf}}}{\partial \mathbf{v}}, \quad \frac{\partial L^{\text{md}}}{\partial \mathbf{v}} = \rho_0 \mathbf{v}, \tag{A11.11}$$

and

$$\frac{\partial L^{\text{emf}}}{\partial \mathbf{v}} = -J_F^{-1}\frac{\partial \hat{\mathbf{B}}}{\partial \mathbf{v}}.\left(\mathbf{C}.\hat{\mathbf{B}}\right) = \frac{1}{c}\left(\mathbf{E}\times\left(\mathbf{F}^{-1}\right)^T\right).\left(\mathbf{C}.\hat{\mathbf{B}}\right) = \frac{1}{c}J_F\mathbf{E}\times\mathbf{B}. \tag{A11.12}$$

Thus (cf. (11.43))

$$\frac{\partial L}{\partial \mathbf{v}} = \rho_0\left(\mathbf{v} + \frac{1}{c}\frac{\mathbf{E}\times\mathbf{B}}{\rho}\right) = \mathbf{p}_R^{\text{tot}}. \tag{A11.13}$$

We further note that $L$ depends on $\mathbf{F}$ through the $\mathbf{C}^{-1}$ and $\mathbf{C}$ present in $L^{\text{emf}}$, and explicitly in $W$ and implicitly via $\tilde{\mathbf{E}}$ and $\tilde{\mathbf{B}}$ also in $W$. We recommend to the reader to go through all the steps. Thus,

$$\frac{\partial L^{\text{emf}}}{\partial \mathbf{F}} = H^{\text{emf}}\mathbf{F}^{-1} - J_F\left(\mathbf{C}^{-1}.\tilde{\mathbf{E}}\right)\otimes\mathbf{E} - \hat{\mathbf{B}}\otimes\mathbf{B}, \quad \frac{\partial L^{\text{md}}}{\partial \mathbf{F}} = -\frac{\partial W}{\partial \mathbf{F}}, \tag{A11.14}$$

with

$$H^{\text{emf}} = \frac{1}{2}J_F\left(\mathbf{E}^2 + \mathbf{B}^2\right) = \frac{1}{2}J_F\tilde{\mathbf{E}}.\mathbf{C}^{-1}.\tilde{\mathbf{E}} + \frac{1}{2}J_F^{-1}\tilde{\mathbf{B}}.\mathbf{C}.\tilde{\mathbf{B}}, \tag{A11.15}$$

and

$$\frac{\partial W}{\partial \mathbf{F}} = \left(\frac{\partial W}{\partial \mathbf{F}}\right)_{\text{expl}} + \frac{\partial W}{\partial \tilde{\mathbf{E}}}.\frac{\partial \tilde{\mathbf{E}}}{\partial \mathbf{F}} + \frac{\partial W}{\partial \tilde{\mathbf{B}}}.\frac{\partial \tilde{\mathbf{B}}}{\partial \mathbf{F}} = \mathbf{T}^E - \boldsymbol{\Pi} \otimes \mathbf{E} + \tilde{\mathbf{B}} \otimes \bar{\mathbf{M}} - \left(\hat{\mathbf{M}}.\tilde{\mathbf{B}}\right)\mathbf{F}^{-1}. \tag{A11.16}$$

Thus,

$$\mathbf{T}^{\text{emf}} = -\frac{\partial L^{\text{emf}}}{\partial \mathbf{F}}, \quad \mathbf{T}^E = -\frac{\partial L^{\text{md}}}{\partial \mathbf{F}} = \left(\frac{\partial W}{\partial \mathbf{F}}\right)_{\text{expl}}, \tag{A11.17}$$

with

$$\mathbf{T}^{\text{emf}} = \left(J_F \mathbf{C}^{-1}.\tilde{\mathbf{E}}\right) \otimes \mathbf{E} + \tilde{\mathbf{B}} \otimes \mathbf{B} - H^{\text{emf}} \mathbf{F}^{-1}, \tag{A11.18}$$

$$\mathbf{T}^{\text{inter}} := \boldsymbol{\Pi} \otimes \mathbf{E} - \hat{\mathbf{B}} \otimes \bar{\mathbf{M}} + \left(\hat{\mathbf{M}}.\bar{\mathbf{B}}\right)\mathbf{F}^{-1}, \tag{A11.19}$$

$$\mathbf{T} = \mathbf{T}^E - \mathbf{T}^{\text{inter}}, \quad \mathbf{T}^{\text{emm}} = \mathbf{T}^f + \mathbf{T}^{\text{inter}}, \tag{A11.20}$$

so that we obtain two equivalent forms of the balance of linear (physical) momentum in the Piola–Kirchhoff format:

$$\frac{\partial}{\partial t}\left(\mathbf{p}_R + \mathbf{p}_R^f\right)\Big|_X - \text{div}_R\left(\mathbf{T}^E + \mathbf{T}^f + \hat{\mathbf{p}}^f \otimes \mathbf{v}\right) = \mathbf{0}, \tag{A11.21}$$

and

$$\frac{\partial}{\partial t}\left(\mathbf{p}_R + \mathbf{p}_R^f\right)\Big|_X - \text{div}_R\left(\mathbf{T} + \mathbf{T}^{\text{emm}} + \hat{\mathbf{p}}^f \otimes \mathbf{v}\right) = \mathbf{0}, \tag{A11.22}$$

wherein

$$\mathbf{T}^{\text{emm}} = J_f \mathbf{F}^{-1}.\mathbf{t}^{\text{emm}}, \quad \mathbf{T}^{\text{inter}} = J_F \mathbf{F}^{-1}.\mathbf{t}^{\text{inter}}. \tag{A11.23}$$

- **Proof of Corollary 11.2:** We could derive this result by direct but painstaking computation from (A11.21) or (A11.22). It is simpler to use the general formulas deduced from Noether's theorem in field

theory (Section 4.2 for a first-order gradient theory). To do this, we need in particular to evaluate the following quantities:

$$\mathbf{v}.\frac{\partial L}{\partial \mathbf{v}}, \quad \frac{\partial L}{\partial \mathbf{v}}.\mathbf{F}, \quad \frac{\partial L}{\partial \mathbf{F}}.\mathbf{F}, \quad \left(\frac{\partial L}{\partial \mathbf{X}}\right)_{\text{expl}}, \tag{A11.24}$$

noting that the identity (11.50) holds true for the free electromagnetic fields. We check that

$$\frac{\partial W}{\partial \mathbf{v}}.\mathbf{F} \equiv -\frac{\partial W}{\partial \mathbf{V}} = -\frac{\partial W}{\partial \tilde{\mathbf{E}}}.\frac{\partial \tilde{\mathbf{E}}}{\partial \mathbf{V}} = \Pi \times \left(\hat{\mathbf{B}} / c\right), \tag{A11.25}$$

so that

$$\frac{\partial L^{\text{md}}}{\partial \mathbf{v}}.\mathbf{F} = -\frac{\partial K}{\partial \mathbf{V}} + \frac{\partial W}{\partial \mathbf{V}} = -\rho_0 \mathbf{C}.\mathbf{V} - \frac{1}{c}\Pi \times \hat{\mathbf{B}} = -\mathbf{P}^{\text{tot}}. \tag{A11.26}$$

We impose objectivity on $W$ so that the latter will depend on $\mathbf{F}$ only through a material strain measure such as $\mathbf{C}$. Gathering all contributions we indeed obtain the result (11.58) since we can write

$$\begin{aligned}\mathbf{T}.\mathbf{F} &= -\frac{\partial L^{\text{md}}}{\partial \mathbf{F}}.\mathbf{F} = \frac{\partial W}{\partial \mathbf{F}}.\mathbf{F} = \left(2\frac{\partial W}{\partial \mathbf{C}}.\frac{\partial \mathbf{C}}{\partial \mathbf{F}} - \Pi \otimes \mathbf{E} + \hat{\mathbf{B}} \otimes \bar{\mathbf{M}} - \left(\hat{\mathbf{M}}.\tilde{\mathbf{B}}\right)\mathbf{F}^{-1}\right).\mathbf{F} \\ &= \left(\mathbf{S}^{E} - \left(\mathbf{C}^{-1}.\tilde{\mathbf{E}}\right) \otimes \Pi + \left(\mathbf{C}^{-1}.\hat{\mathbf{M}}\right) \otimes \tilde{\mathbf{B}} - \left(\hat{\mathbf{M}}.\tilde{\mathbf{B}}\right)\mathbf{C}^{-1}\right).\mathbf{C}.\end{aligned} \tag{A11.27}$$

In the original paper (Maugin, 1990), the contribution $(\hat{\mathbf{M}}.\tilde{\mathbf{B}})\mathbf{1}_R$, which obviously results from the last contribution in (A11.27), was gathered with $W$ in the isotropic contribution to $\mathbf{b}^{\text{tot}}$ so that there appeared a kind of Legendre–Fenchel transformation on the strain–interaction energy such as

$$\hat{W}\left(\mathbf{C}, \tilde{\mathbf{E}}, \tilde{\mathbf{B}}; \mathbf{X}\right) + \hat{\mathbf{M}}.\tilde{\mathbf{B}} = \breve{W}\left(\mathbf{C}, \tilde{\mathbf{E}}, \hat{\mathbf{M}}; \mathbf{X}\right), \tag{A11.28}$$

together with the dual constitutive relations

$$\hat{\mathbf{M}} = -\frac{\partial \hat{W}}{\partial \tilde{\mathbf{B}}}, \quad \tilde{\mathbf{B}} = -\frac{\partial \breve{W}}{\partial \hat{\mathbf{M}}}. \tag{A11.29}$$

This is often an artifact of some thermodynamic presentations in electromagnetic materials (see the discussion in Chapter 3 in Maugin [1988]).

# 12

# *Application to Nonlinear Waves*

## Object of the Chapter

Where waves, which made the great Shakespeare ponder the world of nature, are shown to have fundamental properties that relate to the already introduced notions and make the best use of notions of the accompanying apparatus as they share properties with particles in a dualism that solitonic systems illustrate perfectly.

## 12.1 Wave Momentum in Crystal Mechanics

### 12.1.1 Definition

As a preliminary, we remind the reader of the *small-strain formulation* of Section 3.2. In particular, we have the following in the framework of pure elasticity theory:
*Balance of physical (linear) momentum:*

$$\rho_0 \frac{\partial^2 \mathbf{u}}{\partial t^2} - \operatorname{div} \sigma = \mathbf{0}, \quad \sigma = \frac{\partial W}{\partial \varepsilon}, \quad \varepsilon \equiv \left(\nabla \mathbf{u}\right)_S, \tag{12.1}$$

where $\sigma$ is the symmetric Cauchy stress tensor, $\varepsilon$ is the infinitesimal stress, and $W(\varepsilon)$ is the strain energy per unit volume. Here, we now longer distinguish between actual and reference configurations. This does not mean, however, that the balance of *field* momentum reduces to the same as the balance of *linear* momentum because the former is, of necessity, an equation with the same degree of nonlinearity (or singularity) as the energy equation. Therefore, it remains an equation that is at least quadratic in the fields $\sigma$ and $\varepsilon$. Any "linearization" of this equation is a misconception of the role of that equation (for such a case, see Müller, 1999). Accordingly, the balance of field momentum remains Equation 3.27 with (see also Potapov et al., 2005)

$$P^f = -\rho_0 (\nabla \mathbf{u}).\frac{\partial \mathbf{u}}{\partial t}, \tag{12.2}$$

$$\mathbf{b}^f = -\left(L\mathbf{1} + \sigma.(\nabla \mathbf{u})^T\right), \tag{12.3}$$

$$L = \frac{1}{2}\rho_0 \left(\frac{\partial \mathbf{u}}{\partial t}\right)^2 - W(\varepsilon), \tag{12.4}$$

where $W(\varepsilon)$ need not be restricted to a quadratic function in $\varepsilon$ since, if we neglect geometric nonlinearities here, we may keep physical nonlinearities (expressions of a higher order than quadratic for $W$, even nonconvex ones). In this framework $P^f$ is also referred to as the *crystal momentum* for an elastic crystal, after the pioneering work of Brenig (1955). As a matter of fact, for quantified elastic waves under the name of *phonons* (these are special types of so-called *quasiparticles* that are quantum-mechanically associated with definite types, here elastic, of vibrations), this is the momentum that directly quantifies to *de Broglie's formula*:

$$P^f = \hbar \mathbf{K}, \tag{12.5}$$

where $\hbar$ is Planck's reduced constant, and $\mathbf{K}$ is the wave vector. Notice that in the nonlinear framework, the wave vector is a *covariant vector* (since it is the dual of material position $\mathbf{X}$), and thus we understand the proportionality relation between the naturally covariant vector $P$ or $P^f$ and $\mathbf{k}$ (see Maugin, 1993, pp. 35–37 and Chapter 9). Because of its role in *wave propagation*, $P^f$ is also referred to as the *wave momentum*, $P^w$. Here we discuss this matter in the purely elastic case, but such considerations can be extended to more complicated cases, coupled systems, and so on. In the following, this is considered by way of example in the framework of nonlinear wave propagation associated with some remarkable systems of partial differential equations, in particular those demonstrating both nonlinearity and dispersion. Because of the mathematical difficulties involved, most, if not all, examples are one-dimensional in space. Accordingly, the following remark is spot on.

### 12.2.2 Beware of One-Dimensional Systems!

If we consider the case of linear isotropic homogeneous elasticity in one dimension of space with Hooke's modulus $E$ and characteristic wave speed $c = (E/\rho_0)^{1/2}$, the balance of linear physical momentum yields the ubiquitous wave equation

$$u_{tt} - c^2 u_{xx} = 0, \tag{12.6}$$

in an obvious notation. The corresponding energy equation reads

$$\frac{\partial}{\partial t}\left(\frac{1}{2}\rho_0 u_t^2 + \frac{1}{2}E u_x^2\right) - \frac{\partial}{\partial x}\left((E u_x)u_t\right) = 0. \tag{12.7}$$

From its very definition, the balance of canonical (here field) momentum reads

$$\frac{\partial}{\partial t}\left(-(\rho_0 u_t)u_x\right) - \frac{\partial}{\partial x}\left(\left(\frac{1}{2}E u_x^2 - \frac{1}{2}\rho_0 u_t^2\right) - (E u_x)u_x\right) = 0. \tag{12.8}$$

The last two equations can also be written in the following remarkable form:

$$\frac{\partial H}{\partial t} + c^2\frac{\partial P^f}{\partial x} = 0, \quad \frac{\partial P^f}{\partial t} + \frac{\partial H}{\partial x} = 0. \tag{12.9}$$

Even more remarkably, this shows that both $H$ and $P^f$ satisfy the original wave equation (12.6) since by elimination between the two equations (12.9), one obtains

$$H_{tt} - c^2 H_{xx} = 0, \quad \left(P^f\right)_{tt} - c^2\left(P^f\right)_{xx} = 0. \tag{12.10}$$

Interesting as it is, however, this result is misleading, for it is an artifact of the one-dimensional formulation. In effect, the energy equation is normally a scalar one, while the balance of momentum is co*vectorial*. The misleading symmetry induced by the one-dimensional nature between these two equations was noticed by W.D. Hayes (1974, pp. 23–24) when he wrote down the Equation 12.9 as two quadratic-invariant equations deduced from (12.6) (without the present Eshelbian framework and the consequences in Equation 12.10). Hayes simply comments that the "freedom of generating new solutions by differentiation or integration must be kept in mind, as these generate new conservation laws." This is what happens in the theory of solitonic structures.

## 12.2 Conservation Laws in Soliton Theory

An often-cited exemplary equation in this context is the so-called *Boussinesq equation*, which has origins in both fluid mechanics and crystal mechanics

(cf. Christov et al., 2007). In appropriate units, this may be considered as the field equation of elasticity deduced from a second-gradient of displacement elasticity or strain-gradient elasticity (see Section 4.3.3). It is a one-dimensional (in space) dispersive but nondissipative nonlinear model deduced from the following Lagrangian and energy densities:

$$L = \frac{1}{2}u_t^2 - W\left(u_x, u_{xx}\right), \quad W = \frac{1}{2}\left( u_x^2 + \frac{2}{3}\varepsilon u_x^3 + \varepsilon\delta^2 u_{xx}^2 \right). \tag{12.11}$$

The resulting Euler–Lagrangian equation is the following nonlinear dispersive wave equation (the celebrated Boussinesq equation):

$$u_{tt} - u_{xx}\left(1 + \varepsilon u_x\right) - \varepsilon\delta^2 u_{xxxx} = 0, \tag{12.12}$$

where ε is an infinitesimally small parameter characteristic of the *nonlinearity* and δ is a length characteristic of a weak *nonlocality* (dispersion) of the modeling. This equation is none other than the field equation (balance of linear physical momentum)

$$\frac{\partial}{\partial t}\left(u_t\right) - \frac{\partial}{\partial x}\left(\sigma^{\text{eff}}\right) = 0, \tag{12.13}$$

with

$$\sigma^{\text{eff}} = \frac{\delta W}{\delta u_x} = \sigma - m_x, \quad \sigma = \frac{\partial W}{\partial u_x}, \quad m = \frac{\partial W}{\partial u_{xx}}. \tag{12.14}$$

The energy equation is easily established, while the balance of field momentum is given by

$$\frac{\partial}{\partial t}\left(P^f\right) - \frac{\partial}{\partial x}\left(b^{\text{eff}}\right) = 0, \tag{12.15}$$

with

$$P^f = -u_x u_t, \quad b^{\text{eff}} = -\left(L + u_x\sigma + 2u_{xx}m\right) - \left(u_x m\right)_x. \tag{12.16}$$

Integrating this over the whole real line $R$, we obtain the global conservation of field momentum as

$$\frac{dP(R)}{dt} = \left[b^{\text{eff}}\right]_{-\infty}^{+\infty}, \quad P(R) := \int_R P^f dx. \tag{12.17}$$

This is a Newtonian equation of motion in which the jump between the two end values of the effective Eshelby "tensor," here a scalar, plays the role of a *driving force*. A material inhomogeneity or an additional externally prescribed term in the right-hand side of (12.13) will also bring additional driving forces in the right-hand side of $(12.17)_1$.

But it happens that the Boussinesq equation (12.12), like many equations belonging to the same class (what we called the Boussinesq paradigm; cf. Christov et al., 2007), possesses strongly localized nonlinear solutions (kinks for $u$ and humps for $u_t$) with appropriate space and time derivatives vanishing at infinities. Thus Equation 12.17 reduces to the equation of an *inertial motion* for these solutions:

$$\frac{dP(R)}{dt} = 0 \quad \text{and} \quad \frac{dH(R)}{dt} = 0, \quad H(R) := \int_R H dx. \tag{12.18}$$

If an external force perturbing density $\mu f(x)$ were acting in the right-hand side of (12.12), $\mu$ being a small parameter, then the first of (12.18) would be perturbed in the following way:

$$\frac{dP}{dt} = -\varepsilon^2 \int_R u_x f(x) dx, \tag{12.19}$$

where we took $\mu = 0(\varepsilon)$, and one has to find from (12.19) the modulation of the parameters of the localized nonlinear wave due to the perturbation.

The Boussinesq equation has acquired much of its celebrity through the derived equation called the *Korteweg–de Vries* (*KdV*) *equation*, which is in fact the one-directional wave equation deduced from (12.12) by means of the so-called *reductive perturbation method* (cf. Newell, 1985; Maugin, Pouget et al., 1992). After appropriate nondimensionalization this equation reads

$$\frac{\partial v}{\partial t} + v\frac{\partial v}{\partial x} + \beta\frac{\partial^3 v}{\partial x^3} = 0, \quad \beta = \frac{c_0^2}{2k_0^2} > 0, \tag{12.20}$$

where $c_0$ and $k_0$ are characteristic speed and wave number. This equation (Korteweg, de Vries, Boussinesq, and Rayleigh) admits *exact solitary-waves* solutions in the form of a *hump*, $u(x \to \pm\infty) = 0$, of the type

$$v = v_0 sech^2\left(\frac{x - ct}{\Delta}\right), \tag{12.21}$$

under the condition that speed $c$ and amplitude $v_0$ be related by

$$v_0 = 3c, \quad \Delta^2 = 2c_0/ck_0^2, \quad \text{hence} \quad v_0\Delta^2 = 6c_0/k_0^2 = \text{const.} \tag{12.22}$$

Accordingly, the faster the wave, the narrower its profile. We also note that the wavelike solution is *supersonic* as $c > c_0$. We also remark that a simple-wave trial solution of the type $u \approx \bar{u}(x - ct)$ in (12.12) would have resulted in a kink-like solution in the form of a tanh solution (of which (12.21) is a derivative). The existence of such solutions is due to a strict compensation between nonlinear effects (steepening of a solution to form a shock; signals with higher amplitude would go faster) and dispersive ones (broadening of the signal due to differing speeds of propagation for various Fourier components).

Not only does Equation 12.20 admit exact localized solutions such as (12.21) but such solutions, although truly nonlinear, in some sense practically superimpose each other linearly since two such solutions traveling in opposite direction interact without further perturbation than a change in phase, recovering their individuality after encounter (collision). This is the property of being **solitonic** per se in a strict mathematical sense. In nonexactly solitonic systems, the interactions of "individuals" are usually accompanied by the production of radiation. As a matter of fact, the pioneers (and creators) of soliton theory, such as Kruskal and Zabusky (1966) and Kruskal (1974) for the KdV equation, soon realized that systems of equations prone to the pure solitonic type of dynamic behavior admit new conservation laws in addition to the usual ones. It was further shown that for exactly integrable systems (those indeed admitting true soliton solutions), an infinite number of conservation laws exist, and special algorithms were developed to generate these conservation laws (in this regard, see, e.g., Ablowitz and Segur, 1981, Section 1.6; Calogero and Degasperis, 1982, Chapter 5). If the field equations used to describe solitons are derived in a field-theoretic context from a Lagrangian (or Hamiltonian), then these new conservation laws correspond to *symmetry properties* and result from the application of Noether's theorem (Fokas, 1979). However, only a few of these conservation laws can bear an easily grasped physical significance. The reader may now have realized where we want to lead him since those easily meaningfully interpreted conservation laws are those that pertain to our Eshelbian or canonical framework (this we fully realized and applied in the years 1990–1992, having, of course, buried in the back of our mind the courses and seminars we took with M.D. Kruskal and W.D. Hayes at Princeton some 20 years before). These conservation laws are those that are more critically related to the particle-like features of true solitons—which are thus kinds of *quasiparticles*—in the course of so-called elastic collision or interactions. Canonical *momentum* is one of these features. Other such features are *mass* and *energy*, these three quantities forming, if possible, a true *point mechanics*, the type of which depends on the starting system of partial differential equations. Newtonian

and Lorentzian–Einsteinian point mechanics are examples of such mechanics. Others can be created that no direct evidence could bring to the fore.

Of course, a duality between soliton-like solutions of some systems issued from quantum physics and elementary particles was rapidly established by nuclear and high-energy physicists (see Rebbi and Soliani, 1984). We must also remember the attempts of L. de Broglie and D. Bohm to reconcile quantum physics and a causal interpretation by introducing, in a nonlinear framework, the notion of *pilot wave* guiding the amplitude of the probability ($|\psi|^2$) of presence of a particle as a wave of singularity for which conservation laws and a hydrodynamic analogy play an essential role (see Holland, 1993, pp. 113–124, and also Jammer, 1974). It is possible that the present developments bear some relationship to this, but we emphasize that we are mostly interested in macroscopic problems issued from engineering sciences and phenomenological physics (e.g., in the crystalline state).

## 12.3 Examples of Solitonic Systems and Associated Quasiparticles

Here we follow essentially the contribution of Maugin and Christov (2002).

### 12.3.1 Korteweg–de Vries Equation

The KdV equation (12.20) can also be itself written as a conservation law (here with a different normalization):

$$\frac{\partial v}{\partial t} + \frac{\partial}{\partial x}\left(3v^2 + v_{xx}\right) = 0. \tag{12.23}$$

A straightforward application of the powerful algorithm proposed by Ablowitz and Segur (1981, p. 56) yields the following next-order conservation law:

$$\frac{\partial}{\partial t}\left(v^2 + v_{xx}\right) + \frac{\partial}{\partial x}\left(4v^3 + 8vv_x + 5v_x^2 + v_{xxxx}\right) = 0. \tag{12.24}$$

But in early studies of the KdV equation (cf. Miura, 1974), when such algorithms did not exist, it was proposed to consider the following conservation law:

$$\frac{\partial}{\partial t}\left(\frac{1}{2}v^2\right) + \frac{\partial}{\partial x}\left(2v^3 + vv_{xx} - \frac{1}{2}v_x^2\right) = 0. \tag{12.25}$$

We have shown (Maugin and Christov, 2002) that the difference between (12.24) and (12.25) is also none other than a conservation law. This shows that there exists an infinity of conservation laws associated with (12.23) and containing the contribution $v^2$ in the conserved quantity. Here, also, a false symmetry between successive conservation laws can be built, being merely an arteiact of the one-dimensionality in space of the considered system. For instance, one can build a conservation law where the conserved quantity is nothing but the flux present in (12.23) (cf. Maugin and Christov, 2002). However, the first conserved quantity in (12.23) suggests that we introduce the *potential* $\overline{u}$ of $v$ by $v = \overline{u}_x$, so that we can introduce the conserved mass $M_0$ by

$$M_0 = \int_R v dx = \left[\overline{u}\right]_{-\infty}^{+\infty}, \tag{12.26}$$

where [..] denotes the difference (the "jump") between values of the enclosure at the two infinities along the real line. That is, alternatively, $M_0$ may be qualified as the "difference of potential" or "voltage" of the solution. This seems to be a satisfactory gross "measure" of the solution. It would then seem that $v^2$ would be a good local measure of the energy. But this is not true. Indeed, it is shown that the KdV equation derives, as a Hamiltonian system, from the total Hamiltonian

$$H(R) = -\int_R \left( v^3 - \frac{1}{2} v_x^2 \right) dx. \tag{12.27}$$

while Bhatnagar (1979, p. 126) indeed reports the following conservation law:

$$\frac{\partial}{\partial t}\left( v^3 - \frac{1}{2} v_x^2 \right) + \frac{\partial}{\partial x}\left( \frac{9}{2} v^4 + 3v^2 v_{xx} + \frac{1}{2} v_{xx}^2 + v_x v_t \right) = 0. \tag{12.28}$$

This is the third conservation law in the hierarchy following along the line of (12.23) and (12.25). Applying the canonical definition of momentum to the auxiliary (potential) field $\overline{u}$ already introduced in (12.26), we have

$$P(R) = -\int_R \overline{u}_x \overline{u}_t \, dx, \tag{12.29}$$

and noting that $\bar{u}$ satisfies the following nonlinear evolution equation (NEE)

$$\bar{u}_t + 3\bar{u}_x^2 + \bar{u}_{xxx} = 0, \tag{12.30}$$

we obtain

$$P(R) = \int_R \left(3v^2 + vv_{xx}\right)dx. \tag{12.31}$$

The corresponding local conservation of canonical momentum would be obtained by noting that the second derivative of (12.23), with respect to $x$, reads

$$\frac{\partial}{\partial t}v_{xx} + \frac{\partial}{\partial x}\left(6v^3 + 6vv_x + v_{xxxx}\right) = 0, \tag{12.32}$$

and combining this in some way linearly with (12.25) for traveling wave solutions. This is not extremely useful, and the introduction of the "potential" $\bar{u}$ is tantamount to saying that, insofar as the quasiparticle description of one-directional wave equations such as (12.23) is concerned, the basic form is to be found in the original two-directional wave equation, here the Boussinesq (BO) equation. That is why we next examine the BO equation in its "good" or improved guise.

### 12.3.2 "Good" Boussinesq Equation

This is a nonlinear dispersive wave equation of the form

$$u_{tt} - u_{xx} - \left(u^2 - u_{xx}\right)_{xx} = 0. \tag{12.33}$$

The essential difference with (12.12) is the change in sign in front of the fourth-order space derivative. The reason for that is the bad linear dispersive behavior exhibited by the original equation (so-called *anomalous dispersion*). Equation 12.33 also corresponds to a one-dimensional model of strain-gradient elasticity. Upon introduction of auxiliary variables $q$ and $w$, this can be rewritten as the following Hamiltonian system (see Sanz-Serna and Calvo, 1994):

$$u_t = q_x, \quad w = u_x, \quad q_t = w_x^2 + w_{xx} - w, \tag{12.34}$$

in which the first two are mere definitions of $q$ and $w$. The mass $M$, momentum $P$, and energy $E$ of soliton solutions of (12.33) or (12.34) are given by

$$M = \int_R u\,dx, \tag{12.35}$$

$$P(R) = -\int_R uq\,dx, \tag{12.36}$$

and

$$E(R) = \frac{1}{2}\int_R \left( q^2 + w^2 + u^2 + \frac{2}{3}u^3 \right) dx. \tag{12.37}$$

As the system considered is exactly integrable, the quantities just defined are strictly conserved. But their expressions may look somewhat awkward. However, introducing the potential $\bar{u}$ by $u = \bar{u}_x$ with the condition $\bar{u}(x \to -\infty) = 0$, it is verified that

$$M = \left[\bar{u}\right]_{-\infty}^{+\infty}, \quad \bar{u}_t = q, \quad uq = \bar{u}_x \bar{u}_t, \quad \frac{1}{2}q^2 = \frac{1}{2}\bar{u}_t^2, \tag{12.38}$$

so that $M$ has the same interpretation as in the KdV case, while $P$ and $E$ indeed take their canonical definitions in terms of the potential $\bar{u}$. Simultaneously, in terms of elasticity theory, it is $\bar{u}$ that has the meaning of a displacement while $u$ is a strain per se. But accepting the general philosophy of continuum mechanics, we can also consider Equation 12.33 as a field equation issued from second-grade nonlinear elasticity and multiply it by $u_x$ and integrate by parts to arrive at the equation of field momentum (cf. (12.13))

$$\frac{\partial}{\partial t} P^f - \frac{\partial}{\partial x} b^{\text{eff}} = 0, \quad P^f := -u_x u_t. \tag{12.39}$$

### 12.3.3 Generalized Bousssinesq Equation

There are several ways to generalize the BO equation, obviously leading to nonexactly integrable systems. One such system is obtained while studying the ferroelastic phase transition as a dynamic process in elastic crystals (Maugin, 1987; Pouget, 1988). Here we examine the generalization of this modeling proposed by Christov and Maugin (1993) when approaching the difference scheme of lattice dynamics in a more accurate way than usually done. With $s = v_x$ a *shear strain*, from a lattice-dynamics approach and a long-

wavelength limit, while neglecting coupling with other strain components, one obtains the following type of equation:

$$s_{tt} - c_T^2 s_{xx} - \left(F(s) - \beta s_{xx} + s_{xxxx}\right)_{xx} = 0, \tag{12.40}$$

where $F$ is a polynomial in $s$ starting with second degree (e.g., a nonconvex function admitting three minima), $c_T$ is a characteristic speed, and $\beta$ is a positive scalar. It can be said that both the nonlinearity and dispersion have been increased compared to the classical BO equation (cf. Bogdan et al., 1999). Equation 12.40 is *stiff* in the sense that it involves a sixth-order space derivative, a situation that obviously imposes rather strong limit conditions at infinity or at the ends of a finite interval in numerical simulations. In spite of its apparent complexity (12.40) admits solitary-wave solutions (Christov and Maugin, 1993) that involve the ubiquitous *sech* function (but at the fourth power) for a single value of the phase speed—the existence of different solitary-wave solutions with a continuous spectrum for $c$ was shown numerically (Christov et al., 1996). But it is true that for a velocity too close to $c_T$ these solutions are not able to preserve their shape and eventually transform into pulses that, in turn, exhibit a self-similar (kind of "big bang") behavior as long as the amplitude of the pulse decreases while its support increases (a phenomenon analogous to a *red shift*). These pulses practically pass through each other without changing qualitatively their shapes—save the red-shifting—with perfect conservation of "mass" and "energy," so that these pulses may qualitatively be claimed to be "solitons" (Christov and Maugin, 1993).

The "mass," "momentum," and "energy" of the system (12.40) can be defined thus. Let $F(s) = -dU(s)/ds$. First, we rewrite Equation 12.40 as a *Hamiltonian system* by introducing the triplet $(s, q, w)$ such that Equation 12.40 is equivalent to

$$s_t = q_{xx}, \quad w = s_{xx}, \quad q_t = c_T^2 s + F(s) - \beta w + w_{xx}. \tag{12.41}$$

Then we have

$$M = \int_R s\,dx = \left[v\right]_{-\infty}^{+\infty}, \tag{12.42}$$

$$P(R) = -\int_R s q_x\,dx = -\int_R v_x v_t\,dx, \tag{12.43}$$

$$E(R) = \frac{1}{2}\int_R \left(c_T^2 s^2 + q_x^2 - 2U(s) + \beta s_x^2 + w^2\right)dx, \tag{12.44}$$

that is,

$$E(R) = \frac{1}{2}\int_R \left(c_T^2 s^2 + v_t^2 - 2U(s) + \beta s_x^2 + \left(s_{xx}\right)^2\right) dx. \tag{12.45}$$

Here we have assumed that $v_t(-\infty) = 0$, so that the transformations indicated in the second of (12.43) and (12.45) hold good. Then the following global balance laws hold:

$$\frac{dM}{dt} = 0, \quad \frac{dE}{dt} = 0, \tag{12.46}$$

and

$$\frac{d}{dt}P(R) = \bar{F} := \left[s_{xx}^2\right]_{-\infty}^{+\infty}. \tag{12.47}$$

For solitary-wave solutions, the driving force $\bar{F}$ is in fact equal to zero by virtue of the asymptotic conditions. That force $\bar{F}$, for a long but finite interval of simulation on $R$, is felt only when the solitons "hit" the boundaries and rebound from them. Yet the energy remains unchanged. A strongly implicit conservative finite-difference scheme is used in numerical simulations in order to always preserve both $M$ and $E$. More on the quasiparticle mechanics corresponding to (12.42) through (12.44) can be found in Christov et al. (1996). This particle-like behavior is dominated by an *anti-Lorentzian character* (i.e., while mass varies with the speed, all kinetic quantities go to zero—and not infinity—at a critical speed). A numerical fit has allowed us to uncover this new "point-mechanics," which reduces to a Newtonian one for small speeds; that is, then $M \approx M_0$ and $P \approx M_0 c$ for a definite $M_0$. This is true for solutions of the monotonous *sech*-like shapes (solutions) and also so-called *Kawahara* solitons (localized soliton humplike solutions that acquire oscillatory tails on both sides).

So far we considered only mechanical systems with only one degree of freedom, even though all in kinds of generalized elasticity theory. Because of the additive definition of the canonical entities (remember the summation over $\alpha$ in Chapter 4), the consideration of several degrees of freedom in pure mechanics or in a coupled-field theory is rather simple. This we show in the next section.

### 12.3.4 Mechanical System with Two Degrees of Freedom

When the small coupling between the $v$ degree of freedom of the previous example and the longitudinal displacement $u$ and elongation strain $e = u_x$ is kept (cf. Maugin and Cadet, 1991)—but remember that the ferroelastic phase

transition is driven through $s$, $e$ being only a secondary subsystem—then we have the following coupled wave system:

$$s_{tt} - c_T^2 s_{xx} + \left(s^3 - s^5 + 2\gamma s e + \alpha s_{xx}\right)_{xx} = 0, \tag{12.48a}$$

$$e_{tt} - c_L^2 e_{xx} + \gamma\left(s^2\right)_{xx} = 0, \tag{12.48b}$$

$$s = v_x, \quad e = u_x, \quad (v,u) \in R^2, \tag{12.48c}$$

where $\gamma$ is a coupling coefficient and $c_L$ is a second characteristic speed larger than $c_T$. This system looks formidable. Still it admits exact analytical solitary-wave solutions that do represent the various transitions possible between austenite and two martensitic variants of opposite shear. The sixth-order space derivatives have been discarded. With the quadruplet $(s,q,e,r)$ we can rewrite the system (12.48) as the following Hamiltonian system:

$$s_{tt} = q_{xx}, \quad e_t = c_L r_x, \tag{12.49a,b}$$

$$q = c_T^2 s - s^3 + s^5 - 2\gamma s e - \alpha s_{xx}, \tag{12.49c}$$

$$r_t = c_L e_x - \left(\gamma / c_L\right)\left(s^2\right)_x. \tag{12.49d}$$

The associated total "mass," "momentum," and "energy" are given by

$$M = \int_R s dx = \left[v\right]_{-\infty}^{+\infty}, \tag{12.50}$$

$$P(R) = \int_R \left(s q_x + c_L e_r\right) dx, \tag{12.51}$$

$$E(R) = \frac{1}{2}\int_R \left( \left(q_x^2 + c_L^2 r_x^2\right) + \left(c_T^2 s^2 + c_L^2 e^2\right) - 2\gamma e s^2 - \frac{1}{2}s^4 + \frac{1}{3}s^6 + \alpha\left(s_x\right)^2 \right) dx. \tag{12.52}$$

With the definition (12.51), which we let the reader show to be true in agreement with the canonical definition, with ad hoc conditions at infinity, we obtain a global balance of field momentum in the inhomogeneous form

$$\frac{d}{dt}P(R) = \bar{F} := -\frac{1}{2}\left[\alpha s_x^2 + c_L^2 e^2\right]_{-\infty}^{+\infty}. \tag{12.53}$$

This shows which conditions should apply to have conservation of field momentum strictly enforced so as to have an *inertial motion* of the possible shapes exhibited by the considered system if we work on a necessarily bounded finite interval in a numerical simulation (see Christov and Maugin, 1995).

## 12.4 Sine Gordon Equation and Associated Equations

### 12.4.1 Standard Sine Gordon Equation

This is the one-dimensional (in space) partial differential equation

$$u_{tt} - u_{xx} + \sin u = 0, \tag{12.54}$$

where both nonlinearity and dispersion are contained in the sin function. This ubiquitous equation, which can also be written as *Enneper's equation* of surface geometry as

$$u_{\xi\zeta} - \sin u = 0 \tag{12.55}$$

by introducing right- and left-running characteristic coordinates $\xi, \zeta = x \pm t$, appears in many fields of physics, especially while studying the structure of magnetic domain walls (this can be done on the basis of the spin equation (12.207) in the absence of magneto-mechanical couplings) and Josephson junctions (Christiansen and Olsen, 1982). From the mechanical viewpoint, such an equation can be obtained while studying the torsion of some bars (Wesolowski, 1983) and, above all, as an elementary model of dislocation motion in the so-called Frenkel–Kontorova model (1938)—a linear atomic chain placed in a sinusoidal potential landscape. This remarkable equation is exactly integrable (i.e., admits true soliton solutions) and is Lorentz invariant. It admits single subsonic solitary-wave solutions of the following *kink* form:

$$u(x,t) = \bar{u}(\xi) = 4\tan^{-1}\left(\exp \pm \gamma(\xi - \xi_0)\right), \tag{12.56}$$

wherein

$$\xi = x - ct, \quad \gamma = \left(1 - c^2\right)^{-1/2}, \quad |c| < 1. \tag{12.57}$$

Viewed as an *elastic* system, (12.54) is derivable from the following Lagrangian–Hamiltonian framework where the sinusoidal term should be interpreted as the action of an external source (the already mentioned periodic substrate of the Frenkel–Kontorova modeling) since the classical elastic energy cannot depend explicitly on $u$:

$$L = \frac{1}{2}u_t^2 - \frac{1}{2}u_x^2 - \left(1 - \cos u\right), \quad p = \frac{\partial L}{\partial u_t}, \tag{12.58}$$

$$H = pu_t - L = \frac{1}{2}\left(p^2 + u_x^2\right) + 2\sin^2\left(u/2\right), \tag{12.59}$$

with Hamiltonian equations

$$u_t = \frac{\partial H}{\partial p} = p, \quad p_t = -\frac{\delta H}{\delta u} = u_{xx} - \sin u. \tag{12.60}$$

A kink ($2\pi$ solution in $u$) or an antikink ($-2\pi$ solution) may be considered as a quasiparticle with rest mass $M_0$, momentum $P$, and energy $E$ given by

$$M_0 = 8 = E\left(0\right), \tag{12.61}$$

$$P = P\left(R\right) = \int_R \left(-u_x u_t\right)dx = 8\gamma c = Mc = \frac{M_0 c}{\left(1 - c^2\right)^{1/2}}, \tag{12.62}$$

$$E = E\left(R\right) = \int_R H dx = 8\gamma = E\left(c\right), \tag{12.63}$$

with the classical relationship between the triplet ($M_0$, $P$, $E$) typical of Lorentzian point-mechanics (the characteristic speed of relativity, the light velocity in vacuum, here is one):

$$E^2\left(c\right) = M_0^2 + P^2\left(c\right), \tag{12.64}$$

while for Newtonian point mechanics we would have

$$E = P^2/2M_0, \quad P = M_0 c. \tag{12.65}$$

Equations 12.62 and 12.64 apply the canonical definitions of Chapter 4, and the given estimates are based on the form of the kink solutions (12.56). Here the amplitude of the solution is independent of the speed: We have a so-called *topological* soliton. Because of this the solutions (12.56) exist in *statics*, and they can, therefore, represent the structure of a magnetic domain wall at rest. However, a quantity sometimes called the "charge" and defined by

$$q = (2\pi)^{-1} \int_R u_x dx = \frac{1}{2\pi} [u]_{-\infty}^{+\infty} = \pm 1 \tag{12.66}$$

can be introduced that pertains to the sense of "rotation" of $u$ through the solitonic structure, hence its "helicity."

Of course, for a fixed $c$, the three quantities $M$, $P$, and $E$ are strictly conserved, that is, for kink and antikink solutions; in particular, we have a standard *inertial* equation of motion for a relativistic quasiparticle:

$$\frac{dP}{dt} = \frac{d}{dt}\left( \frac{M_0 c}{\sqrt{1-c^2}} \right) = 0. \tag{12.67}$$

### 12.4.2 Sine Gordon–d'Alembert Systems

While studying magnetic domain walls in elastic ferromagnets (Maugin and Miled, 1986a) on the basis of the equations set forth in Section 11.10.2, we were led to introducing systems of the following type:

$$\phi_{tt} - \phi_{xx} - \sin\phi = \eta u_x \cos\phi, \quad u_{tt} - c_T^2 u_{xx} = -\eta (\sin\phi)_x . \tag{12.68}$$

Here $\phi$ is twice the angle of rotation (of magnetic spins in a plane parallel to the $x$-axis of propagation and the polarization of the transverse elastic displacement $u$; the so-called *Néel wall* in ferromagnetism), $c_T$ is a characteristic (transverse) elastic speed, and $\eta$ is representative of a magnetostrictive magneto-mechanical coupling. A similar problem arises in the ferroelectricity of deformable crystals of the polar type where $\eta$ is then related to electrostriction in electroelasticity (cf. Pouget and Maugin, 1984). The system in (12.68) couples linearly a sine–Gordon equation and a linear wave equation and thus deserves its name (coined by Kivshar and Malomed, 1989). Accordingly, this system is *not* exactly integrable from the point of view of soliton theory because the $u$-subsystem induces *radiations* during soliton interactions (cf. Pouget and Maugin, 1985b), but exact one-soliton solutions are known to exist analytically (Pouget and Maugin, 1984).

From our viewpoint in this book, ignoring the physical origin of the function $\phi$, we may consider (12.68) as a two-degrees-of-freedom nonlinear elastic dispersive system with displacement components $u$ and $\phi$. We can then exploit the canonical formalism of Chapter 4, while noting the additive property over field components of the canonical expressions. We write thus

$$L = \frac{1}{2}\left(u_t^2 + \phi_t^2\right) - W\left(u_x, \phi_x, \phi\right), \tag{12.69}$$

$$W = \frac{1}{2}\left(\phi_x^2 + c_T^2 u_x^2\right) + \eta u_x \sin\phi - \left(1 + \cos\phi\right), \tag{12.70}$$

$$H = p_u u_t + p_\phi \phi_t - L, \quad p_u = u_t, \quad p_\phi = \phi_t, \tag{12.71}$$

$$\sigma = \frac{\partial W}{\partial u_x}, \quad \mu = \frac{\partial W}{\partial \phi_x}, \tag{12.72}$$

and

$$P^f = -\left(u_x u_t + \phi_x \phi_t\right), \quad b = -\left(L + \sigma u_x + \mu \phi_x\right). \tag{12.73}$$

Therefore, the following local and global balances of field (wave) momentum hold, in the now-canonical form

$$\frac{\partial P^f}{\partial t} - \frac{\partial b}{\partial x} = 0 \quad , \frac{d}{dt} P(R) = \left[b\right]_{-\infty}^{+\infty}, \quad P(R) := \int_R P^f dx. \tag{12.74}$$

For solitary-wave solutions for which all derivatives vanish at infinity, $b$ vanishes at infinity, and $P(R)$ is strictly constant for a fixed velocity. Exact solutions are given in Pouget and Maugin (1984) and the interactions of individuals (with accompanying radiation) are exhibited in Pouget and Maugin (1985b). Elastic systems with a kind of micropolar internal structure (microstructure of the rotational type) exhibit solitonic solutions with a similar dynamic behavior (cf. Maugin and Miled, 1986b; Pouget and Maugin, 1989a, 1989b). The quasiparticle dynamics remains essentially Lorentzian but with perturbations due to the wave component $u$.

## 12.5 Nonlinear Schrödinger Equation and Allied Systems

### 12.5.1 The Standard Cubic Nonlinear Schrödinger Equation

Another well-known exactly integrable equation (cf. Calogero and Degasperis, 1982) is the cubic Schrödinger equation (sometimes called *NLS* without specializing to the cubic case). This reads in one-dimensional (space) setting:

$$ia_t + a_{xx} + 2\lambda|a|^2 a = 0, \tag{12.75}$$

where $a(x, t)$ is a complex-valued amplitude and $\lambda$ is a real scalar parameter. This is a somewhat universal (canonical) equation that governs the slowly varying complex amplitude of the envelope of a carrier wave (fast oscillations) in a *dispersive*, *weakly nonlinear* medium. Thus we were able to show that this is the case for shear horizontal (SH) *surface elastic waves* propagating on top of a thin film glued on a more rigid nonlinear elastic substrate although the quantum origin of Equation 12.75 is also obvious. This equation admits so-called bright and dark solitons as solutions (of which the exact form here is quite irrelevant; see Maugin, Pouget et al., 1992, for these), for which, to start with, the mass $M$, canonical momentum $P(R)$, and energy $E(R)$ are given by (cf. Drazin and Johnson, 1989)

$$M = \int_R |a|^2 \, dx, \tag{12.76}$$

$$P(R) = \int_R i\left(a a_t^* - a^* a_t\right) dx, \tag{12.77}$$

$$E(R) = \int_R \frac{1}{2}\left(|a_x|^2 - \lambda|a|^4\right) dx, \tag{12.78}$$

where the asterisk indicates the complex conjugate. The quantum physicist will recognize in Equation 12.76 the total probability of presence of a particle of wave function $a$ according to Max Born's interpretation (this should be normalized to one). In our mechanical frame of mind, this, without normalization, may be called the *number of surface phonons* or also the *wave action*. The canonical momentum $P$ was introduced in the causal reinterpretation of quantum mechanics (see Holland, 1993, p. 113) by treating $a$ as a classical but complex-valued field. Remarkably, the point mechanics associated with Equations 12.76 through 12.78 is Newtonian; that is, if $c$ is the propagation

velocity of bright solitons, we have the following Newtonian relations among the triplet ($M$, $P$, $E$):

$$P = Mc, \quad E = P^2/2M. \tag{12.79}$$

This is shown by substituting the bright-soliton solution obtained by Zakharov and Shabat (1972) in the set (12.76) through (12.78).

### 12.5.2 Zakharov and Generalized Zakharov Systems

The *Zakharov (Z) system* obtained in optical propagation couples linearly, in one dimension of space, a complex-valued field $a$ and a real-value field $n$, as follows (Zakharov, 1972):

$$ia_t + a_{xx} = na, \quad n_{tt} - c_T^2 n_{xx} = 2\left(|a|^2\right)_{xx}, \tag{12.80}$$

where $c_T$ is the characteristic speed of the $n$ subsystem, and the coupling parameter has been set equal to one. Since the $n$ subsystem is linear in $n$, the dispersion comes from the $a$ subsystem and the nonlinearity from the coupling. For the one-soliton solution (traveling wave), it is clear that the system (12.80) is equivalent to a NLS equation (12.75). The mass $M$ may be defined just as in this case, and the canonical momentum, recalling the additive nature of field momentum for several degrees of freedom, is obtained by combining expressions of the type (12.77) and the standard form for $n$. Thus,

$$M = \int_R |a|^2 \, dx, \quad P(R) = \int_R \left(i\left(aa_t^* - a^* a_t\right) - n_x n_t\right) dx. \tag{12.81}$$

We shall come back to the energy $E$ for a more complex case (in the following). The Zakharov system, just like the cubic NLS, is exactly integrable and admits multiple soliton solutions.

The *generalized Zakharov (GZ) system* was obtained by not neglecting the coupling between the SG component and the so-called Rayleigh component (polarized in the sagittal plane) in the previously mentioned surface wave problem (Maugin, Hadouaj, et al., 1992). With $n = u_x$, where $u$ stands for the elastic component in the sagittal plane and an appropriate scaling, this system reads

$$ia_t + a_{xx} + 2\lambda|a|^2 a + 2an = 0, \quad n_{tt} - c_0^2 n_{xx} + \mu\left(|a|^2\right)_{xx} = 0, \tag{12.82}$$

where dispersion has two sources, self-dispersion and dispersion caused by the coupling.

Complicated as it is, the system (12.82) admits exact analytical solitary-wave solutions of the bright-soliton type for $a$ accompanied by a solitary wave in $n$, but obviously it is not exactly integrable. Noting again the additional character of some canonical definitions, the mass $M$, canonical momentum $P$, and energy $E$ of soliton-like solutions will be of the following form:

$$M = \int_R |a|^2 \, dx, \tag{12.83}$$

$$P(R) = \int_R \left( i\left( a a_t^* - a^* a_t \right) - u_x u_t \right) dx, \tag{12.84}$$

$$E(R) = \int_R \frac{1}{2}\left( |a|^2 - \lambda |a|^4 - 2u_x |a|^2 + \mu^{-1}\left( u_t^2 + c_0^2 u_x^2 \right) \right) dx. \tag{12.85}$$

Here, $M$, the "number of surface phonons" (in our specific application) or the total wave action, is the same as for the NLS equation and for the Z system, while $P$ obviously is formally the same as for the Z system. The system (12.82) was studied in great detail by Maugin, Pouget et al. (1992) and Hadouaj et al., (1992a, 1992b). In particular, the integration of (12.82) for the exact solitary-wave solution given by these authors provides the looked-for relationship between the momentum $P$, the "mass" $M$, and the speed $c$ of the quasiparticles associated via (12.83) through (12.85) with such localized wave solutions, in the original form

$$P(M,c) = Mc + \frac{2}{3}\mu M^3 c \left( \frac{\lambda + \mu\left( c_0^2 - c^2 \right)^{-1}}{\left( c_0^2 - c^2 \right)^2} \right). \tag{12.86}$$

Here one may identify a typical "Newtonian" first contribution $Mc$, which is that obtained for the pure cubic NLS equation (cf. (12.79)), and a neither Newtonian nor Lorentzian contribution due to the $\mu$ coupling. Accordingly, for small $c$'s, this quasiparticle behaves almost like a Newtonian particle, but assuming $\mu > 0$, $\lambda > 0$, there exists a window in speeds between $c_0$ and $c^* \equiv \left( c_0^2 + (\mu/\lambda) \right)^{1/2}$ for which no propagation is possible, the "Newtonian" behavior being recovered for high speeds, while the behavior looks more like a Lorentzian one for a speed approaching $c_0$ from below. This strange dynamic behavior is illustrated in the original papers.

A further physically motivated generalization of the Z system may also appear in studying the nonlinear elastic problems of surface waves on a crystal, when an additional discrete (weakly nonlocal) effect can be felt in the

direction of propagation $x$. One then has to contemplate the coupling of a GZ system with a Boussinesq-like subsystem, yielding the system

$$2ia_t + 3a_{xx} + 2\lambda|a|^2 a - na = 0, \tag{12.87a}$$

$$n_{tt} - c_0^2 c_{xx} + \left(|a|^2 + n^2 + n_{xx}\right)_{xx} = 0, \tag{12.87b}$$

in which, to our knowledge, exact analytic one-soliton solutions are known only in the $\lambda = 0$ case.

## 12.6 Driving Forces Acting on Solitons

We have already seen examples of "configurational" forces driving soliton solutions in noninertial motion. Such forces are a priori exhibited in the right-hand side of Equations $12.17_1$, 12.19, 12.47, 12.53, and $12.74_2$, but apart from the case of (12.19), these equations are rendered *inertial* (i.e., with constant momentum) by the vanishing values of the source terms. Here we are interested in cases such as (12.79) where the source term comes from the perturbing actions in the original physical system described by partial differential equations. These sources may be external sources, inhomogeneities placed on the path of the wave, and additional terms due to the modeling of the material (e.g., additional viscosity, additional coupling). Examples of perturbed systems are

- *Perturbed Boussinesq equation:*

$$u_{tt} - u_{xx}(1 + \varepsilon u_x) - \varepsilon\delta^2 u_{xxxx} = \gamma u_{xxxt}, \tag{12.88}$$

  where the perturbation is due to viscosity

- *Perturbed sine Gordon equation:*

$$\phi_{tt} - \phi_{xx} + \sin\phi = \varepsilon f(x, \phi, \ldots), \tag{12.89}$$

  of which an example is given by

$$\phi_{tt} - \phi_{xx} - \sin\phi = -F(t)\cos(\phi/2), \tag{12.90}$$

where the perturbation is due to an applied magnetic torque resulting from an applied magnetic field of time-varying intensity in the magnetic model

- *Perturbed GZ system:*

$$ia_t + a_{xx} + 2\lambda|a|^2 a + 2an = 0, \quad n_{tt} - c_T^2 n_{xx} = -\mu\left(|a|^2\right)_{xx} + \gamma n_{xxt}, \qquad (12.91)$$

where the perturbation is due to viscosity in the $n$-subsystem such that $n_{xxt} = u_{xxxt}$

In the case (12.88), the balance of field momentum will read

$$\frac{d}{dt}P(R) = -\int_R \gamma u_x u_{xxxt}\,dx. \qquad (12.92)$$

In the case of (12.90) or with the same perturbation applied to the sine Gordon system, we will have balances of canonical energy and momentum perturbed as

$$\frac{d}{dt}E(R) = -\int_R \phi_t F(t)\cos(\phi/2)\,dx, \quad \frac{d}{dt}P(R) = \int_R \phi_x F(t)\cos(\phi/2)\,dx. \qquad (12.93)$$

Finally, in the case of (12.91),

$$\frac{d}{dt}P(R) = (4\gamma/\mu)\int_R n_t n_x\,dx. \qquad (12.94)$$

We take a closer look at the cases (12.93) and (12.94). The method we are applying is none other than the method of "balance equations" as exposed by Malomed (1985) and exploited by Pouget and Maugin (1985a) and Kivshar and Malomed (1989) for nonexactly integrable systems. That is, the variations (modulations, perturbations) of the global energy and momentum of solitary-wave solutions are established in terms of the perturbations by leaving free some typical parameter (e.g., the speed) of the exact solitary-wave solution and finding its variation (in the form of an ordinary differential equation in terms of the perturbations). The ideal solitary wave that was propagating inertially in the absence of perturbation will be slowed down, accelerated, or even modulated in time, depending on the cause of the perturbation. To find the modulation of the velocity, by virtue of the consistency between energy and momentum, we can apply the method to either of these two balance laws. Of course, "conservation" would be a more exact qualification than "balance" in the present book.

For example, Pouget and Maugin (1985a), and then Sayadi and Pouget (1990), apply the method to the energy equation $(12.93)_1$. In particular, since soliton solutions at rest exist for this system, a function $F(t) = FH(t - t_0)$, where $F$ is a constant and $H$ is a Heaviside function, will simulate a suddenly applied magnetic field that will affect the soliton (the magnetic domain wall in the magnetic image) position by putting it in motion if it was previously at rest. It will alter the speed, and at a higher order it will modify the shape, as phonon radiations will take place. Because of the Lorentzian invariance of the pure sine Gordon equation, the result, as shown by Pouget and Maugin (1985a), is practically a *uniformly accelerated* motion in a constant field of force, governed by the "relativistic" equation

$$\frac{d}{dt}\left(\frac{c(t)}{\sqrt{1-c^2(t)}}\right) = \frac{F}{2} = \hat{F}, \tag{12.95}$$

where, now, $c = dx_{\text{sol}}/dt$ is variable in time, and $x_{\text{sol}}$ is the center of "mass" of the now-moving kink. Equation 12.95 classically integrates to

$$x(t) = x_0 + \hat{F}^{-1}\left(1 + \hat{F}^2 t^2\right)^{1/2}. \tag{12.96}$$

A direct numerical check on the discrete system equivalent to the sine-Gordon system shows that this is an excellent approximation (Pouget and Maugin, 1985a). Thus we have an approximate, but sufficiently accurate, dynamic representation of the starting motion of a magnetoelastic domain wall under the action of a suddenly applied magnetic field.

In the case of (12.94) pertaining to the perturbed motion of a solution of the generalized Zakharov system, using the known unperturbed one-soliton solution (cf. Maugin and Hadouaj, 1991) in the right-hand side of (12.94), it is shown (Hadouaj et al., 1992a, 1992b) that this forced equation of momentum follows:

$$\frac{d}{dt}P(R) = F_{\text{visc}} = -\gamma\frac{3\mu M^5 c}{20}\left(\frac{\lambda + \mu\left(c_0^2 - c^2\right)^{-1}}{\left(c_0^2 - c^2\right)^2}\right). \tag{12.97}$$

This represents the dissipation-induced rate of change of field momentum. It should be noted that the "mass" of the solution given by Equation 12.83 is formally left unaltered by dissipation and is computed to be given by

$$M = 4\eta\left(\lambda + \mu\left(c_0^2 - c^2\right)^{-1}\right)^{-1}, \tag{12.98}$$

where η is the amplitude of the solution, which is, therefore, proportional to $M$ for a fixed speed $c$. As a consequence, we can state that the damped GZ system still conserves the "mass," but of course, the amplitude is affected where the speed $c$ varies in time while keeping the relationship (12.98). Extracting the amplitude from Equation 12.98

$$\eta(t) = \frac{M}{4}\left(\lambda + \mu\left(c_0^2 - c^2(t)\right)^{-1}\right), \tag{12.99}$$

this provides one of the looked-for equations (once we know $c$) for an initially prescribed $M$. Of course the solitary-wave solution, when it exists, is slowed down by viscosity γ considered as a small parameter. For a certain range of initial speeds and "masses" (amplitudes), the qualitative discussion of (12.97), on account of the $P(c)$ curve, shows that a new scenario of solitonic behavior is exhibited, a so-called perestroika of the solution, which has been corroborated by direct simulation on the associated discrete system (Hadouaj and Maugin, 1992). Its shows that in such nonlinear dispersive systems a *weak dissipation* may cause a *violent* rearrangement of the dynamic solutions. This is enough to emphasize the interest in the global canonical conservation laws of solitonic systems.

## 12.7 A Basic Problem of Materials Science: Phase-Transition Front Propagation

### 12.7.1 Some General Words

A full understanding of the phenomenon of the propagation of phase-transition fronts in deformable crystals—metals, alloys—is one of the essential problems of contemporary materials science and mechanics at both theoretical and application levels. This unique problem can be examined at three different scales: (i) a *microscopic scale* (lattice dynamics) in the absence of thermodynamic irreversibility, (ii) a *mesoscopic scale* (exploitation of continuum thermomechanical equations in a structured front), and (iii) a *macroscopic scale*, that of engineering applications. The first scale, inspired by the Landau–Ginzburg theory, although discrete to start with, deals with nonlinear localized waves (solitonic structures: solitary wave, soliton complexes) where nonlinearity and dispersion (discreteness) are the main ingredients. The developments given in the present chapter deal with such wave dynamics. The second scale involves nonlinearity, dispersion, *and* dissipation (viscosity). The third scale is that one at which the front is seen as an irreversibly driven singular surface—as examined in Chapter 7—and where macroscopic thermodynamics (theory of irreversible processes) and numerical methods

such as finite-element and finite-volume methods are used in conjunction with a criterion of progress.

The three scales are reconciled by the fact that all solutions satisfy the same *Hugoniot conditions* sufficiently far away from the front, whether structured as a solitonic or dissipative structure, or without thickness such as a singular surface. This multilevel, multiphysics approach gathers the viewpoints of condensed-matter physicists (microscale), applied mathematicians (mesoscale), and engineers (macroscale), and even that of the theoretical physicist via the inclusive notion of quasiparticles (this chapter) and the underlying and pervasive invariant-theoretical framework. In all cases the notion of *driving force* is involved, being either set equal to zero or being very active indeed.

### 12.7.2 Microscopic Condensed Matter–Physics Approach: Solitonics

The first approach considered is that dealing with the *microscale* of lattice dynamics *in a perfect lattice*, so that there is no dissipation and effects of temperature are not involved, except perhaps in the phase-transition parameter. Following works by Falk (1983), Pouget (1988), and Maugin and Cadet (1991), this allows one to readily obtain a dynamic representation of a phase boundary (here a kink) as a *solitonic structure* for a two-degrees-of-freedom, but essentially one-dimensional system. The reason for this is that, unless one wants to study the *lateral stability of this system*, the "theorem of the flea" applies: At its scale the "flea" sees only the *first-order geometric description* of the transition layer, hence essentially the normal direction to a layer of constant thickness. Notice that the continuum model obtained in the *long-wavelength limit* is that of a *nonlinear elastic body with first gradients of strains* taken into account but no dissipation. This long-wave limit is admissible because the transition layer between two phases, although thin (perhaps a few lattice spacings), is nonetheless large enough. Numerical simulations can be performed *directly* on the lattice. The elastic potential is nonconvex in general. To exemplify this approach, we consider a one-dimensional ($x$), two-degrees-of-freedom, lattice with transverse (main effect) and longitudinal (secondary effect) displacements from the initial position. In the so-called *long-wave limit* where the discrete dependent variables (strains) $s_n$ and $e_n$ vary slowly from one lattice site to the next and they can be expanded about the reference configuration ($na$,0), the discrete equations yield a system of two (nondimensionalized) coupled partial—in ($x$,$t$)—differential equations (with an obvious notation for partial $x$ and $t$ derivatives), which is none other than the system of equations (12.48), where, we remind the reader, $s$ and $e$ are the shear and elongation strains, $\gamma$ is a coupling coefficient, and $\alpha$ is a nonlocality parameter. Parameters $c_T$ and $c_L$ are the characteristic speeds of the linear elastic system. This corresponds to stresses and energy density given by

$$\sigma_S = \bar{\sigma}_S - m_x, \quad \sigma_e = \frac{\partial W}{\partial e}, \quad \bar{\sigma}_S = \frac{\partial W}{\partial s}, \quad m = \frac{\partial W}{\partial s_x} \tag{12.100}$$

and

$$W(s,e,s_x)=\frac{1}{2}\left(c_T^2 s^2-\frac{1}{2}s^4+\frac{1}{3}s^6+c_L^2 e^2-2\gamma s^2 e+\alpha(s_x)^2\right). \tag{12.101}$$

In other words, Equation 12.48a and b are none other than the $x$-derivatives of the balance of (physical) linear momentum for a continuum made of a nonlinear, homogeneous elastic material with strain gradients—with both nonlinearity and strain gradients relating only to the *shear* deformation. As already noticed this apparently complicated system still admit exact dynamic solutions of the *solitonic type*. A thorough discussion of the existence of solitary-wave-like solutions—such solutions connecting two different or equivalent minimizers (i.e., two phases) of the potential energy—was given by Maugin and Cadet (1991), to whom we refer the reader. The remarkable fact is that such complicated solutions are shown (by computation) to satisfy the following (temperature-independent) *HUGONIOT* condition between *states at infinity*:

$$\text{Hugo}:=\left[\bar{W}(s,e \text{ fixed})-\langle\bar{\sigma}_S\rangle s\right]=0, \tag{12.102}$$

where $\bar{\sigma}_s$ is the shear strain *without* strain-gradient effect, and $\bar{W}$ is the elastic energy with such effects similarly neglected. Obviously, gradient effects play a significant role only within the rapid transition zone that the kink solution represents, while outside this zone the state is practically spatially uniform, although different on both sides of the localized front. Here we have used the following definitions for the jump and mean value of any quantity $a$:

$$[a]:=a(+\infty)-a(-\infty),\quad \langle a\rangle:=\frac{1}{2}\left(a(+\infty)+a(-\infty)\right) \tag{12.103}$$

Equation 10.102 is typical of the *absence of dissipation* during the transition, in general a working hypothesis that is *not* realistic. Furthermore, it can in fact be rewritten as the celebrated *Maxwell's rule of equal areas.*

Under the same conditions the corresponding dynamic solitary-wave-like solution satisfies the quasiparticle inertial motion

$$\frac{d}{dt}P(R)=0, \tag{12.104}$$

with vanishing driving force in the right-hand side—Equation 12.53 with a vanishing right-hand side because of the asymptotic behavior of the solutions.

### 12.7.3 Macroscopic Engineering Thermodynamic Approach

This is a local viewpoint exposed in Chapter 7, which refers to the fact that it is assumed at each instant of time that the thermoelastic solution is known by any means—analytical but very frequently numerical—on both sides of the singular surface $\Sigma$ so that one can compute a *driving force* acting on $\Sigma$. Further progress of $\Sigma$ must not contradict the second law of thermodynamics. The latter, therefore, governs the local evolution of $\Sigma$, which is generally *dissipative*, although no microscopic details are made explicit to justify the proposed expressions. The approach is *thermodynamic* and *incremental* (in total analogy with modern plasticity). All physical mechanisms responsible for the phase transformation are contained in the *phenomenological-macroscopic* relationship given by the *local criterion of progress* of $\Sigma$. Without going into details, which can be found in several papers (Maugin and Trimarco, 1995; Maugin, 1997, 1998), and considering from the outset the finite-strain framework, we remind the reader that at any regular point in the body (i.e., on both sides of $\Sigma$), we have the balance of (physical) linear momentum and the future heat equation written in the Piola–Kirchhoff form for a *heat-conducting thermoelastic material* (in general, $W(\mathbf{F},\theta)$ is different on both sides of $\Sigma$, and generally nonconvex in its first argument and concave in the second one—the thermodynamic temperature $\theta$). But while each phase is materially homogeneous, the presence of $\Sigma$ is a patent mark of a loss of translational symmetry on the overall body, hence the consideration of a global material inhomogeneity. The field equation capturing this breaking of symmetry is the jump relation associated with the equation of momentum *on the material manifold*, that is, what we have called the balance of material momentum in previous chapters. This jump equation, together with that for entropy, governs the phase-transition phenomenon at $\Sigma$. These equations a priori read

$$\mathbf{N}.\left[\mathbf{b}+\bar{\mathbf{V}}\otimes\mathbf{P}\right]+\mathbf{f}_{\Sigma}=\mathbf{0},\quad \mathbf{N}.\left[\bar{\mathbf{V}}S-\left(\mathbf{Q}/\theta\right)\right]=\sigma_{\Sigma}\geq 0, \tag{12.105}$$

where the last inequality is a statement of the second law of thermodynamics at $\Sigma$, $\mathbf{N}$ is the unit normal to $\Sigma$ oriented from the *minus* to the *plus* side, and we defined the jumps and mean values at $\Sigma$ by (compare to (12.103)):

$$\left[a\right]:=a^{+}-a^{-},\quad \left\langle a\right\rangle:=\frac{1}{2}\left(a^{+}+a^{-}\right), \tag{12.106}$$

where $a^{\pm}$ are the uniform limits of $a$ in approaching $\Sigma$ on its two faces along $\mathbf{N}$. $\bar{\mathbf{V}}$ is the material velocity of $\Sigma$, $S$ is the entropy density, $\theta$ is the thermodynamic temperature; $\mathbf{P}$ is the material momentum, and $\mathbf{b}$ is the Eshelby stress tensor. We have shown that for a coherent homothermal front we have

$$\mathbf{f}_{\Sigma}.\bar{\mathbf{V}}=f_{\Sigma}\bar{V}_{N}=\theta_{\Sigma}\sigma_{\Sigma}\geq 0 \tag{12.107}$$

and

$$f_\Sigma = -\mathrm{Hugo}_{\mathrm{PT}}, \quad \mathrm{Hugo}_{\mathrm{PT}} := \mathbf{N}.\left[\mathbf{b}_S\right].\mathbf{N} = \left[W - \left\langle \mathbf{N}.\mathbf{T} \right\rangle.\mathbf{F}.\mathbf{N}\right], \tag{12.108}$$

where $\mathbf{b}_S$ is the quasistatic part of $\mathbf{b}$ (although the computation is made without neglecting inertia). If this inertia is really neglected, then we have following reduction:

$$\mathrm{Hugo}_{\mathrm{PT}} = \left[W - \mathrm{tr}\left(\left\langle \mathbf{T} \right\rangle.\mathbf{F}\right)\right]. \tag{12.109}$$

In this canonical formalism the driving force $\mathbf{f}_\Sigma$ happens to be purely normal, but it is constrained to satisfy, together with the propagation speed $\bar{V}_N$, the surface dissipation inequality indicated in the last of (12.107). In other words, any relationship between these two quantities must be such that the inequality (12.107) is verified. This is the basis of the formulation of a *thermodynamically admissible criterion of progress* for $\Sigma$. Indeed, we should look for a relationship $\bar{V}_N = g\left(f_\Sigma\right)$ that satisfies the last of (12.107). For illustrative purposes we may consider the *cartoonesque* case where the phase-transition process does not involve any characteristic time (just like rate-independent plasticity), in which case the dissipation in (12.107) must be homogeneous of degree one only in $\bar{V}_N$; the threshold type of progress criterion corresponds to this. That is, $\bar{V}_N \in \partial I_f = N_C\left(f_\Sigma\right)$, where $I_f$ is the indicator function of the closed segment $F = [-f_c, +f_c]$—a convex set—and $N_C$ is the "cone of outward normals" to this convex set, with the symbol $\partial$ denoting the so-called subgradient (see Maugin, 1992, Appendix). If we "force" the system evolution to be such that there is effective progress of the front at $\mathbf{X} \in \Sigma$ while there is *no* dissipation, then we must necessarily enforce the following condition:

$$f_\Sigma = 0 \quad \text{i.e.,} \quad \mathrm{Hugo}_{\mathrm{PT}} \equiv \left[W - \left\langle \mathbf{N}.\mathbf{T} \right\rangle.\mathbf{F}.\mathbf{N}\right] = 0. \tag{12.110}$$

Because temperature ($\theta_\Sigma$) is fixed, and the thickness of the front is taken as zero, so that uniform states are reached immediately on both sides of $\Sigma$, (12.110) is none other than the condition of "Maxwell" (12.102) in the one-dimensional pure-shear case. Thus a macroscopic approach dear to the engineer has allowed us to obtain, in general, a more realistic (in general, dissipative) progress of the front. The case of Section 12.7.2 then appears as a "*zoom*"—in the nondissipative case—on the situation described in the present section since the front acquires, through this zoom magnification (asymptotics), a definite, although small, thickness and a structure while rejecting the immediate vicinity of the zero-thickness front to infinities. The next approach allows one to introduce both a *thickness* and *dissipation*.

### 12.7.4 Mesoscopic Applied-Mathematics Approach: Structured Front

Here the front of phase transformation is looked upon as a mixed "*viscous-dispersive*" structure at a "mesoscale." We refer to this as the *applied-mathematician approach.* This dialectical approach, in which one applies macroscopic concepts at a smaller scale to obtain an improved phenomenological description, is finally fruitful. Here we follow Truskinowsky (1994), to whom we refer the reader for details. We therefore consider a one-dimensional model (along the normal to the structured front—"theorem of the fly"), and we envisage a *competition* between viscosity (i.e., a simple case of dissipation) and some *weak nonlocality* accounted for through a strain-gradient theory (compare Section 12.7.2). The critical nondimensional parameter that compares these two effects is defined by

$$\omega = \eta/\sqrt{\varepsilon}. \tag{12.111}$$

where $\eta$ is the viscosity and $\varepsilon \approx L^2$ is the nonlocality parameter (size effect). Progressive-wave solutions $u = u(\xi = x - \bar{V}_N t)$ of the continuous system that relate two minimizers (uniform solutions at infinities that minimize $\bar{W}$) over a distance of the order of $\delta = \sqrt{\varepsilon}$ are discussed in terms of this parameter. The mathematical problem reduces to a *nonlinear eigenvalue problem* of which the specification of the points of the discrete spectrum constitutes the looked-for *kinetic relation* $\bar{V}_N = g(f;\varepsilon)$, where $f = \bar{\sigma} - \bar{\sigma}(+\infty)$ plays the role of *driving force.* As a matter of fact the speed of propagation $\bar{V}_N$ satisfies the *Rankine–Hugoniot equation* $\bar{V}_N^2 = [\bar{\sigma}]/[s]$, where strain gradients and viscosity play no role and the jumps are taken between asymptotic values at infinity (cf. (12.103)). The evolution obtained for the kinetic law is strongly nonlinear function and evolves with the value of the parameter $\omega$.

### 12.7.5 Theoretical Physics Approach: Quasiparticle and Transient Motion

The approach of Section 12.7.3 simply accepts the value of $\bar{V}_N$, whatever its evolution, as it is computed from the full field solution at each instant of time and each material point $\mathbf{X} \in \Sigma$. In contrast, the approaches of Sections 12.7.2 and 12.7.4 provide *progressive-wave* solutions, that is, waves that are steady in the sense that the propagation speed, although a property of the solution (and not only of the material as in linear-wave propagation), does not vary in time along the propagation path. This is a type of *inertial motion.* What about a *noninertial motion*? To look at such a case, we view the problem in the framework of Sections 12.5 and 12.6. The localized—but with nonzero thickness—dynamic solutions of Section 12.7.2 are looked on as global entities behaving like mass particles in motion in the appropriate *point mechanics*, that is, as so-called *quasiparticles* or, as we like to say, ***wavicles***. All perturbing effects such as dissipation, inhomogeneities, and so on will then be treated as *perturbing*

*forces* acting on the inertial motion, which thus becomes *noninertial.* To understand this viewpoint, it is sufficient to envisage the presence of a viscous (more generally, dissipative) contribution in the right-hand side of the classical balance of linear momentum. As indicated in Section 12.5 this results in the presence of an additional *material* force $\mathbf{f}_D^{\text{inh}} = -\mathbf{f}_D.\mathbf{F}$ in the right-hand side of the canonical momentum equation. The latter equation is used, after integration over the path of the wave, to treat the material force as a perturbation on the solution in the absence of $\mathbf{f}_D$. The essential problem consists then in identifying the *point mechanics* that is associated with a particular system of partial differential equations on account of some of its exact integrals. This point mechanics—that is, a coherent system of relations between the mass, momentum, and energy of a point particle—can be completely new and a priori unforeseeable. In particular, a perturbative approach of the canonical, quasiparticle type was suggested by Fomethe and Maugin (1997) to study the varied motion of a phase-transition front under the action of a temperature gradient (since the latter creates a material thermal force; cf. Chapter 5).

### 12.7.6 Thermodynamically Based Continuous Automaton

Recently, in order to treat numerically the progress of phase-transition fronts in thermoelasticity, Berezovski and the author (cf. Berezovski and Maugin, 1999, etc.) have introduced a numerical strategy that, while based on the thermodynamic, no-thickness singular surface of Section 12.7.3 (engineering approach), allows for the automatic application of the criterion of transformation during the progression while providing simultaneously a more reasonable (nonlinear) kinetic law, which is here part of the solution.

This is a performing finite-volume method (FVM) adapted so as to include the balance of material momentum and its jump at the phase boundary. This is all the more appropriate given that the fixed FVM cells thus considered may also be viewed as the elementary blocks of a thermodynamics of so-called *discrete systems* in the manner of Schottky (1961; cf. Muschik, 1990). In this thermodynamics the state in one discrete system (e.g., one of the computing cells) is defined in terms of its environment, which may or may not be in thermodynamic equilibrium. *Contact thermodynamic quantities* (e.g., contact temperature, contact stresses, contact velocity) are introduced to characterize the state of the discrete system (in fact defined at the boundary surface of a cell in the FVM). This idea of making a cell's state depend on that of its neighbors is tantamount to introducing a *strategy* for the propagation of the thermodynamic state, hence the notion of *cellular automaton* (Berezovski, 1997). Although discretization here is based on continuous balance laws, we may refer to this method as that of *continuous cellular automata.* The strategy referred to in the preceding is essential in the case of the dynamics of a *phase-transition front*. It is along this line of thought that many recent works developed (Berezovski, 1997; Berezovski and Maugin, 1999a, 1999b). In this new scheme, all thermomechanical balance laws are expressed for each cell

(see Chapter 13 in this book), and the bulk quantities within each cell are related to the contact ones through the thermodynamics of discrete systems. Thereby a high-performance wave-propagation algorithm is exploited—combining Lax–Wendroff and Godunov's ideas (Berezovski and Maugin, 1999)—that yields extremely good results in the simulation of the rapid progression of sharp wave fronts in 2D thermoelasticity under the external action of an applied stress shock. The thermodynamic justification of the scheme is given in Berezovski and Maugin (2004). The kinetic relation obtained by computing separately the driving force and the velocity of the front compares favorably with that deduced from the mesoscopic approach recalled in Section 12.7.4.

## Appendix A12.1: Eshelbian Kinematic-Wave Mechanics

### A12.1.1 Some Words of Introduction

Since the space–time parametrization ($\mathbf{X}$,$t$) provides the natural background for the canonical thermomechanics of continua (Chapter 5) and the accompanying theory of motion of defects, one may naturally wonder what happens in the dual space–time manifold spanned by a material wave vector $\mathbf{K}$ and an angular frequency $\omega$ since a space–time invariant *phase* is defined by $\phi = \mathbf{K}.\mathbf{X} - \omega t$. The observation of the invariance of this scalar quantity was an essential tool in the intellectual construct of Louis de Broglie that yielded *quantum wave mechanics*, with further works by this author, Erwin Schrödinger, and others in the 1920s (cf. Holland, 1993). This strictly applies to a monochromatic linear wave process. Dispersion may be envisaged but no nonlinearity. However, the kinematic-wave theory, due essentially to Lighthill (1965a, 1965b), Whitham (1965, 1974a, 1974b), and Hayes (1970a, 1970b, 1973), allows one to introduce a more inclusive definition of wave vector and angular frequency from a general space–time-dependent phase function. The cited authors also noticed the interest of variational formulations and the exploitation of basic theorems of field theory (the theory of the averaged Lagrangian) in the solution of nonlinear wave problems with almost monochromatic features but including some degree of dispersion and nonlinearity, with refinements by Benney and Newell (1967) and Newell (1985). Very few applications have followed in fluid mechanics where this started, probably due to the difficulty of grasping some of the basic ideas. This is even truer in wave-like phenomena in deformable solids, where the only available problem solution seems to be the one given by the author and a coworker (Maugin and Hadouaj, 1991) in a complicated nonlinear surface wave problem.

In this appendix, which follows essentially Maugin (2007), exploiting the noticed duality between the parametrization ($\mathbf{X}$,$t$) and the wave-like

entity (**K**,ω) and remembering the basic structure of variational continuum mechanics in finite strains (the ideal paragon case, Chapter 4), we examine the related wave-kinematics in the theory of the averaged Lagrangian theory of Whitham and Hayes and show how, via the application of Noether's theorem, such notions as those of wave action, material wave momentum (quite similar to the wave momentum of de Broglie), and an Eshelby "wave" material tensor emerge naturally with corresponding continuum conservation laws of wave action, material wave momentum, and wave energy. One can even show the existence of a Hamilton–Jacobi equation. By way of application the case of one-dimensional dispersive weakly nonlocal elasticity is considered with the possibility of the existence of modulated localized nonlinear solutions akin to bright solitons. This work has been preceded by reflections on the relative nature of waves (phonons) in the Eulerian and material descriptions (Maugin, 1993, pp. 34–38)—works in cooperation with C. Trimarco, further elaboration in Potapov et al. (2005), and first considerations on wave-kinematics in Maugin (2003). Recent works by Kienzler and Herrmann (2004) and Herrmann and Kienzler (2005) go in the same direction.

### A12.1.2 Kinematic-Wave Theory and Elasticity

First, the reader is reminded that the phase of a *plane* linear wave in a continuum is defined in the material description by

$$\varphi(\mathbf{X},t) = \tilde{\varphi}(\mathbf{K},\omega) = \mathbf{K}.\mathbf{X} - \omega t, \tag{A12.1}$$

where **K** is the material wave vector and ω is the associated circular frequency. But in the kinematic-wave theory a general phase function

$$\varphi = \bar{\varphi}(\mathbf{X},t). \tag{A12.2}$$

is introduced, from which the material wave vector **K** and the frequency ω are defined by

$$\mathbf{K} = \frac{\partial \bar{\varphi}}{\partial \mathbf{X}} = \nabla_R \bar{\varphi}, \quad \omega = -\frac{\partial \bar{\varphi}}{\partial t}, \tag{A12.3}$$

From this there follows at once the two equations (curl-free nature of **K**, and conservation of the wave vector)

$$\nabla_R \times \mathbf{K} = \mathbf{0} \tag{A12.4}$$

$$\frac{\partial \mathbf{K}}{\partial t} + \nabla_R \omega = \mathbf{0}. \tag{A12.5}$$

In particular, the equations (A12.3) are trivially satisfied for plane wave solutions for which the last of (A12.1) holds true. For an *inhomogeneous rheonomic* linear behavior with dispersion we have the dispersion relation

$$\omega = \Omega(\mathbf{K};\mathbf{X},t). \tag{A12.6}$$

Accordingly, the *conservation of wave vector* (A12.5) becomes

$$\frac{\partial \mathbf{K}}{\partial t} + \mathbf{V}_g . \nabla_R \mathbf{K} = -\left.\frac{\partial \Omega}{\partial \mathbf{X}}\right|_{\text{expl}}, \quad \mathbf{V}_g = \frac{\partial \Omega}{\partial \mathbf{K}}, \tag{A12.7}$$

and thus the *Hamiltonian system* (Maugin, 2003)

$$\frac{D\mathbf{X}}{Dt} = \frac{\partial \Omega}{\partial \mathbf{K}}, \quad \frac{D\mathbf{K}}{Dt} = -\left.\frac{\partial \Omega}{\partial \mathbf{X}}\right|_{\text{expl}}, \tag{A12.8}$$

where we have set

$$\frac{D}{Dt} \equiv \frac{\partial}{\partial t} + \mathbf{V}_g . \nabla_R . \tag{A12.9}$$

Simultaneously we have the *Hamilton–Jacobi equation* (compare $(A12.3)_2$)

$$\frac{\partial \varphi}{\partial t} + \Omega\left(\mathbf{X}, t; \mathbf{K} = \frac{\partial \varphi}{\partial \mathbf{X}}\right) = 0. \tag{A12.10}$$

If we now consider a wave in an inhomogeneous rheonomic dispersive *nonlinear* material, the frequency will also depend on the amplitude. Let **a** denote the $n$-vector of $R^n$ that characterizes this small, slowly varying amplitude of a complex system (in general with several degrees of freedom). Thus, now,

$$\omega = \Omega(\mathbf{K},\mathbf{X},t,\mathbf{a}). \tag{A12.11}$$

Accordingly, the second of Hamilton's equations (A12.8) will now read (Maugin, 2003)

$$\frac{D\mathbf{K}}{Dt} = -\left.\frac{\partial \Omega}{\partial \mathbf{X}}\right|_{\text{expl}} + \mathbf{A}.\left(\nabla_R \mathbf{a}\right)^T, \quad \mathbf{A} := -\frac{\partial \Omega}{\partial \mathbf{a}}. \tag{A12.12}$$

The relationship with the developments in Chapter 4 follows from the remarkable considerations of Whitham on a so-called *averaged Lagrangian*. For a wave motion depending on the phase (A12.2) and with all characteristic quantities varying slowly over space–time (derivatives of **a**, ω, and **K** are small in an appropriate mathematical sense and can thus be neglected), Whitham proposes to replace the initial variational problem (4.1) by one pertaining to the averaged Lagrangian, that is,

$$\delta \int \tilde{L} d\mathbf{X} dt = 0 \quad , \quad \tilde{L} = \frac{1}{2\pi} \int_0^{2\pi} L d\varphi, \tag{A12.13}$$

with

$$\tilde{L} = \tilde{L}\left( \frac{\partial \overline{\varphi}}{\partial \mathbf{X}} = \mathbf{K}, \frac{\partial \overline{\varphi}}{\partial t} = -\omega, \mathbf{a}; \mathbf{X}, t \right), \tag{A12.14}$$

where the *fields* are the amplitude **a** and the phase φ. Accordingly, the associated field (variational) equations

$$\frac{\partial \tilde{L}}{\partial \mathbf{a}} = \mathbf{0}, \tag{A12.15}$$

$$\frac{\partial \tilde{S}}{\partial t} - \nabla_R . \mathbf{W} = 0, \tag{A12.16}$$

for the variational (i.e., field) equations, and the canonical energy and momentum equations

$$\frac{\partial \tilde{H}}{\partial t} - \nabla_R . \tilde{\mathbf{Q}} = \tilde{h}, \quad \frac{\partial \tilde{\mathbf{P}}}{\partial t} - \mathrm{div}_R \tilde{\mathbf{b}} = \tilde{\mathbf{f}}^{\mathrm{inh}} \tag{A12.17}$$

follow from Noether's theorem for the translational invariance under $t$ and **X**, where we have set

$$\tilde{S} := \frac{\partial \tilde{L}}{\partial \omega}, \quad \mathbf{W} := \frac{\partial \tilde{L}}{\partial \mathbf{K}}, \tag{A12.18}$$

$$\tilde{H} = \omega \tilde{S} - \tilde{L}, \quad \tilde{\mathbf{Q}} = \omega \mathbf{W}, \quad \tilde{h} = -\left. \frac{\partial \tilde{L}}{\partial t} \right|_{\mathrm{expl}}, \tag{A12.19}$$

$$\tilde{\mathbf{P}} = \tilde{S}\mathbf{K}, \quad \tilde{\mathbf{b}} = -\left(\tilde{L}\mathbf{1}_R - \mathbf{W}\otimes\mathbf{K}\right), \quad \tilde{\mathbf{f}}^{\text{inh}} = \left.\frac{\partial \tilde{L}}{\partial \mathbf{X}}\right|_{\text{expl}}. \tag{A12.20}$$

Dimensionally, $\tilde{S}$ is an *action* and may be called the *wave action*, while (A12.16) may be referred to as a strict *conservation law for the wave action* in which **W** is the *action flux*. Note that in continuum mechanics the *action* density *S* would be given in terms of the canonical momentum **P** and Hamiltonian *H* by $S = \mathbf{P}.\mathbf{X} - Ht$; compare the discussion in Maugin (2003). But here in the preceding the material covector $\tilde{\mathbf{P}}$ may be called the ***material wave momentum*** (notice that its formula reminds us of the quantum wave-mechanics relationship due to de Broglie: $\tilde{\mathbf{P}} = \hbar\mathbf{K}$, where **h** is the reduced elementary quantum of action [Planck's constant]), and $\tilde{\mathbf{b}}$, the associated flux, may be called the ***material wave Eshelby stress***. This tensor is not symmetric unless **W** is proportional to **K**.

The Equation A12.17 are a consequence of Noether's identity. But the wave action conservation equation (A12.16) plays here the central role (equivalent to the balance of linear physical momentum,

$$\frac{\partial \mathbf{p}}{\partial t} - \text{div}_R \mathrm{T} = 0, \tag{A12.21}$$

for hyperelasticity). Indeed, in the same way as the analogs for elasticity in (4.80) and (4.81) can be deduced from (A12.21) by right scalar multiplication by **v** and **F**, respectively, and some further manipulations on account of the expression for *L*, Equations $\text{A12.17}_{1-2}$ can be deduced from Equation A12.16 by scalar and tensorial multiplication, respectively, by ω and **K** on account of the functional dependency assumed for $\tilde{L}$ and (A12.15). This we show explicitly for the second (covectorial) equation. Indeed, we have

$$\mathbf{0} = \left\{\frac{\partial \tilde{S}}{\partial t} - \left(\nabla_R.\mathbf{W}\right)\right\}\mathbf{K} = \frac{\partial\left(\tilde{S}\mathbf{K}\right)}{\partial t} - \tilde{S}\frac{\partial \mathbf{K}}{\partial t} - \text{div}_R\left(\mathbf{W}\otimes\mathbf{K}\right) + \left(\mathbf{W}.\nabla_R\right)\mathbf{K}. \tag{A12.22}$$

But

$$\tilde{S}\frac{\partial \mathbf{K}}{\partial t} = -\tilde{S}\nabla_R\omega \tag{A12.23}$$

and

$$\left(\mathbf{W}.\nabla_R\right)\mathbf{K} = \frac{\partial \tilde{L}}{\partial \mathbf{K}}.\nabla_R\mathbf{K} = \frac{\partial \tilde{L}}{\partial \mathbf{K}}.\left(\nabla_R\mathbf{K}\right)^T, \tag{A12.24}$$

where we used the definitions of ω and **K** in terms of the phase. Furthermore, from the total material gradient of $\tilde{L}$, we obtain that

$$\begin{aligned}\frac{\partial \tilde{L}}{\partial \mathbf{K}}.\left(\nabla_R \mathbf{K}\right)^T &= \nabla_R \tilde{L} - \left.\frac{\partial \tilde{L}}{\partial \mathbf{X}}\right|_{\text{expl}} - \frac{\partial \tilde{L}}{\partial \omega}\nabla_R \omega - \frac{\partial \tilde{L}}{\partial \mathbf{a}}.\left(\nabla_R \mathbf{a}\right)^T \\ &= \operatorname{div}_R\left(\tilde{L}\mathbf{1}_R\right) - \left.\frac{\partial \tilde{L}}{\partial \mathbf{X}}\right|_{\text{expl}} - \tilde{S}\nabla_R \omega.\end{aligned} \tag{A12.25}$$

Accordingly, combining (A12.23) through (A12.25) in (A12.22) yields

$$\mathbf{0} = \left\{\frac{\partial \tilde{S}}{\partial t} - \left(\nabla_R .\mathbf{W}\right)\right\}\mathbf{K} = \frac{\partial \tilde{\mathbf{P}}}{\partial t} - \operatorname{div}_R \tilde{\mathbf{b}} - \left.\frac{\partial \tilde{L}}{\partial \mathbf{X}}\right|_{\text{expl}} \tag{A12.26}$$

with the definitions (A12.20). As a matter of fact, here one of Noether's identities is none other than

$$\left\{\frac{\partial \tilde{S}}{\partial t} - \left(\nabla_R .\mathbf{W}\right)\right\}\mathbf{K} - \left\{\frac{\partial \tilde{\mathbf{P}}}{\partial t} - \operatorname{div}_R \tilde{\mathbf{b}} - \left.\frac{\partial \tilde{L}}{\partial \mathbf{X}}\right|_{\text{expl}}\right\} \equiv \mathbf{0}. \tag{A12.27}$$

### A12.1.3 Application to Nonlinear Dispersive Waves in Elastic Crystals

For the sake of example we consider a one-dimensional nonlinear elastic bulk motion in a dispersive crystal. With $u_t$ and $u_X$ replacing **v** and **F**, we have the following rheonomic Lagrangian density:

$$L = \frac{1}{2}\rho_0 u_t^2 - \frac{1}{2}E\left(u_X^2 - \frac{1}{6}\beta u_X^4\right) + \frac{1}{2}E\delta^2\left(u_{XX}\right)^2 \tag{A12.28}$$

where $\rho_0$ is a fixed density, $E$ is an elasticity coefficient, β is coefficient of nonlinearity for elasticity (it may be of any sign), and δ is a characteristic (intrinsic) length. The model (A12.28) belongs in the class of models described by (4.119), for which (4.121) through (4.130)) apply. The elastic component is not necessarily longitudinal (i.e, along x). The variational field equation (4.121) reads

$$u_{tt} - c_E^2 u_{XX}\left(1 - \beta u_X^2\right) - c_E^2\delta^2 u_{XXXX} = 0, \tag{A12.29a}$$

in which we recognize a modified Boussinesq (crystal) equation (compare to the standard Boussinesq equation (12.12); see Christov et al. [2007] for the so-called "Boussinesq paradigm"). Here $c_E = (E/\rho_0)^{1/2}$ is the linear elastic speed. The crystal is cut in such a way that no cubic term appears in the expression

(A12.28) so that the first nonquadratic term is quartic. In appropriate nondimensional form (A12.29a) is rewritten as

$$u_{tt} - u_{XX}\left(1 - \beta u_X^2\right) - \delta^2 u_{XXXX} = 0. \tag{A12.29b}$$

In the linear case, trying a solution $u = a\exp(i\varphi)$, with $\varphi = KX - \omega t$, we deduce from (A12.29) the following "linear" dispersion relation:

$$D_L(\omega, K) := \omega^2 - K^2\left(1 - \delta^2 K^2\right) = 0. \tag{A12.30}$$

It is readily checked that the averaged Lagrangian is given by

$$\tilde{L} = \frac{1}{2\pi}\int_0^{2\pi} L d\varphi = D_L(\omega, K)a^2. \tag{A12.31}$$

Accordingly, the associated Euler–Lagrange variational equations (A12.15) and (A12.16) for the amplitude $a$ and the phase $\varphi$ read (for $a \neq 0$)

$$D_L(\omega, K) = 0 \tag{A12.32}$$

and

$$\frac{\partial(\omega a^2)}{\partial t} + \frac{\partial(Ka^2)}{\partial X} = 0, \tag{A12.33}$$

which are the linear dispersion relation and the conservation of wave action, respectively.

Now we look for the influence of the elastic nonlinearity. First, following Newell (1985) or Maugin and Hadouaj (1991), we construct an amplitude-dependent dispersion relation (remember Equation 3.11). For this purpose we consider the following asymptotic solution with slow space $x$ and time $T$ variables:

$$u(X,t) = a\exp(i\varphi) + \varepsilon u_1 + \varepsilon^2 u_2 + \ldots., \quad x = \varepsilon X, \quad T = \varepsilon t, \tag{A12.34}$$

where $\varepsilon$ is an order parameter and the phase is defined in a general way by (A12.2) and (A12.3). We immediately have

$$\frac{\partial}{\partial t} = -\omega\frac{\partial}{\partial\varphi} + \varepsilon\frac{\partial}{\partial T}, \quad \frac{\partial}{\partial X} = K\frac{\partial}{\partial\varphi} + \varepsilon\frac{\partial}{\partial x}. \tag{A12.35}$$

On substituting (A.12.34) and (A12.35) in (A12.3) and (A12.29), at the order zero in $\varepsilon$ we obtain ($D_L \neq 0$)

$$\frac{\partial^2 u_0}{\partial \varphi^2} + \nu^2 u_0 = 0, \tag{A12.36}$$

where

$$u_0 = a \exp(i\nu\varphi), \quad \nu^2 = -\frac{\beta a^2}{D_L(\omega, K)}. \tag{A12.37}$$

The zeroth-order solution is only $2\pi$ periodic with no smaller period when $\nu^2 = 1$, that is, when there holds the following *amplitude-dependent dispersion relation*:

$$\bar{D}_{NL}(\omega, K; a) := D_L(\omega, K) + \beta a^2 = 0. \tag{A12.38}$$

Alternatively, this equation may be considered as providing the slowly varying amplitude in terms of $\omega$, $K$, and the material parameters. However, following Newell (1985) or Maugin (1999, Appendix A6) and in anticipation of more generality, it is worthwhile to view (A12.38) as a first (zeroth) approximation and write the general dispersion relation in the perturbed form of a *"dispersive" nonlinear dispersion relation*:

$$D_{NL}(\omega, K; a, a_x, a_T, \ldots) := \bar{D}_{NL}(\omega, K; a) + (\varepsilon g_1 + \varepsilon^2 g_2 + \ldots) = 0, \tag{A12.39}$$

where the ellipsis in the arguments of $D_{NL}$ on the left-hand side stand for higher-order space and time derivatives in the slow variables. The first-order term in the expansion of (A12.34) indeed yields $u_0 = a\exp(i\varphi)$. The next order yields $g_1 = 0$, $u_1 = 0$, and none other than the wave-action conservation (A12.34). The fact that $u_1$ vanishes is not surprising since the quartic nonlinearity of the initial potential is a third-harmonic generator. At order two, we will obtain that $g_2$ must be given by

$$g_2 = -a^{-1}\left(\frac{\partial^2}{\partial T^2} - \frac{\partial^2}{\partial x^2}\right)a. \tag{A12.40}$$

Gathering these results in (A12.49) we finally have the following *"wave-like" equation* for the dispersive nonlinear dispersion relation:

$$\omega^2 - K^2(1 - \delta^2 K^2) + \beta a^2 - \varepsilon^2 a^{-1}\left(\frac{\partial^2}{\partial T^2} - \frac{\partial^2}{\partial x^2}\right)a = 0. \tag{A12.41}$$

We have thus constructed a set of partial differential equations for the unknown triad ($\omega$, $K$ $a$), a system that consists of Equations A12.33, A12.34,

and A12.41. The general solution of this is impracticable. That is why an interesting approximation consists in considering an almost monochromatic regime ($\omega_0$, $K_0$) whose point belongs to the linear dispersion relation in Equation A12.32—that is, when $\beta$ and $\varepsilon$ vanish. But in the nonlinear case we have to consider couples ($\omega$, $K$) in the neighborhood of this working point. On account of the representation (A12.3) we shall therefore write

$$K = K_0 + \varepsilon\phi_x, \quad \omega = \omega_0 - \varepsilon\phi_T, \tag{A12.42}$$

where $\phi$ is the perturbation phase. Moreover, we introduce a moving coordinate $\xi$ and a new scaling by

$$\xi = x - \omega_0' T, \quad \tau = \varepsilon T, \quad a \to \varepsilon a, \tag{A12.43}$$

where a prime denotes the derivative with respect to $K$ at $K_0$. Then (A12.34) and (A12.41) first yield the following two equations:

$$\frac{\partial}{\partial T}\left(\left(\omega_0 - \varepsilon\phi_T\right)a^2\right) + \frac{\partial}{\partial x}\left(\left(K_0 + \varepsilon\phi_x\right)a^2\right) = 0 \tag{A12.44}$$

and

$$a^{-1}\left(\frac{\partial^2}{\partial T^2} - \frac{\partial^2}{\partial x^2}\right)a - \left(\phi_T^2 - \phi_x^2 + \beta a^2 + \delta\phi_\xi^4\right) + 2\left(\omega_0\phi_T + K_0\phi_x\right) = 0. \tag{A12.45}$$

Then using (A12.43) these two equations provide two first-order time differential equations:

$$2\omega_0 a a_\tau + \left(1 - \omega_0'^2\right)a\left(2a_\xi\phi_\xi + a\phi_{\xi\xi}\right) + \text{h.o.t.} = 0 \tag{A12.46}$$

and

$$\left(1 - \omega_0'^2\right)a^{-1}\left(a_{\xi\xi} - \phi_\xi^2\right) - \left(\beta a^2 + \delta\phi_\xi^4\right) + 2\omega_0\phi_\tau + \text{h.o.t.} = 0, \tag{A12.47}$$

where h.o.t. stands for higher-order terms. These two equations therefore yield ($\omega_0 \neq 0$)

$$a_\tau = \frac{\omega_0'^2 - 1}{2\omega_0}\left(a_\xi\phi_\xi + a\phi_{\xi\xi}\right), \tag{A12.48}$$

and

$$\phi_\tau = \frac{1-\omega_0'^2}{2\omega_0}\left(a^{-1}a_{\xi\xi} - \phi_\xi^2\right) + \frac{\beta a^2}{2\omega_0} \tag{A12.49}$$

Finally, introducing a complex amplitude $A = a\exp(i\phi)$, (A12.48) and (A.12.49) combine to give a single *nonlinear Schrödinger equation* (NLS equation; the asterisk denotes complex conjugacy):

$$iA_\tau + pA_{\xi\xi} + q|A|^2 A = 0. \tag{A12.50}$$

with the definitions

$$p = \frac{1}{2}\omega_0'', \quad q = \frac{\beta}{2\omega_0}. \tag{A12.51}$$

Here $\omega_0''$ is the curvature of the linear dispersion relation at the working point $(\omega_0, K_0)$ . As already mentioned (A12.50) is a canonical equation of the theory of envelope waves; that is, it always obtains but with different values of $p$ and $q$. According to the celebrated result of Zakharov and Shabat (1972), this equation admits stable "bright" envelope solitons as solutions whenever the product $pq$ is positive, that is, when the product of the curvature of the linear dispersion relation and of the quartic nonlinearity parameter is positive. If the curvature is negative, then the material must be selected to have a negative parameter β to allow for the propagation of these "bright" solitons. Thus the choice of the working point and of the specific material is crucial for the existence of this wave phenomenon. Now, solutions of this type should not come here as a surprise—except for the exploited methodology, which is seldom used in solid mechanics—because the original modified Boussinesq equation has associated with it an evolution equation (one-directional equation deduced by means of the so-called reductive perturbation method), which is a modification of the traditional Korteweg–deVries equation, and the latter itself will provide modulated envelope waves in the appropriate conditions of slow variation of the modulation of a small amplitude almost monochromatic signal (Benney and Newell, 1967; Ostrovsky and Potapov, 1999).

### A12.1.4 Return to the Notion of Eshelby Stress

Now, before concluding, we briefly return to the notion of Eshelby stress. The model (12.29) fits into the second-gradient scheme of Equations 4.119, 4.121, and 4.125. According to (4.49) and after a short computation, the material Eshelby stress (here reduced to a scalar) is

$$b = -\left[\frac{u_t^2 + u_X^2}{2} + \frac{3}{2}\delta^2 u_{XX}^2 - \frac{\beta}{4}u_X^4 - \delta^2 u_X u_{XXX}\right], \tag{A12.52}$$

and the balance of *material (or field) momentum* (here a strict conservation law) reads

$$\frac{\partial\left(-u_t u_X\right)}{\partial t}+\frac{\partial}{\partial X}\left[\frac{u_t^2+u_X^2}{2}+\frac{3}{2}\delta^2 u_{XX}^2-\frac{\beta}{4}u_X^4-\delta^2 u_X u_{XXX}\right]=0. \qquad \text{(A12.53)}$$

Here some of the groupings of terms are misleading and due to the specific one-dimensional nature of the problem (see our remark in Section 12.1.2). But now if we try to think in terms of the averaged Lagrangian, in the linear (but dispersive) case the latter will be provided by (A12.14) in which $D_L$ is given by the left-hand side of (A12.30). On using the definitions in (A12.17) we shall find that the general balance of *wave momentum* is given by

$$\frac{\partial\left(\omega K a^2\right)}{\partial t}+\frac{\partial}{\partial X}\left[\left(\frac{\omega^2+K^2}{2}-\frac{3}{2}\delta^2 K^4\right)a^2\right]+\ldots=0, \qquad \text{(A12.54)}$$

where the ellipsis in the left-hand side stands for unknown terms due to the nonlinear nature of the full problem. Noting $\tilde{P}=-u_t u_X \approx \omega K a^2$ in the zeroth approximation we obviously identify the analogies between Equations A12.53 and A12.54. To go further in the exploitation of (A12.54) we would have to find the missing nonlinear terms and enforce the already indicated perturbation of the dispersion relation, introduce an averaged Lagrangian that depends also on the time derivative and space derivative of the amplitude, and apply the almost monochromatic approximation (A12.42).

By way of conclusion, we note that Equation A12.50 itself partakes of the wave–particle dualism in the sense that, via a new application of the canonical formalism, a *quasiparticle* having Newtonian mechanics as its "point particle" mechanics (see Section 12.5) can be associated with that equation. The "point mass" involved in this mechanics is none other than the "wave action" or "number of phonons" defined by

$$M=\int_R |A|^2\, dX \qquad \text{(A12.55)}$$

on the real line $R$. Thus, successive application of the wave–mechanics dualism, averaged Lagrangian method, and perturbation techniques led us again to some kind of particle–wave dualism. Although quantization in the linear wave case with the concept of phonons applies directly, here the path has been long and indirect. Further elaboration of analytical continuum mechanics is needed to warrant further progress along this line. Some analogies between canonical continuum mechanics and continuum wave-kinematics may still be noted. For instance, for homogeneous systems, if the action flux **W** is either zero or everywhere tangential to the material body $B$ at its surface

$\partial B$, integration over material space of Equations A12.16 and A12.17$_2$ yields the global balance equations

$$\frac{d}{dt}\int_B \tilde{S}dV = 0, \quad \frac{d}{dt}\int_B \tilde{\mathbf{P}}dV + \int_{\partial B} \tilde{L}\mathbf{N}dA = \mathbf{0}; \tag{A12.56}$$

that is, total wave action is conserved and total material wave momentum is driven by the flux of averaged Lagrangian, in the same way as total physical momentum is conserved and total material momentum is driven by the flux of physical Lagrangian in material mechanics for a vanishing or tangential applied traction at the boundary. This is one of the analogies that can be easily established.

# 13

# *Numerical Applications*

## Object of the Chapter

Where we find out that the Eshelby canonical stress is not only a theoretical concept but that its introduction kindled the improvement of various numerical methods, not the least being the ubiquitous finite-element method, while the finite-difference method and the finite-volume method gain in accuracy and practicality thanks to its consideration.

## 13.1 Introduction

It is usually, and correctly, remarked that at all regular material points, the balance of material momentum in pure mechanics is "equivalent" to the balance of physical momentum. The reason for this is that at all such points, the former can be deduced from the latter by some algebraic and analytic operations allowed by the smoothness of the fields. That is, at such points the balance of material momentum is an *identity.* However, it is not exactly true that both equations of momentum are operationally equivalent, being then only two different "projections" on different manifolds of the same equation, because they *cannot* play the same role in *problem solving.* This is due to the fact that, whether we like it or not, applied forces—which are real physical forces in the Newtonian–Euler–Cauchy sense—are prescribed in physical space (a world to which they belong by definition) so that they intervene in problem solving in the equations (field equations and boundary conditions) expressed in that space. Therefore, initial-value boundary-value problems are, of necessity, solved, analytically or numerically, in physical space. The question then arises of the usefulness of the balance of material momentum at regular material points, its role in capturing singularities being clear at singular points (cf. foregoing chapters). This usefulness resides in the redundancy between the two (essentially vectorial) equations as it can be exploited thus. While the balance of physical momentum—and other equations governing other

fields than deformation—are used in direct problem solving, the balance of material momentum (or its "equilibrium" form where this applies) is to be exploited either in the form of a *criterion* to be satisfied by the already obtained point-wise field solution (e.g., in fracture, phase-transition, anelasticity, etc.) or as a way of checking globally the accuracy and quality of the obtained solution. This is very similar to the exploitation of the energy balance in the numerics of hyperbolic systems where the accuracy of the adopted scheme is measured by a global energy criterion (i.e., one asks whether the scheme conserves energy). In the following we focus attention on such an application of the balance of material momentum in various numerical techniques, noting in passing that the notion of momentum is vectorial, and therefore "directional," and thus richer than that of energy (a scalar), which addresses only magnitude. Three numerical techniques are briefly examined in the light of recent advances. These are the known techniques—also called *methods*—of (i) **finite differences** (hence the finite-difference method (FDM)), which is the oldest one, introduced initially for solving the Laplacian and wave-like problems (essentially hyperbolic problems); (ii) **finite elements** (hence the finite-element method (FEM)), conceived in the 1960s, which have a strong engineering flavor initially due to the aeronautical structural-mechanics background although very much related to the principle of virtual work and the notions of generalized functions (test functions), and (iii) **finite volumes** (hence the finite-volume method (FVM)), which carry with them the spirit of balance laws and thus are intimately related to continuum physics. Dynamics is the preferred realm of the first and third techniques, which we shall examine first, while the FEM has found favor among many engineers in solving equilibrium mechanical situations because of the existence of many handy ready-to-use packages. However, it seems to be the one that most benefited from the new notion of material forces in recent developments, and therefore it will be examined at a little greater length.

## 13.2 Finite-Difference Method

The *finite-difference method* (FDM) is the numerical realm of nonlinear hyperbolic systems. This discretization method finds its origin in analysis and the approximation of space derivatives of various orders by finite differences. Most often the method has to be especially designed (hence we speak of different numerical *schemes*) for the system of partial differential equations under consideration. That is why FDM is often considered as an art with its technicalities such as implicit and explicit schemes, the choice of steps (integer, half, mixed), the comparison between steps in space and time (the so-called Courant number), and so on. The school of Courant (Lax, Wendroff, etc.) in the United States and that of Godunov and Yanenko in Russia are responsible for

its successes in treating problems including sharp field discontinuities such as shock waves in fluids. The accuracy of the devised FDM schemes is measured by their ability to more or less conserve the global energy of the system. That is, in the present case, the numerical simulation of nonlinear-wave propagation is performed on the FDM discretized version of the *field* equations. For a *conservative system* it is checked whether the global (space integral) version of the energy equation holds good for the numerically obtained solution. The result of this check is expressed by announcing that for example, "energy is conserved up to x%," values of the order of 0.1 percent or $10^{-3}$ being quite normal. From that viewpoint, checking that the global version of the here redundant material—or canonical or field-momentum—balance law holds good for the numerical solution obtained is also a valid criterion for the accuracy of the FDM scheme, except that, because of the *vectorial nature* of that equation, the check is made along three different axes instead of that of the conservation of a single scalar entity as is the case for the energy equation. This places energy and canonical momentum on equal footing or, as we like to say, on the same *ontological level*. In particular, for *systems* of field equations, both canonical equations and accuracy criteria concern the *global* physical system and not only one degree of freedom in spite of the 3D vectorial nature of canonical momentum. Thus, following Christov and Maugin (1995), we may speak of FDM schemes that more or less conserve *both* energy and canonical momentum.

As exemplified by cases examined in Chapter 12, with the introduction of localized nonlinear waves of the solitary-wave type (kinks, humps, bound states, soliton complexes) in nonlinear *dispersive* systems of field equations, the exploitation of the canonical momentum balance law is even more fruitful. This is easily understood by examining two specific questions. First, in a general way, for such systems, the field equations present both nonlinearities and high-order space or mixed derivatives. This is the case when treating an elastic crystal in which both nonconvexity of the strain energy and a weak nonlocality (gradient effects) are taken into account (e.g., in shape-memory alloys). An example of such systems is the following 1-D generalized Boussinesq equation (cf. Maugin and Christov, 2002) where subscripts $t$ and $x$ stand for partial derivatives, $s$ is a strain (e.g., one shear component), $F(s)$ is a polynomial in $s$ starting with second degree, and $\beta$ is a positive or negative parameter:

$$s_{tt} - c_T^2 s_{xx} - \left[F(s) - \beta s_{xx} + s_{xxxx}\right]_{xx} = 0. \tag{13.1}$$

A *stiff* mathematical system such as this one, although one-dimensional in space, requires devising a high-performance FDM scheme (see, e.g., Christov and Maugin, 1995). This means that FDM is also an art. We do not write here the field-momentum balance equation that corresponds to the field equation (13.1) because its formal expression suffices for our general purpose. Imagine that we have obtained analytically (with some luck) or numerically strongly localized solitary-wave-like solutions of (13.1) that we call "shapes" $S$. These

usually correspond to spatially uniform solutions at infinity. First, the writing of the global form—by integration over the real line $R$ in the absence of applied force—of the field or wave–momentum equation provides theoretically an equation of the following type:

$$\frac{d\mathbf{P}}{dt} = \mathbf{0}; \quad \mathbf{P} := \int_R P\,dX. \tag{13.2}$$

This is a Newtonian-like equation of *inertial motion* for the "shape" $S$. There is no term in the right-hand side of Equation $13.2_1$ because all field derivatives go to zero at infinity for these solutions $S$, which, therefore, are steadily progressing. As a matter of fact, imposing the vanishing of the right-hand side of $(13.2)_1$ reveals the *natural limit* conditions on higher-order field derivatives, which classical types of boundary conditions do not consider. But in the numerical simulation of the steady propagation of "*shapes*" $S$, we have to work either on a periodic landscape arrangement or on a finite space interval. The satisfaction of these conditions is a necessity for the realization of the inertial motion globally governed by (13.2). Otherwise, the nonzero values at the interval boundaries will in fact create a perturbing *driving force* that will accelerate or slow down the supposedly steadily moving shape, with a motion equation

$$\frac{d\mathbf{P}}{dt} = \mathbf{F}^{\text{driving}} \neq \mathbf{0} \tag{13.3}$$

then replacing $(13.2)_1$. Making $\mathbf{F}^{\text{driving}}$ zero or minimal in some sense is a justified endeavor. But it is clear that the same scheme—Equations $13.2_1$ and 13.3—can also be exploited to treat the influence of nonzero applied forces (or any term that can be viewed as a perturbation on the inertial motion of undeformed "shapes" present in the right-hand sides of the basic field equations to start with). Then the initial "shape" solutions are found—with some freedom left to some of their parameters—on the basis of the homogeneous form of these equations. Equation 13.3, where the right hand-side is then given by the space-integrated, materially convected form of this perturbing force, provides the time-evolution equation of these gross parameters (e.g., speed) in solutions (transient nonlinear localized wave forms) that cannot be obtained through any other known method. Examples of application of this technique have been presented in the preceding chapter—see also Christov et al. (1996), Maugin (1999), and Maugin and Christov (2002). Note that, as mentioned in the introduction to this chapter, and in accordance with the general philosophy of this presentation, the field equations, per se, serve one purpose, while the energy and/or canonical momentum equations serve another. Note by way of conclusion that (13.2) and (13.3) do not presuppose that the *point mechanics* (relationships between mass, momentum, velocity, and energy) satisfied by the "shapes" in question is Newtonian. These relationships are part of the problem as shown in the examples of nonlinear-wave propagation treated in Chapter 12.

## 13.3 Finite-Volume Method—Continuous Cellular Automata

The *finite-volume method* (FVM) considers a fixed grid and cells, rather than discrete points, as discrete elements. It directly reflects the notion of conservation laws, which apply to these cells. The continuum theories of physics clearly emphasize the notions of balance laws and conservation laws. Therefore, the FVM seems, at the price of some adjustments, appropriate for the treatment of dynamic problems issuing from continuum mechanics. This is all the more true given that cells thus considered may also be viewed as the elementary blocks of the thermodynamics of so-called *discrete systems* in the manner of Schottky (cf. Muschik, 1990). In this thermodynamics the state in one discrete system (e.g., one of the above cells) is defined in terms of its environment, which may or may not be in thermodynamic equilibrium. *Contact thermodynamic quantities* (e.g., contact temperature, contact stresses) are introduced to characterize the state of the discrete system (in fact defined at the boundary surface of a cell in the FVM). This idea of making a cell's state depend on that of its neighbors is tantamount to introducing a *strategy* for the propagation of the thermodynamic state. This is akin to introducing the notion of *cellular automaton*, although discretization here is based on continuum balance laws, so that we may refer to this method as that of *continuous cellular automata.* The strategy referred to in the preceding is essential in some dynamic thermomechanical problems such as that of the propagation of a *phase-transition front*. It is along this line of thought that recent works develop.

To illustrate the notion of the FVM, it is interesting to give a very few elements of that type of approach, for instance, in linear isotropic but materially inhomogeneous thermoelasticity, where the basic field equations are those given in Section 2.3. All thermomechanical balance laws must be expressed for each cell, and the bulk quantities within each cell are related to the contact ones through the thermodynamics of discrete systems. A high-performance wave-propagation algorithm can be exploited—using or astutely mixing Lax–Wendroff and Godunov's ideas (cf. Berezovski and Maugin, 2001)—that yields extremely good results in the simulation of the rapid progression of sharp wave fronts in 2D elasticity or thermoelasticity (cf. Berezovski and Maugin, 2001, 2002). Here, the balance of linear (physical) momentum, the time-rate of change of the Hooke–Duhamel constitutive equation, and the heat-propagation equation read as follows at any regular material point $\mathbf{x}$ in the absence of body force and heat source:

$$\frac{\partial\left(\rho_0(\mathbf{x})v_i\right)}{\partial t}-\frac{\partial\sigma_{ji}}{\partial x_j}=0, \tag{13.4}$$

$$\frac{\partial\sigma_{ji}}{\partial t}=\lambda(\mathbf{x})\frac{\partial v_k}{\partial x_k}\delta_{ij}+\mu(\mathbf{x})\left(\frac{\partial v_i}{\partial x_j}+\frac{\partial v_j}{\partial x_i}\right)+m(\mathbf{x})\frac{\partial T}{\partial t}\delta_{ij}, \tag{13.5}$$

$$\frac{\partial(C(\mathbf{x})T)}{\partial t} = \frac{\partial}{\partial x_i}\left(k(\mathbf{x})\frac{\partial T}{\partial x_i}\right) + m(\mathbf{x})\frac{\partial v_k}{\partial x_k}. \tag{13.6}$$

where $\rho_0$ is the density of matter, $\sigma$ is Cauchy's stress, $\lambda$ and $\mu$ are Lamé coefficients, $m = -\alpha(3\lambda + 2\mu)$ is the thermoelastic coupling coefficient if $\alpha$ is the dilatation coefficient, $C$ is the heat capacity, and $k$ is the heat-conduction coefficient; $T$ here denotes the small deviation of temperature. The material inhomogeneity is explicitly indicated by the **x**-dependence of some of these coefficients. Note that even the (Hooke–Duhamel) constitutive equation is rewritten as a kind of local conservation law (13.5). By integration over a cell or finite-volume element $V$ of Equations 13.4 through 13.6, we obtain the following system of FVM balance equations:

$$\frac{\partial}{\partial t}\int_V \rho_0 v_i \, dV = \int_{\partial V} \Sigma_{ij} n_j \, dA, \tag{13.7}$$

$$\frac{\partial}{\partial t}\int_V \varepsilon_{ij} dV = \int_{\partial V} H_{ijk} n_k dA, \tag{13.8}$$

$$\frac{\partial}{\partial t}\int_V \sigma_{ij} dV = \int_{\partial V} \left(2\mu H_{ijk} n_k + \lambda \delta_{ij} V_k \, n_k\right) dA + \varphi_{ij}, \tag{13.9}$$

$$\frac{\partial}{\partial t}\int_V CT dV = \int_{\partial V} \left(k(\mathbf{n}.\nabla)T + mV_k \, n_k\right) dA + \varphi^{\text{inh}}, \tag{13.10}$$

where we have set

$$H_{ijk} \equiv (1/2)\left(\delta_{ik} V_j + \delta_{jk} V_i\right) \tag{13.11}$$

and source terms due to material inhomogeneities (labeled *"inh"*) and thermoelastic couplings (labeled *"te"*) are given by

$$\varphi_{ij} = \varphi_{ij}^{\text{te}} + \varphi_{ij}^{\text{inh}}, \tag{13.12}$$

$$\varphi_{ij}^{\text{te}} = \int_V m\delta_{ij} \frac{\partial T}{\partial t} dV, \tag{13.13}$$

$$\varphi_{ij}^{\text{inh}} = -\int_V \left(v_k \frac{\partial \lambda}{\partial x_k}\delta_{ij} + v_i \frac{\partial \mu}{\partial x_j} + v_j \frac{\partial \mu}{\partial x_i}\right) dV, \tag{13.14}$$

$$\varphi^{\text{inh}} = -\int_V v_k \frac{\partial m}{\partial x_k} dV. \tag{13.15}$$

In the preceding, $V_i$ (trace of $v_i$ at the boundary) and $\Sigma_{ij}$ (trace of $\sigma_{ij}$ at the boundary) are the "contact" velocity and Cauchy stress defined at the FV element boundary of unit outward normal $n_i$. $\Theta$ denotes the "contact temperature." Contact and bulk quantities are related by thermodynamic constraints, which express the continuity of some partial derivatives of the internal energy (cf. Berezovski and Maugin, 1999), such as the following one for the stress—labels (1) and (2) refer to two neighboring cells:

$$\sigma_{ij}^{(1)} + \Sigma_{ij}^{(1)} - T^{(1)}\left(\frac{\partial \sigma_{ij}^{(1)}}{\partial T}\right)_{\varepsilon} - \Theta^{(1)}\left(\frac{\partial \Sigma_{ij}^{(1)}}{\partial T}\right)_{\varepsilon} = \text{same with label}\,(2). \quad (13.16)$$

The reader is referred to Berezosvki (1997) and Berezovski and Maugin (2001, 2002) for the application to the numerics of smooth elastic and thermoelastic 2D wave propagation. What about the application to the propagation of phase-transition fronts where, of necessity, a criterion of progress (change of thermoelastic phase as the front progresses) is involved? This must necessarily exploit the *balance of canonical momentum* in a form adapted to the continuous-cellular automaton formalism. As a matter of fact, in the present case, this additional balance law reads, at each regular material point:

$$\frac{\partial p_i^w}{\partial t} - \frac{\partial b_{ji}^w}{\partial x_j} = f_i^{\text{inh}} + f_i^{\text{th}}, \quad (13.17)$$

where we have set ($W$ is the free energy per unit volume)

$$p_i^w = -\rho_0 v_j u_{j,i}, \quad b_{ji}^w = -\left(L^{\text{th}}\delta_{ji} + \sigma_{jk}u_{k,i}\right), \quad (13.18)$$

$$L^{\text{th}} = \frac{1}{2}\rho_0(\mathbf{x})\mathbf{v}^2 - W\left(\varepsilon_{ij}, T; \mathbf{x}\right), \quad f_i^{\text{inh}} = \left(\frac{\partial L^{\text{th}}}{\partial x_i}\right)_{\text{expl}},$$

$$f_i^{\text{th}} = S\frac{\partial T}{\partial x_i}, \quad S = -\frac{\partial W}{\partial T}. \quad (13.19)$$

The two source terms in (13.17) are due, respectively, to true material inhomogeneities and pseudo-inhomogeneities caused by thermal effets; $p_i^w$, the purely quadratic part of canonical momentum, is the w*ave* or *crystal momentum*, and $b_{ji}^w$ is the corresponding part of the Eshelby stress tensor, with $u_i$ the infinitesimal displacement. The integral of (13.17) over a VE cell yields

$$\frac{\partial}{\partial t}\int_V p_i^w dV - \int_{\partial V} n_j B_{ji}^w dA = \Phi_i^w, \quad (13.20)$$

where

$$\Phi_i^w = \int_V \left( f_i^{\text{inh}} + f_i^{\text{th}} \right) dV, \tag{13.21}$$

and $B_{ji}^w$ is the "contact" Eshelby stress tensor. Together with the Eshelby tensor of the neighboring cell, the Eshelby stress $b_{ji}^w$ satisfies the following time-evolution equation and thermodynamic constraint:

$$\frac{\partial b_{ji}^w}{\partial t} = -\left( \frac{\partial L^{\text{th}}}{\partial t} \delta_{ji} + \frac{\partial \sigma_{jk}}{\partial t} \frac{\partial u_k}{\partial x_i} + \sigma_{jk} \frac{\partial v_k}{\partial x_i} \right) \tag{13.22}$$

and

$$-\frac{\partial}{\partial t} \left( \frac{\partial u_j}{\partial x_p} \right) \left( B_{pj}^w - b_{pj}^{w*} \right) \geq 0, \tag{13.23}$$

where the minus sign in (13.23) originates from the fact that the Eshelby stress expends power in the "inverse-motion" velocity field. A short algebra allows one to show that the volume-element integral of (13.22) yields the following expression:

$$\begin{aligned} \frac{\partial}{\partial t} \int_V \left( b_{ji}^w + \frac{1}{2} \rho_0 \mathbf{v}^2 \delta_{ji} \right) dV = -\int_{\partial V} \left( \Sigma_{jk} V_k n_i \right) dA + \\ + \int_V \left( \left( \sigma_{pq} \frac{\partial v_p}{\partial x_q} - C \frac{\partial T}{\partial t} \right) \delta_{ji} - \frac{\partial \sigma_{jk}}{\partial t} \frac{\partial u_k}{\partial x_i} + \frac{\partial \sigma_{jk}}{\partial x_i} v_k \right) dV. \end{aligned} \tag{13.24}$$

The integrand in the left-hand volume integral is none other than the *"quasi-static"* Eshelby stress, which indeed governs the phase transition, as already seen in Chapter 7. The criterion of progress must, therefore, exploit Equations 13.23 and 13.24. This technique has been used repeatedly by Berezovski, Maugin, and coworkers in propagation involving phase transformations as well as simply continuously inhomogeneous materials or randomly inhomogeneous materials (e.g., Berezovski, Engelbrecht and Maugin, 2003, 2008).

NOTE: The "balance laws" rewritten in the preceding over a cell element are in a form ready for discretization since they are of the general form in FVM: The time derivative of a volume average computed at the center of a cell is balanced by flux terms evaluated at the boundary of the cell element and source terms again evaluated at the center of each cell element. If cells are labeled by means of integers, their flat boundaries are labeled by half integers. In the reduced one-dimensional case, this reminds us of known

finite-difference schemes using the notion of half-integer numeration (leap-frog steps and so on).

**Numerical Illustrations**

**EXAMPLE 1:** Wave interaction with martensitic inclusion (all figures after Maugin and Berezovski, 2009). This is a 2D propagation problem that provides the simulation of the wave interaction with a martensitic inclusion in an austenite environment (see Section 12.7 for this general nonlinear wave problem). The initial shape of the martensitic inclusion is shown in Figure 13.1. (This is a cylinder of long length orthogonally to the plane of the figure.) The pulse loading is applied at a part of the left boundary of the computation domain by prescribing a time variation of a normal component of the stress tensor. The snapshot of the stress distribution at 30 time steps (Figure 13.2) shows the form of the pulse after its departure and short-time propagation in the austenite. Upper and bottom boundaries are stress free, and the right boundary is assumed to be rigid. The material properties of austenite and martensite correspond to Cu-14.44Al-4.19Ni shape-memory alloy (Escobar and Clifton, 1993). In the austenitic phase, the density is equal to 7100 kg/m$^3$, the elastic modulus $E$ is 120 GPa, the shear wave velocity has the value of 1187 m/s, and the dilatation coefficient is $6.75 \cdot 10^{-6}$ 1/K. For the martensitic phase, $E$ is 60 GPa, and the shear wave velocity is 1055 m/s, with the same density and dilatation coefficient as in the preceding.

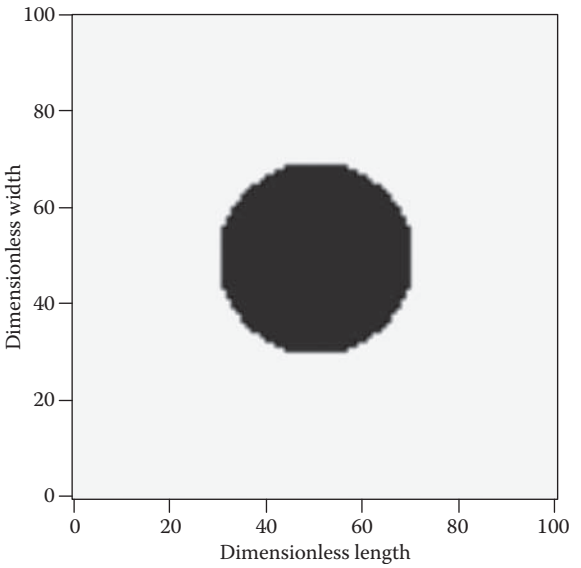


**FIGURE 13.1**
**(See color insert following page 434.)** Initial shape of martensitic inclusion (dark zone).

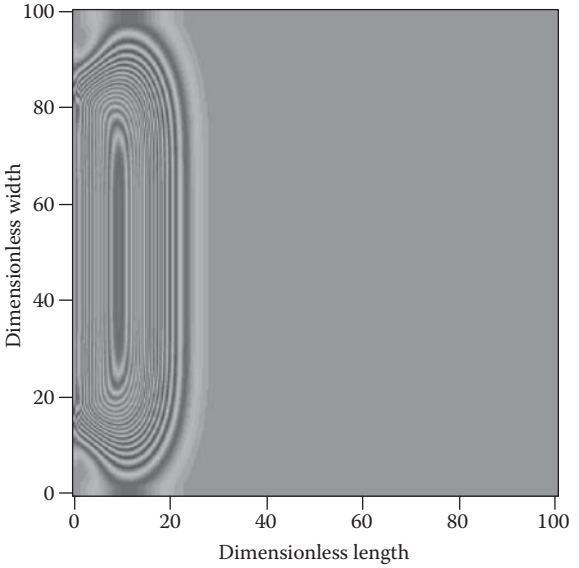


**FIGURE 13.2**
**(See color insert following page 434.)** Initial pulse shape.

The next figure, Figure 13.3, shows the interaction of the pulse with the martensitic inclusion. Due to the difference in material properties of martensite and austenite, the velocity of the wave in martensite is less than in austenite. Simultaneously, the phase transformation process is induced at the boundary between martensite and austenite (Figure 13.4). The final stage of the interaction is presented in Figure 13.5 in terms of the stress distribution. The changed shape of the martensitic inclusion after the interaction with the stress pulse is shown in Figure 13.6. One can see the growth of the martensitic inclusion in all directions, but the growth in the rear side of the inclusion (right part in the figure) is more than in its front side (left part on the figure). Note that in this simulation the FVM discretization is rather coarse but sufficient to exhibit the main effects.

**EXAMPLE 2:** Plate under stepwise constant loading (all figures after Maugin and Berezovski, 2009). Now we consider the application of a constant velocity stepwise loading only at a part of the left boundary of a plate, with the upper and bottom boundaries being stress free. At the right boundary we apply a nonreflective boundary condition (Figure 13.7). Calculations are performed for the Cu–Zn (25.63 wt. %)-Al (4.2 wt. %) shape-memory alloy (Goo and Lexcellent, 1997). The corresponding mechanical properties are the following: The density has the value of 8228 kg/m$^3$, the Young modulus values in austenite and in martensite are 67.25 GPa and 32 GPa, respectively, and Poisson's ratio is 0.33 in both phases.

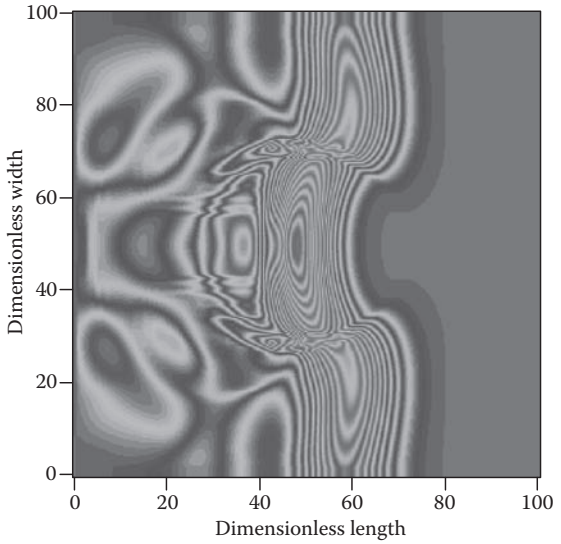


**FIGURE 13.3**
**(See color insert following page 434.)** Contour plot of stress distribution at 80 time steps.

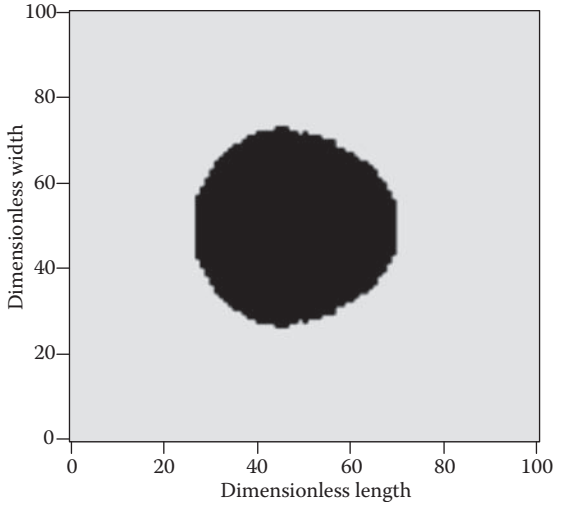


**FIGURE 13.4**
**(See color insert following page 434.)** Shape of martensitic inclusion at 80 time steps.

In an elastic material, the stepwise loading with constant velocity leads to a stepwise constant stress distribution. However, due to the martensitic transformation, here we obtain a more complicated distribution of the stress inside the plate. Snapshots of wave fronts and the corresponding location of the phase boundary at different time instants are shown in Figures 13.8

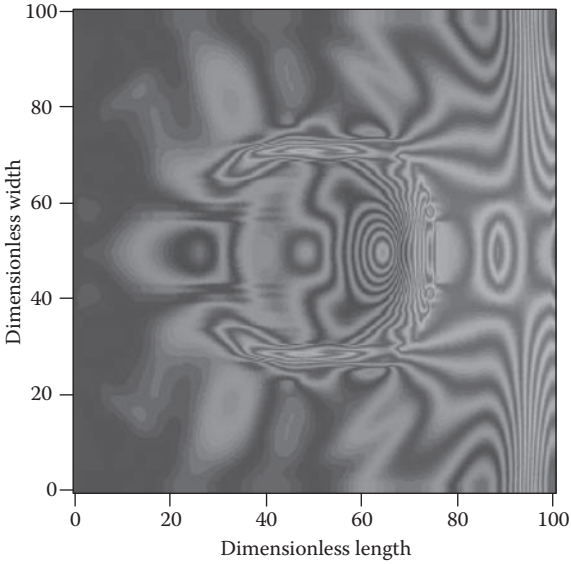


**FIGURE 13.5**
**(See color insert following page 434.)** Contour plot of stress distribution at 120 time steps.

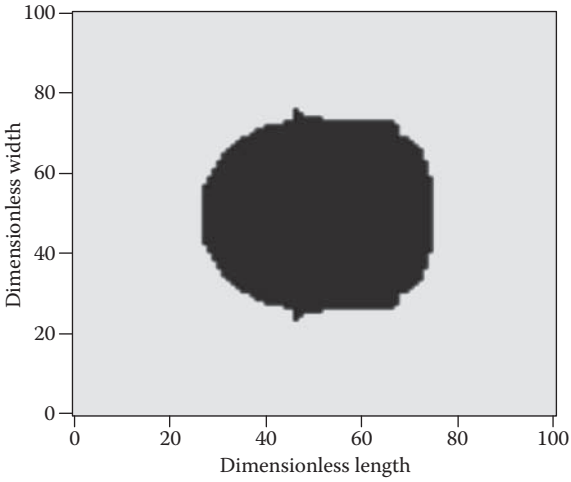


**FIGURE 13.6**
**(See color insert following page 434.)** Final shape of martensitic inclusion.

through 13.10. As one can see, the propagation of stress waves, their reflections from upper and bottom boundaries, and the interaction with the moving phase-transition front form the shape of the front itself. This shows clearly how the loading conditions affect the propagation of the phase-transition front in the two-dimensional case. Approximately after 240 ms, the whole

**FIGURE 13.7**
**(See color insert following page 434.)** Nonplane loading of a plate.

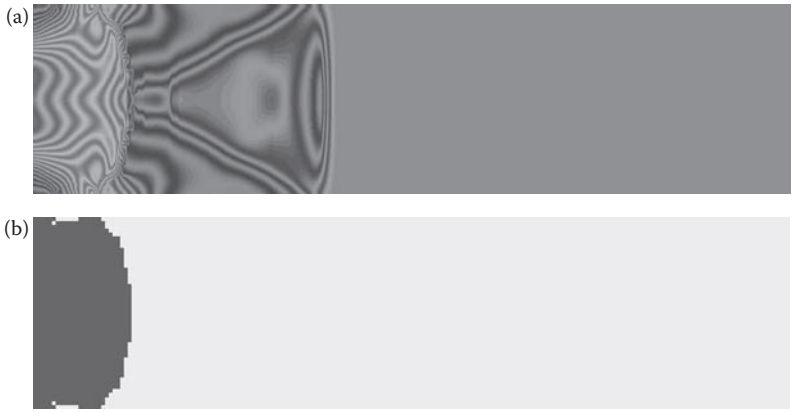


**FIGURE 13.8**
**(See color insert following page 434.)** Snapshot of wave distribution and front location in Cu–Zn–Al plate at 25 microseconds. Red color (lighter in black and white) corresponds to high stress and blue color (darker in black and white) to low stress values.

plate will be transformed into the martensitic state, and further it will be deformed elastically.

## 13.4 Finite-Element Method

### 13.4.1 General Principle

To illustrate our purpose in this section, we remind the reader of the basic equations of equilibrium, energy, and material momentum in finite-strain elasticity (applied body force $\mathbf{f}^0$; corresponding material force $\mathbf{F}^0 = -\mathbf{f}^0 \,.\mathbf{F}$):

$$\mathrm{div}_R \mathbf{T} + \mathbf{f}^0 = \mathbf{0}, \tag{13.25}$$

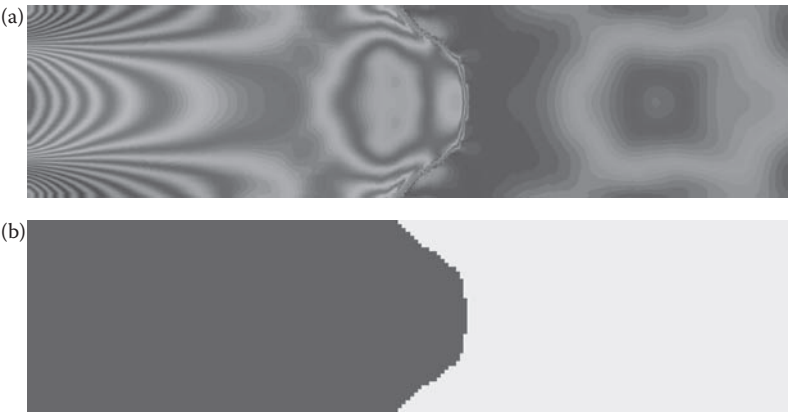


**FIGURE 13.9**
**(See color insert following page 434.)** Snapshot of wave distribution and front location in Cu–Zn–Al plate at 125 microseconds.


**FIGURE 13.10**
**(See color insert following page 434.)** Snapshot of wave distribution and front location in Cu–Zn–Al plate at 225 microseconds.

$$\left.\frac{\partial W}{\partial t}\right|_{\mathbf{x}} = \nabla_R.\left(\mathbf{T}.\mathbf{v}\right) + \mathbf{f}^0.\mathbf{v}, \tag{13.26}$$

$$\mathrm{div}_R\,\mathbf{b} + \mathbf{F}^0 = \mathbf{0}, \tag{13.27}$$

respectively. At all regular material points $\mathbf{X}$ we have the following *Ericksen–Noether identity*:

$$\left(\mathrm{div}_R \mathbf{T} + \mathbf{f}^0\right).\mathbf{F} + \left(\mathrm{div}_R \mathbf{b} + \mathbf{F}^0\right) = \mathbf{0}. \tag{13.28}$$

Note that Equation 13.25, valid at all regular points $\mathbf{X}$ in $\Omega_t$, and the associated *natural boundary* condition at $\partial\Omega_t$,

$$\mathbf{N}.\mathbf{T} = \mathbf{t}^0, \tag{13.29}$$

are equivalent to the following *weak formulation* (principle of virtual power with inertia discarded):

$$P^*_{(i)} + P^*_{(c)} + P^*_{(v)} = 0, \tag{13.30}$$

where

$$P^*_{(i)} = -\int_{\Omega_t} \mathbf{T}:\left(\nabla_R \mathbf{v}^*\right)^T d\Omega, \quad P^*_{(c)} = \int_{\partial\Omega_t} \mathbf{t}^0.\mathbf{v}^* dS, \quad P^*_{(v)} = \int_{\Omega_t} \mathbf{f}^0.\mathbf{v}^* d\Omega. \tag{13.31}$$

Equation 13.30 holds for all sufficiently smooth vectorial test functions (physical velocity fields) $\mathbf{v}^*$. In classical elastic engineering computations, when true material inhomogeneities or defects (field singularities) are absent, the *finite-element method* (FEM) is based on a discretization of Equation 13.30 by introducing interpolations of test functions. Imagine that the computation is also made in the absence of applied body forces ($\mathbf{f}^0 = 0$). Then $\mathrm{div}_R\, \mathbf{T} = 0$ is solved by the FEM, and this yields a solution that depends on the location of nodes of the FEM net on the material manifold. Knowing such an FEM field solution, the quantities $\mathbf{b}$ and $\mathrm{div}_R\, \mathbf{b}$ can be evaluated, and this may yield

$$\mathrm{div}_R \mathbf{b} \neq \mathbf{0} \ \left(\text{say } \mathbf{f}^{\mathrm{err}}\right); \tag{13.32}$$

that is, there may exist a spatial distribution of spurious material forces $\mathbf{f}^{\mathrm{err}}$, where there should be none according to the Ericksen–Noether identity. Equation 13.32 says something about the faithfulness of the FEM grid, and the question naturally arises of the tailoring of a finite-element grid in such a way that these spurious *configurational forces* are made to vanish. They are *configurational* forces, as they do depend on the location of nodes on the material manifold. One may think to release the inner material nodes (or make them float) so as to make these spurious material forces vanish, or at the least minimize them. This idea stems from M. Braun (1997), G.A. Maugin (2000), and P. Steinmann (2001) and steinmann et al. (2001). In particular, the first author has shown that a distribution of practically vanishing configurational nodal forces could be obtained. Figure 13.11 (from Braun, 1997, who started it all after reading our book (Maugin, 1993)) exhibits the two finite-element meshes with fixed and floating nodes for a simple problem of plane elasticity

solved by triangular finite elements. In the left picture a fixed mesh is prescribed. Then the nodes are allowed to float into new positions, shown in the right part of the picture, where the configurational forces are (nearly) zero. To preserve the shape of the body the boundary nodes should be kept fixed or at least confined to the fixed boundary, while the inner nodes have been released to take a position free of configurational forces. This is the essence of the method. Of course, the boundary nodes still perceive configurational forces, which are normal to the boundary and prevent the body from shrinking. Simultaneously, the total energy is reduced in the process and, therefore, becomes closer to the minimum attained by the exact solution. Unfortunately, this optimization procedure may be accompanied by the formation of badly shaped elements, which may not improve the finite-element

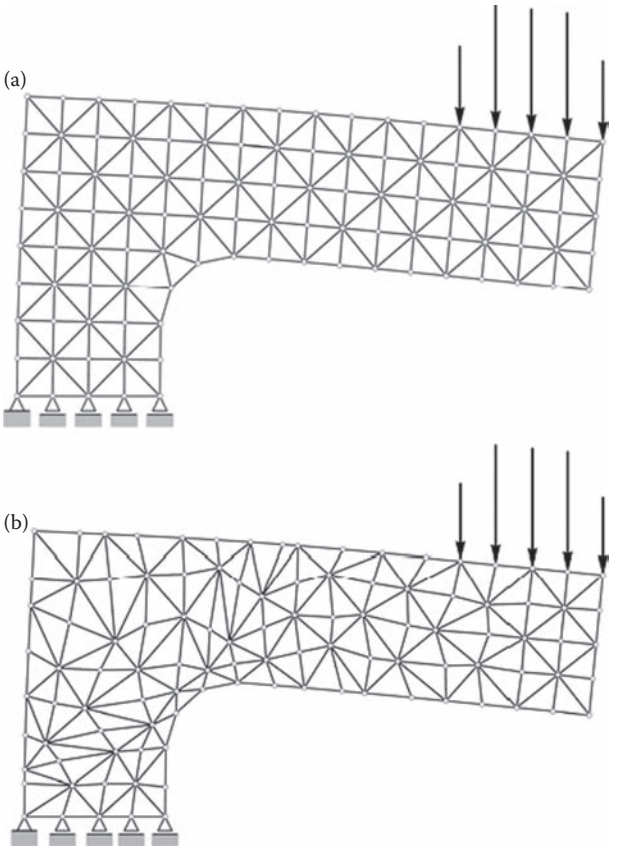


**FIGURE 13.11**
Finite elements with (a) fixed nodes—deformed configuration—and (b) floating nodes. In b, the internal nodes are free, and the boundary nodes are shifted along the boundary. (Courtesy of Braun, M., Universität Duisburg-Essen; After Braun, M., *Proc. Est. Acad. Sci. Phys. Math.*, Figure 3, 46, 24–31, 1997.)

solution altogether. In the process of the preceding FEM, since all required quantities are already computed in this optimization procedure, a particularly economical and rapid means of computing the energy-release rate is offered. To see this, multiply (13.28) by $\mathbf{F}^{-1}$ to the right, multiply the result scalarly by the test function $\mathbf{v}^*$, and account for (13.30) to obtain the following expression (compare to (3.17)):

$$-\int_{\Omega_t} \mathbf{b}:\left(\nabla_R \mathbf{V}^*\right)^T d\Omega + \int_{\partial\Omega_t} \mathbf{N}.\mathbf{b}.\mathbf{V}^* dS + \int_{\Omega_t} \mathbf{F}^0.\mathbf{V}^* d\Omega = 0, \tag{a}$$

for all *virtual material* velocity fields $\mathbf{V}^* = -\mathbf{F}^{-1}.\mathbf{v}^*$. This is formally equivalent to (13.30). But one should note that the second term in (a) does not correspond to a prescribed surface stress. Because of this, equation (a) is not applicable as such, that is, as a weak formulation of the original boundary-value problem. Rather, we note that for any velocity field we have

$$\int_{\partial\Omega_t} \mathbf{N}.\mathbf{b}.\mathbf{V}^* dS = \int_{\partial\Omega_t} \left(\mathbf{N}.\mathbf{V}^*\right) W dS + \int_{\Omega_t} \mathbf{t}^0.\mathbf{v}^* d\Omega, \tag{b}$$

so that we obtain the following **original** result (note that $\mathbf{N}$ is directed outward):

$$G\left(\Omega_t;\mathbf{V}^*\right) := \int_{\Omega_t} W\left(\mathbf{N}.\mathbf{V}^*\right) dS = \int_{\Omega_t} \mathbf{b} : \left(\nabla_R \mathbf{V}^*\right)^T d\Omega - \int_{\Omega_t} \mathbf{T} : \left(\nabla_R \mathbf{v}^*\right)^T d\Omega\,. \tag{c}$$

For a self-equilibrated (Piola–Kirchhoff) stress field ($\mathbf{f}^0 = 0$, $\mathbf{t}^0 = 0$), we have

$$\int_{\Omega_t} \mathbf{T}:\left(\nabla_R \mathbf{v}^*\right)^T d\Omega \equiv 0, \tag{13.33}$$

so that (c) reduces to the following formula for the *flux of elastic energy outward* the material volume $\Omega_t$ for a material velocity field $\mathbf{V}^*$:

$$G\left(\Omega_t;\mathbf{V}^*\right) = \int_{\Omega_t} \mathbf{b} : \left(\nabla_R \mathbf{V}^*\right)^T d\Omega. \tag{13.34}$$

The quantity $G$ is usually called an *energy-release rate* (compare to the general definition involving the influx of the Hamiltonian density in Equation 8.25).

Equation 13.34 can be generalized to more involved cases including additional degrees of freedom (e.g., a microstructure such as in micropolar elastic bodies; Maugin, 1998) or *nonsimple* elastic media accounting for the second gradient of strain (so-called *second-gradient* theory; cf. Maugin and Trimarco, 1992).

### 13.4.2 Implementation

We consider the quasistatics of inhomogeneous bodies acted on by external body forces. Consequently, the equilibrium form of the balance of material momentum reads

$$\operatorname{div}_R \mathbf{b} + \mathbf{g} = \mathbf{0}, \quad \mathbf{g} := -(\nabla \mathbf{u}).\mathbf{f}^0 + \mathbf{f}^{\text{inh}}, \quad \mathbf{f}^{\text{inh}} = -\left.\frac{\partial W}{\partial \mathbf{X}}\right|_{\text{expl}}. \tag{13.35}$$

Introducing (material-vectorial) test functions $\eta$, we can write the weak formulation of the first of these as

$$G(\eta_i) := \int_B g_i \, \eta_i \, dV = \int_B b_{ji} \, \eta_{i,j} dV \tag{13.36}$$

where we use only lowercase Latin indices, and there appears no surface contribution as we shall consider only stationary boundaries, that is, boundaries that remain the same for all times. Consequently, the test function $\eta$ vanishes at the material boundary $\partial B$. Note the identity of (13.36) and (13.34). Now, the standard discretization procedure of the FEM is implemented (see, e.g., Wriggers, 2001). An element-wise interpolation of the test function $\eta$ and its gradient is introduced by

$$\eta_i = \sum_I N^I \eta_i^I, \quad \eta_{i,j} = \sum_I N^I_{,j} \eta_i^I, \tag{13.37}$$

where the $\eta^I$ are the nodal values of the test function and the $N^I$ are the shape functions. Evaluating, then, (13.36) for each element of area $\Omega_e$, and the result being true for any test function, we obtain the *nodal* configurational force $\mathbf{G}^I$ with components

$$G_i^I = \int_{\Omega_e} N^I g_i \, d\Omega = \int_{\Omega_e} b_{ji} \, N^I_{,j} d\Omega. \tag{13.38}$$

This can be used to evaluate $\mathbf{G}^I$ in every integration point once the standard problem in physical space is solved, that is, once the nodal displacements $\mathbf{u}^I$ are known, so that $\nabla \mathbf{u}$, $W$, and $\mathbf{b}$ can be evaluated in every integration point. Then the contributions from each element at a node have to be assembled to give the discrete value of the configurational force at that node, that is,

$$\mathbf{G}^I = \bigcup_{e=1}^{N_e} \mathbf{G}^I(\Omega_e). \tag{13.39}$$

In the case where there are no physical body forces, a direct interpretation of the discrete configurational force $\mathbf{G}^I$ is possible. Indeed, for a linear elastic

material, the elastic potential $\prod^h$ of a body discretized with finite elements is given by

$$\Pi^h = \frac{1}{2}\mathbf{U}.\mathbf{K}\mathbf{U} - \mathbf{U}.\mathbf{P}, \tag{13.40}$$

where **U** is the vector of the global node displacements, **P** is the vector of the global node forces, and **K** is the stiffness matrix. Consequently, the discrete equivalence of Equation $13.35_2$ defines the discrete values of the configurational forces as

$$G_i^I = \frac{\partial \Pi^h}{\partial x_i^I}, \tag{13.41}$$

where $\mathbf{x}^I$ stands for the node positions. Of course, $\mathbf{G}^I$ should vanish for a homogeneous material, so that (13.41) can be used to obtain a better finite-element discretization, when the finite-element mesh is changed in such a way as to make $\mathbf{G}^I$ tend to zero everywhere, a strategy that will be illustrated in the sequel.

It was also remarked by some authors (Steinmann, 2000; Steinmann et al., 2001; Mahnken, 2007) that in the neighborhood of some critical points—e.g., the crack tip—it may be advantageous to sum the configurational nodal forces of the FEM discretization over a finite region Ω, so that an additional summation over nodes will be applied to (13.39), that is,

$$\mathbf{G}^I = \sum_{n=1}^{N_{pe}} \bigcup_{e=1}^{N_e} \mathbf{G}^I\left(\Omega_e^n\right), \tag{13.42}$$

where $N_{pe}$ is the number of nodes lying in the domain Ω, this domain being possibly not directly related to the original discretization, a fact that can be exploited advantageously in adaptively refined finite-element meshes (see the following).

### 13.4.3 First Example: Homogeneous Block under Pressure

This very simple example illustrates pedagogically the effect of displacing nodes by considering the case of displacing *one* node only. The body is a homogeneous linear elastic isotropic block (with artificially equal Lamé coefficients, $\lambda = \mu$) under uniform pressure on part of its top side; cf. Mueller and Maugin (2002) and Figure 13.12a). To simulate the frictionless support of the block, only the vertical displacements on the bottom edge are fixed. The extremely simple discretization with four-node displacement elements is shown in Figure 13.12b. With an assumed plane strain state, the obtained distribution of nodal-configuration forces is shown in Figure 13.13. Of course, relatively large configurational forces are necessary to keep particles in a

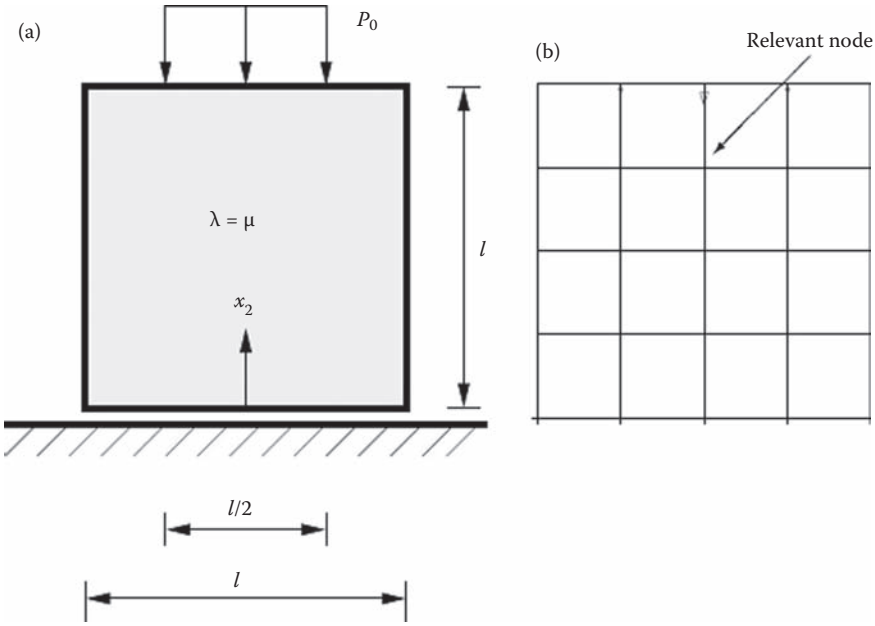


**FIGURE 13.12**
Homogeneous block under pressure: (a) Setting, (b) discretization. (From Mueller, R., Kolling, S., and Gross, D., *Int. J. Numer. Methods Eng.*, 53, 1557–74, 2002. With permission.)

fixed place at the boundary while almost zero spurious configurational forces appear at internal points since the body is homogeneous (and they should theoretically be strictly zero). Now we envisage displacing only one node, in fact changing the vertical $x_2$-coordinate of the second central node from the top (the "relevant" node in Figure 13.12b). This change is made in the range $0.5 < x_2/l < 1.0$, where $l$ is the height of the block. The result of this change is shown in Figure 13.4 as concerns the configurational force $G_2$ at this node in comparison with the numerical estimate of the expression (13.41). The results coincide as expected. From this simple analysis there follows the existence of a specific $x_2$ position of the relevant node at which the potential energy $\Pi^h$ is extremized and $G_2$ vanishes. Here this corresponds to a value $x_2 = 0.9l$ approximately. In summary, due to the noncontinuous strain approximation in the finite element, nodal configurational forces occur although they should not. This indicates that the standard equilibrium field equations are not exactly solved. This hinders achieving a better approximation by displacing the nodes. This displacement can be made according to the simplest rule, that of the steepest descent such that the new points are deduced from the previous ones by the operation

$$\mathbf{x}^I \rightarrow \mathbf{x}^I - c\mathbf{G}^I, \tag{13.43}$$

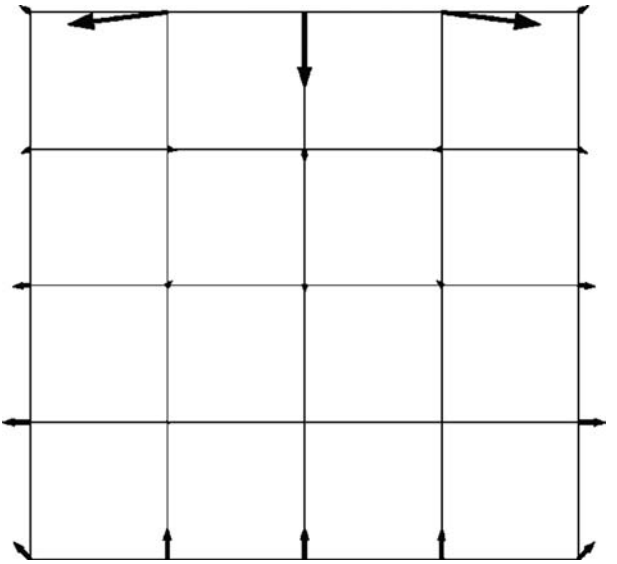

**FIGURE 13.13**
Homogeneous block under pressure: Distribution of nodal configurational forces. (From Mueller, R., Kolling, S., and Gross, D., *Int. J. Numer. Methods Eng.*, 53, 1557–74, 2002. With permission.)

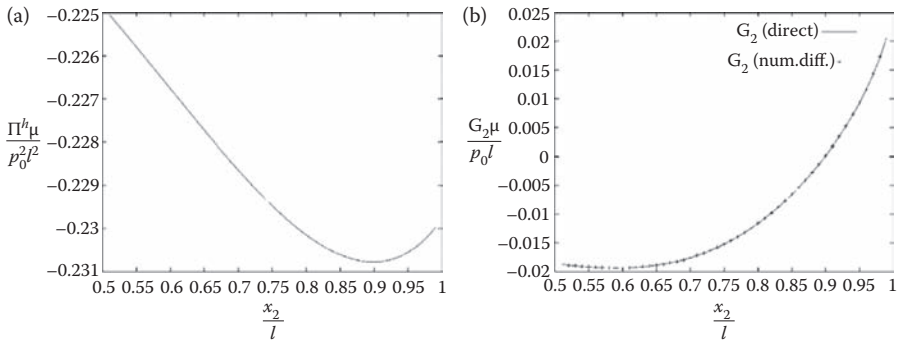


**FIGURE 13.14**
Homogeneous block under pressure: (a) Total potential vs. $x_2$-coordinate of relevant node position, (b) comparison between $G_2$ and numerical differentiation of $\Pi^h$. (From Mueller, R., Kolling, S., and Gross, D., *Int. J. Numer. Methods Eng.*, 53, 1557–74, 2002. With permission.)

where $c$ is a sufficiently small chosen value. Equation 13.43 is the simplest *update rule* or "kinetic relation" for the "evolution" of the position of nodes. Here it is without a time scale, having simply an incremental but oriented (vectorial) nature. The rule (13.43) can be applied to all interior nodes, but a different strategy may apply to nodes on the boundary if this boundary is to remain unchanged. We may forbid any position change in any direction, or we may accept only changes in the tangential direction to the boundary.

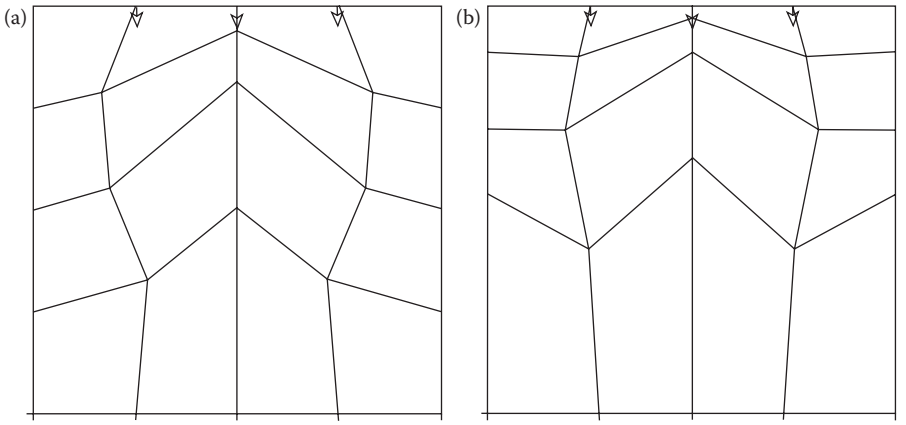


**FIGURE 13.15**
Homogeneous block under pressure, stationary state of updated meshes: (a) Fixed nodes, (b) tangentially free nodes. (From Mueller, R., Kolling, S., and Gross, D., *Int. J. Numer. Methods Eng.*, 53, 1557–74, 2002. With permission.)

The resulting changed meshes are exhibited in Figure 13.15. If the boundary nodes are allowed to move in the tangential direction (see the side faces), the system has a higher degree of freedom to relax the configurational stresses, hence a higher reduction of the potential energy, as shown in Figure 13.16.

### 13.4.4 Second Example: Clamped Block under Tension

This considers the same elastic material as in the first example and serves to illustrate the difference between a very fine finite-element mesh and a coarse one that applies the proposed node-updating technique. The loading corresponds to one edge loaded with a tensile stress $\sigma_0$ (see Figure 13.17a). A numerical reference solution is obtained with a very fine finite-element mesh involving 10,000 elements and 10,201 nodes. The result is the $\sigma_{22}$ stress distribution exhibited in Figure 13.17b. Then a regular coarse mesh of 36 elements and 49 nodes is implemented to evaluate the same stress distribution, but the node-updating technique is applied, allowing the boundary nodes to move in the tangential direction, while the nodes on the edge where the load is applied are kept fixed. Remarkably enough (Figure 13.18), the iterative update aligns the mesh along the contour lines of the stress distribution. It is observed that the value of the displacement approaches the reference solution of the fine mesh as the coarse mesh is continuously updated, but this limit cannot be reached as it seems that the coarse mesh is unable to come arbitrarily close the "exact" reference solution.

These examples bring up the following remarks. Due to the requirement that the test function for the material force balance vanishes at the boundary, discrete material forces occur at the boundary as *reaction forces* to this constraint. Inside the body that is supposed to be homogeneous, discrete

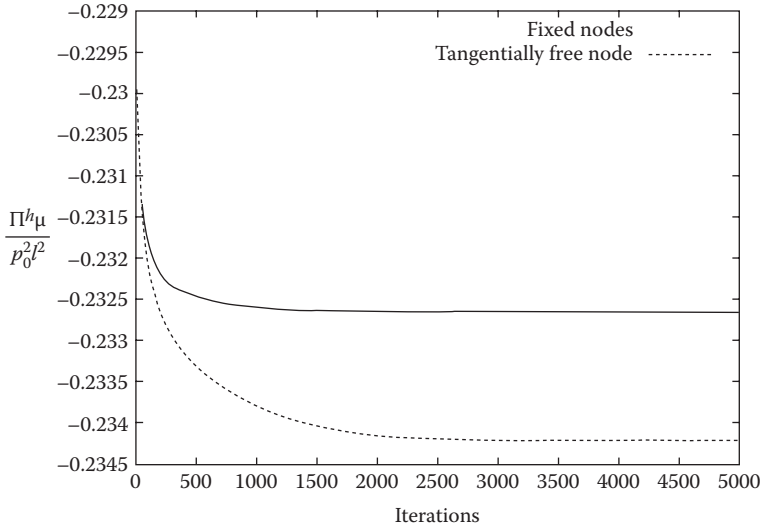


**FIGURE 13.16**
Homogeneous block underpressure: Energy change during update iterations. (From Mueller, R., Kolling, S., and Gross, D., *Int. J. Numer. Methods Eng.*, 53, 1557–74, 2002. With permission.)

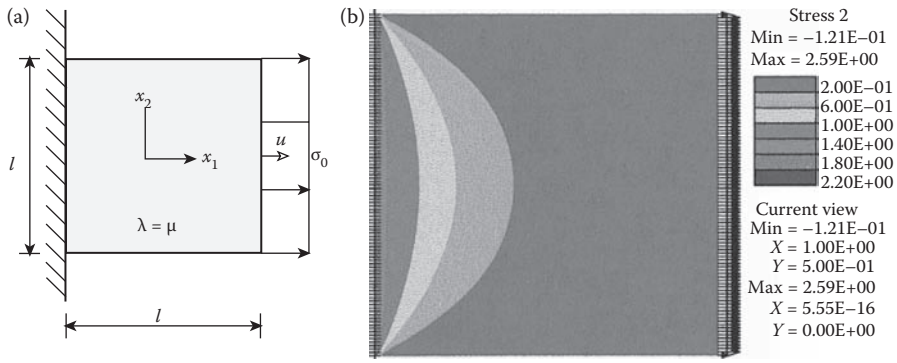


**FIGURE 13.17**
**(See color insert following page 434.)** Homogeneous block under tension: (a) Setting, (b) fine discretization with $\sigma_{22}$ distribution. (From Mueller, R., Kolling, S., and Gross, D., *Int. J. Numer. Methods Eng.*, 53, 1557–74, 2002. With permission.)

material forces should identically vanish. But this is not exactly the case. The reason for this is that material forces are basically energetic quantities, since the Eshelby stress tensor is computed from strain energy, stresses, and strains. But in a standard finite-element discretization only the displacements are approximated continuously (i.e., in $C^0$ class), which is not the case for their derivatives, and therefore the resulting strains and strain energy are not continuous. Accordingly, discontinuities between the elements lead to numerically caused material forces. As a result a strategy of adaptation of

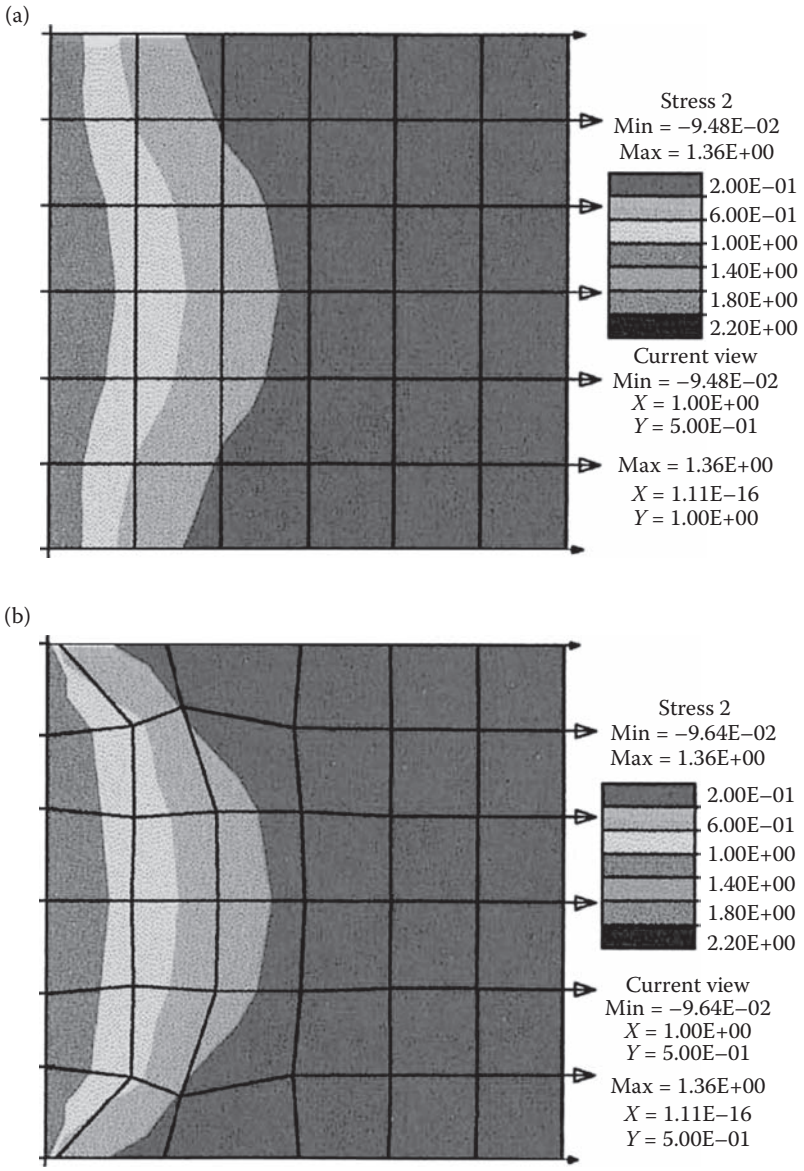


**FIGURE 13.18**
**(See color insert following page 434.)** Homogeneous block under tension: (a) Initial coarse mesh with $\sigma_{22}$ distribution, (b) update mesh with $\sigma_{22}$ distribution. (From Mueller, R., Kolling, S., and Gross, D., *Int. J. Numer. Methods Eng.*, 53, 1557–74, 2002. With permission.)

the meshing must be implemented. The material forces themselves provide a basis to assign new mesh sizes. This is realized by the introduction of refinement factors, $r^I$, from which new nodal values of the mesh size are defined by the rule (compare to (13.43))

$$h^I_{\text{new}} \to h^I_{\text{old}} r^I .$$

The rule for determining this refinement factor as well as other technicalities such as an extrapolation scheme for nodes on the boundary are discussed in Mueller et al. (2004). In particular, the influence of the boundary-node refinement on the numerics of the problem of a notch stretched in hyperelasticity is examined in that paper, showing that the proposed extrapolation captures better the high gradients in the vicinity of the notch tip.

### 13.4.5 Third Example: Inhomogeneous Cantilever Beam

Here the inhomogenity in fact is a square hole as depicted in Figure 13.19a. This illustrates the relation between a defect, in this case the hole, and the associated material (or configurational) forces. The beam is clamped on the left side and loaded by a vertical displacement on the opposite side. This resembles a cantilever beam, hence the naming. Figure 13.19b gives the distribution of the $\sigma_{11}$ stress component together with the starting position of the hole. This stress distribution is similar to the distribution of the bending stress known from the technical beam theory. As the hole is initially placed in the vertical center near the neutral phase, it disturbs the stress distribution only slightly. The resulting material force on the hole is evaluated by computing the sum

$$\mathbf{G}_{\text{hole}} = \sum_{K=1}^{N_{\text{hole}}} \mathbf{G}^K , \tag{13.44}$$

where $N_{\text{hole}}$ is the set of nodes located on the boundary of the hole. Parodying (13.43) we may propose a simple "kinetic relation" in the form

$$\mathbf{X}^{\text{new}}_{\text{hole}} = \mathbf{X}^{\text{old}}_{\text{hole}} - c\mathbf{G}_{\text{hole}} , \tag{13.45}$$

where $c$ is chosen such that

$$\left| \mathbf{X}^{\text{new}}_{\text{hole}} - \mathbf{X}^{\text{old}}_{\text{hole}} \right| = b = \text{const.} \tag{13.46}$$

This can be interpreted as a motion of the hole with "constant velocity" or an evolution without time scale. It should be noted that this example is

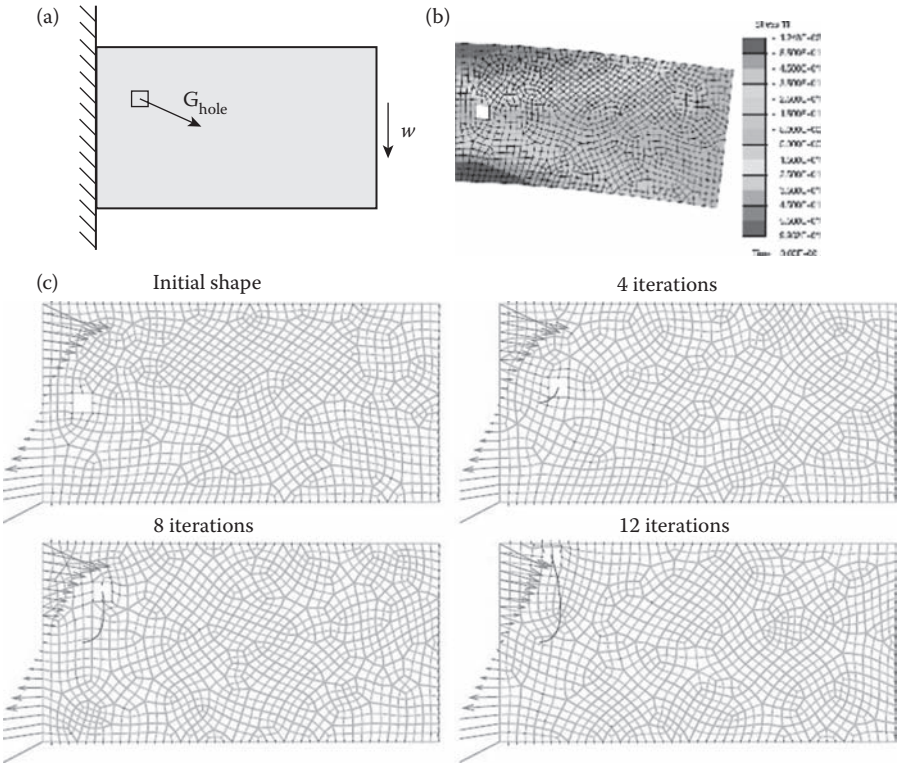


**FIGURE 13.19**
**(See color insert following page 434.)** (a) Cantilever beam, (b) distribution of $\sigma_{11}$ stress. (Adapted from Mueller, R. and Maugin, G.A., *Comput. Mech.*, 29, 52–60, 2002.) (c) Material forces and trajectory of the square hole "leaving" the cantilever beam from the top. The result is a more homogeneous body.

purely academic in the sense that no physical process has been specified yet. In particular, if the hole is interpreted as an oversimplified model of a vacancy or a void, then one may think of diffusion or corrosion processes that allow the hole to move through the material body. Figure 13.19c illustrates this possible motion—path trajectory—as being that of an inhomogeneity being *driven out* of the body by the material forces. Here, after each new position of the hole reached by application of (13.45) a new finite-element mesh is generated to avoid any deterioration of the discretization. After 12 iterations the calculation is stopped as the hole reaches the boundary and the automatic mesh generation breaks down. If one tries different starting points for the hole position, the material forces will always act in such a way as to try to drive the inhomogeneity out of the body, thus rendering the body "more homogeneous." For instance, a slightly shifted-down starting point will result in a trajectory where the hole leaves the body at the lower boundary.

### 13.4.6 Fourth Example: Crack Propagation Using Material Forces

This 2D simulation resembles a compact-tension (CT) specimen that is loaded by a dead displacement $w$ along the $x_2$ direction (see setting in Figure 13.20). A state of plane strains is assumed. A circular hole is introduced in the specimen out of the $x_1$-axis in order to break the symmetry of the setting and simulate a localized inhomogeneity as a void. This allows one to study the interaction of material forces at the crack tip with the material forces caused by this special type of inhomogeneity. The initial distribution of material forces $\mathbf{G}$ is plotted in Figure 13.20b. As now usual, large material (configurational) forces are observed where the displacement boundary conditions are applied and at the crack tip. In the close vicinity of the crack tip, material forces occur due to the inaccurate approximation of the solution with large gradients in this region. These forces should vanish since the body is theoretically homogeneous at those points. In the situation of Figure 13.20b the hole is placed relatively far from the crack tip. Crack propagation is assumed to take place according to the simple rule (compare to (13.45))

$$\mathbf{X}^{\text{new}}_{\text{crack tip}} = \mathbf{X}^{\text{old}}_{\text{crack tip}} - c\mathbf{G}_{\text{crack tip}}. \tag{13.47}$$

Here the proportionality constant $c$ of this schematic "kinetic relation" has to be chosen in an appropriate way; that is, the crack propagation has to be sufficiently small and, at the same time, large enough to ensure a proper mesh generation for the new geometry. Here no threshold for crack initiation is introduced (we are satisfied with qualitative results). Such crack-initiation

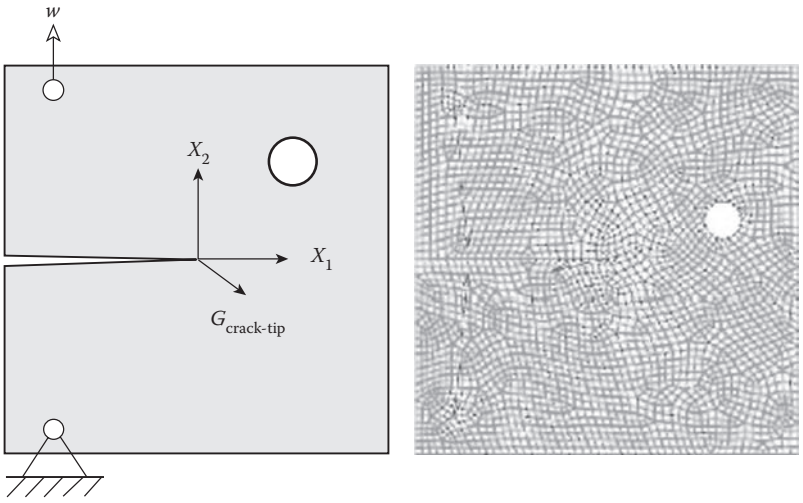


**FIGURE 13.20**
**(See color insert following page 434.)** 2D crack propagation in presence of a hole: (a) Setting, (b) material force distribution. (Adapted from Mueller, R. and Maugin, G.A., *Comput. Mech.*, 29, 52–60, 2002.)

criteria as well as other criteria (e.g., maximal circumferential stress) for the propagation direction can be found in the technical literature (e.g., Gross, 1996). All simplifications being accounted for, two quite different initial situations have been analyzed (Mueller and Maugin, 2002). In the first situation, when the crack is placed sufficiently far away from the hole, the crack "has sufficient time" to orient toward and finally reach the hole, although in the simulation the automatic mesh generation fails when the crack reaches the very vicinity of the hole (Figure 13.21). In the second situation, when the crack tip is closer to the hole, while the crack is necessarily "irresistibly attracted" by the hole (material with a weaker—in fact vanishing—elasticity), the crack tip does not change direction rapidly enough to reach the hole, and it misses it, creating a possibly dangerous situation with a ligament (see Figure 13.22). We show only snapshots but an animated film of these propagations can be produced (ask the author).

The problem of the refinement of the mesh in the vicinity of a crack tip cannot be overlooked. It has been examined in detail by Mueller et al. (2004); see also Rütter and Stein (2005). The transformation to domain integrals was recently reexamined by Mahnken (2007). This is accompanied by the additional summation mentioned in (13.42).

The hole introduced in the preceding may be replaced by an inclusion of softer (this is the case of the hole) or harder elasticity than the matrix in which the crack tends to expand. This problem can be studied in terms of three parameters, which are the inclusion size, the anisotropy ratio, and the stiffness ratio. Kolling et al. (2002) have given the relevant results. In terms of the stiffness ratio and the distance (nondimensionalized as $b/r$) between inclusion and the crack tip, we have the results sketched out in Figure 13.23, which provides both the material force (driving force on the crack tip) and the distribution of material forces over the boundary of the inclusion. Here the latter is aligned with the direction of the crack. Due to the presence of the crack, there exists a resultant driving force $\mathbf{R}_\tau$ on the inclusion. This force here is equivalent to the $J$-integral (with opposite sign) because a virtual movement of the inclusion toward the crack results in the same energy change as a movement of the crack tip toward the inclusion. For a short distance to the crack and a hard inclusion, the driving force is significant—it is an attraction—but it decreases rapidly for a larger distance and for a soft inclusion, respectively. In particular, the elastic energy tends to zero for a very soft inclusion while it converges to a finite limit value for a very hard inclusion. Furthermore, if we assume the velocity of the inclusion toward the crack tip to be small compared to its shape evolution, then we can also obtain the equilibrium shape of the inclusion for different stiffness and anisotropy ratios at a fixed distance by applying the considerations of Section 7.8.1 due to Schmidt and Gross (1997). The interpretation of these results is that, independent of the anisotropy ratio, the hard inclusion always shows a tendency to move toward the crack tip. A possible agglomeration of inclusion-like defects may thus take place near the crack tip. If no migration of the hard inclusion is

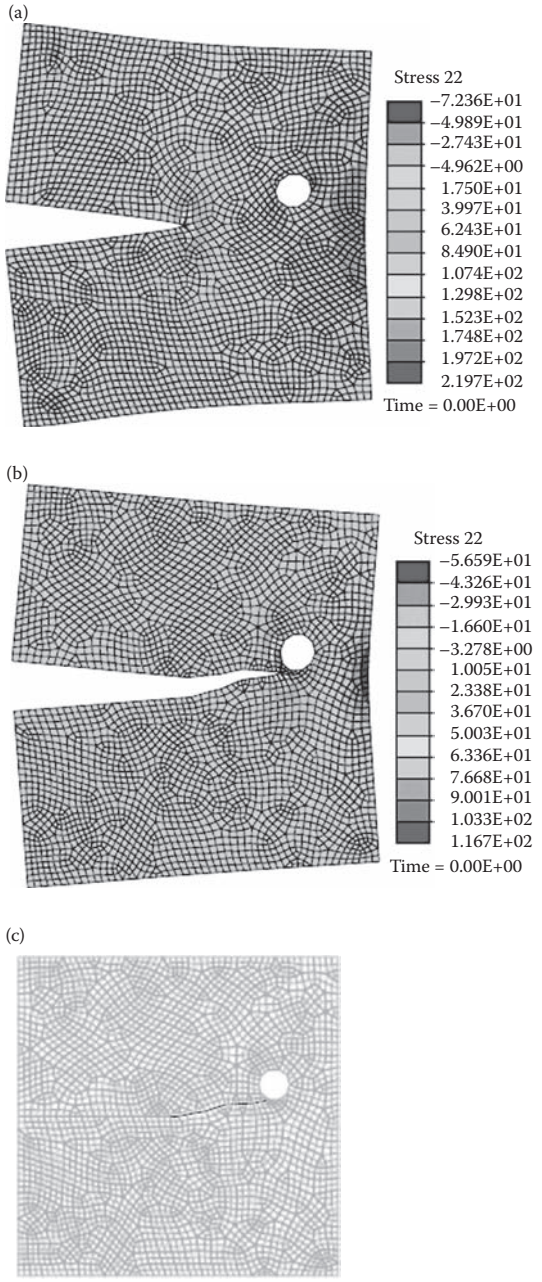


**FIGURE 13.21**
**(See color insert following page 434.)** 2D crack propagation in the presence of a hole in the deformed configuration: Distribution of $\sigma_{22}$ stresses, (a) initial position of crack tip, (b) final position of crack tip, and (c) crack path meeting the hole. (Adapted from Mueller, R. and Maugin, G.A., *Comput. Mech.*, 29, 52–60, 2002.)

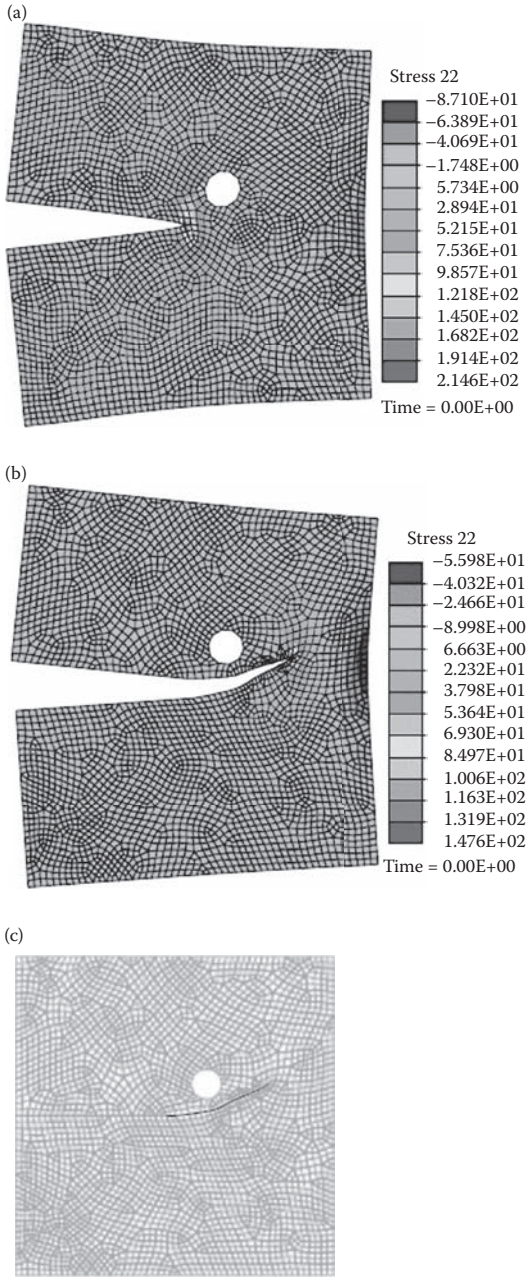


**FIGURE 13.22**
**(See color insert following page 434.)** 2D crack propagation in the presence of a hole in the deformed configuration: Distribution of $\sigma_{22}$ stresses, (a) initial position of crack tip, (b) final position of crack tip, and (c) crack path missing the hole. (Adapted from Mueller, R. and Maugin, G.A., *Comput. Mech.*, 29, 52–60, 2002.)

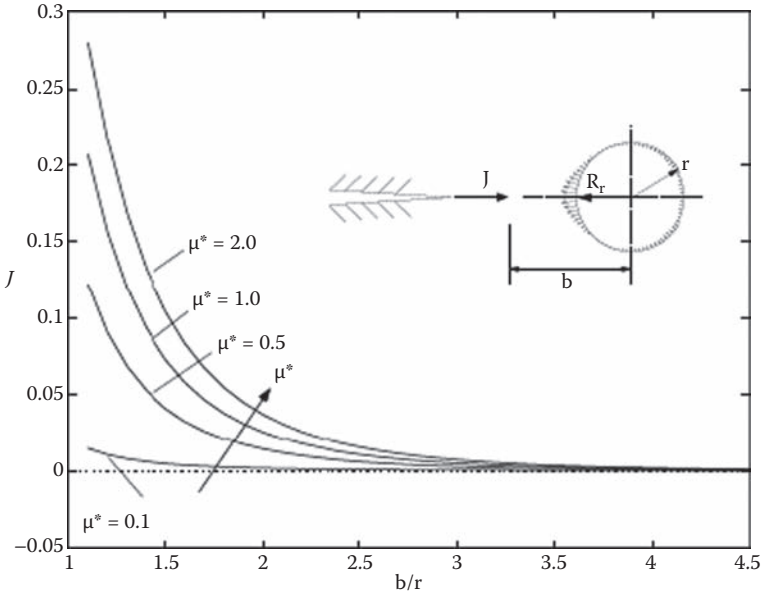


**FIGURE 13.23**
Crack-inclusion interaction: Material force (*J*-integral) versus distance between inclusion and crack tip and influence of the stiffness ratio. (From Kolling, S., Baaser, H., and Gross, D., *Int. J. Fract.*, 118, 229–38, 2002. With permission.)

assumed, then the equilibrium shape has a characteristic distortion toward the crack tip.

#### *13.4.6.1 3D Crack Propagation*

This is illustrated by Figure 13.24, which gives (Figure 13.24a) the distribution of $\sigma_{33}$ stress in the load direction (vertical displacement on the top surface) and the material forces in the ligament (Figure 13.24b) for a typical specimen. There obviously is a high-stress concentration at the crack tip. Large discrete material forces appear along the tip line, and this is shown by the cut along the ligament in Figure 13.24b. If the material forces are large enough to force the crack front to move, the latter will move in the negative direction of the material forces, thus yielding a crack expansion. For the movement of the crack front, only the component normal to the crack front is relevant, thus resulting in crack propagation that is more pronounced in the middle than on the free surface. This is observed experimentally and predicted by damage models of the Gurson type. Spectacular colored 3D simulations are given in Kuhl (2004) with applications to biomechanical structures. Other works aiming at a refinement of the FEM are by Miehe et al. (2007), Thoutireddy (2004), and Thoutireddy and (2003), and with special attention to the *extended* FEM (X-FEM), for example, by Andriyana (2006) and Legrain (2006).

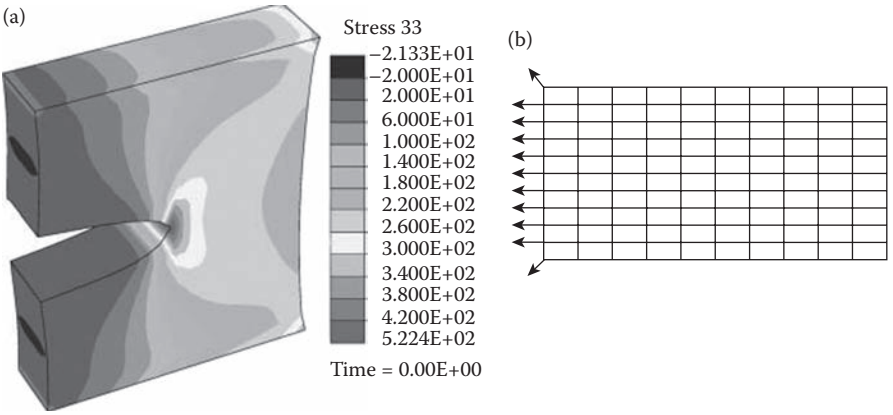


**FIGURE 13.24**
3D cracked specimen: (a) Distribution of $\sigma_{33}$ stress, (b) material forces in the ligament. (Adapted from Mueller, R. and Maugin, G.A., *Comput. Mech.*, 29, 52–60, 2002.)

### 13.4.7 Fifth Example: Layer on a Base Material

This example is due to Mueller, Kolling et al. (2002). Various cases must be considered depending on whether the layer is softer than the bulk material (case i) or stiffer than the bulk material (case ii). A remote stress $\sigma_0$ is applied to the bulk material; the bonding between base material and layer is assumed to be perfect. The setting is shown in Figure 13.25a. The resulting $\sigma_{11}$ stress distributions in the deformed configuration for the two cases are shown in Figure 13.25b and c. The different stress states at the bonding interface for the two types of stiffness ratios cause different configurational forces to occur. These are shown in Figure 13.15d and e. In case i, the configurational forces on the interface point into the layer material. But in case ii, if the layer is stiffer, the direction of the configurational forces is toward the base material; that is, this agrees with a previously made general statement on the direction of material *inhomogeneity* forces: The configurational forces at the interface act as driving force on the material inhomogeneity. If the interface were mobile due to some transport mechanism (diffusion, phase transition), it would move in the direction opposite to the configurational force in order to reduce the total potential.

### 13.4.8 Sixth Example: Misfitting Inhomogeneity in Two-Phase Materials

We have already reported on the theoretical aspects of this problem in Section 7.8.1. In this morphology problem the main ingredient is the variation of potential energy given by

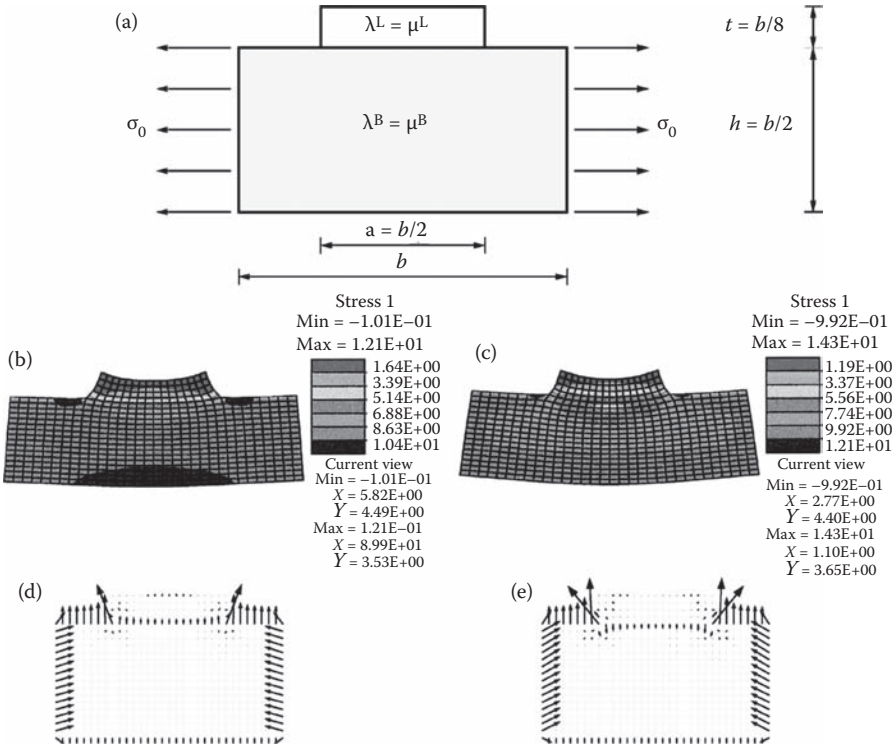


**FIGURE 13.25**
**(See color insert following page 434.)** Inhomogeneous substrate problem: (a) Setting, (b) stress distribution for soft layer, (c) stress distribution for stiff layer, (d) configurational forces for soft layer, and (e) configurational force for stiff layer. (From Mueller, R., Kolling, S., and Gross, D., *Int. J. Numer. Methods Eng.*, 53, 1557–74, 2002. With permission.)

$$\delta\Pi = -\int_{\partial B} \tau_n \delta n ds, \tag{13.48}$$

where $\delta n$ denotes a shape variation of the interface along its outward unit normal vector $\mathbf{n}$, and the generalized thermodynamic driving force $\tau_n$ is given by the normal jump of the Eshelby stress at the interface of the precipitate, that is,

$$\tau_n = \mathbf{n}.[\mathbf{b}].\mathbf{n}. \tag{13.49}$$

We remind the reader that an analytical solution can be found to this if the matrix is assumed to be isotropic and infinite (this is the celebrated Eshelby inclusion problem; cf. Eshelby, 1957). In the general case, however, one must resort to numerics to obtain the equilibrium shapes of the precipitate. This

was achieved by Schmidt and Gross (1997). Special attention must be paid to the numerical scheme. To that purpose one must note the definition (13.41) of the discrete values $\mathbf{G}^I$ of the configurational forces. Accounting for (13.48), the variation of the potential yields

$$\delta\Pi = \frac{\partial \Pi}{\partial \mathbf{x}^I}.\delta\mathbf{x}^I = \mathbf{G}^I.\delta\mathbf{x}^I = -\int_{\partial B} \tau_n \delta n ds, \tag{13.50}$$

in terms of the nodal coordinates $\mathbf{x}^I$. To obtain discrete values of the continuous normal variation $\delta n$, linear shape functions $N^I(s)$ are introduced such that $\delta n = N^I(s)\delta n^I$. Furthermore, the configurational force $\mathbf{G}^I$ itself is projected in its normal direction by using $\delta\mathbf{x}^I = \mathbf{n}\,\delta n^I$ because of the preferred direction of $\tau_n$. Thus,

$$\mathbf{G}^I.\delta\mathbf{x}^I = -\int_{\partial B} \tau_n N^I(s)\delta n^I ds, \tag{13.51}$$

hence for any $\delta n^I$ (Mueller et al., 2002),

$$G_n^I \equiv \mathbf{G}^I.\mathbf{n} = -\int_{\partial B} \tau_n N^I(s) ds. \tag{13.52}$$

A typical distribution of material forces acting along the interface of the precipitate is shown in Figure 13.26 for an isotropic inhomogeneity (inclusion) in an anisotropic matrix (for which no analytical solution exists) comparing two techniques for computing $\tau_n$. This shows a tendency to a cubic equilibrium shape, a fact corroborated by shape optimization where the cuboidal shape extremizes the total free energy (see Mueller and Gross, 1998; Schmidt and Gross, 1997).

### 13.4.9 Note on Topological Optimization

In recent works dealing with the technical subject of topological optimization and the sensitivity analysis of variational design (see Barthold, 2005; Barthold and Materna, 2007; Materna and Barthold, 2007a, 2007b), it was noticed that the variational approach using the notion of "topological derivative" was akin to a "configurational derivative" yielding the notion of Eshelby stress tensor. This is easily understood if we remember that, technically and on the classical example of optimization of weight, the method used consists in introducing successive appropriate "holes" to make the structure lighter. The notion of topological derivative in this optimization framework is due to Sokolowski and Zhochowski (1999). It certainly is related to the notion of

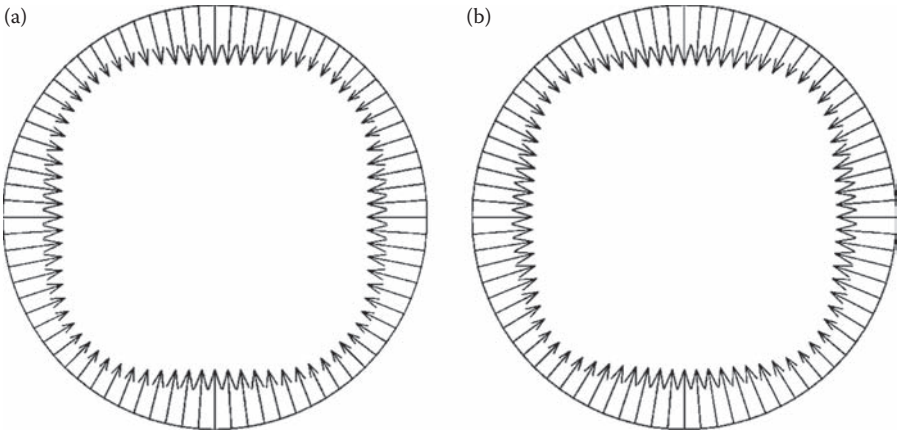


**FIGURE 13.26**
Distribution of the driving force along the arc length of the interface of an isotropic inclusion in an anisotropic matrix: (a) $\tau_n$ computed via $G_n$, (b) $\tau_n$ computed via a standard finite-element method. (From Mueller, R., Kolling, S., and Gross, D., *Int. J. Numer. Methods Eng.*, Figure 14, 53, 1557–74, 2002. With permission.)

"Hadamard derivative" (cf. Clarke, 1983) introduced early in the twentieth century by Jacques Hadamard (1907) for functional variations involving variations of integration domains. We do not dwell further in this technical matter, but it is instructive to note the *necessary* appearance of *material forces* along the boundary of an optimized hook—cf. Figure 13.27—due to Materna and Barthold, 2007.

## 13.5 Conclusive Remarks

We do not dwell further on the technical aspects of numerical schemes because this relates to a real scientific profession by itself. What has been implemented here is the basic idea that the coexistence of two equations sharing a similar ontological status, the balance of physical linear momentum or its equilibrium form on the one hand and the balance of canonical momentum or its equilibrium form on the other hand, favors a strategy by which the second type of equations is typically used in the study of the motion of defects (this last notion being granted in a generous manner) by applying a "kinetic law" once the classical solution is known. Not only do the various numerical techniques need to be exploited in order to implement this strategy, but they themselves benefit from the spirit of Eshelbian mechanics. In particular, they can exploit the notion of driving force to check the accuracy of some of the techniques (case of finite differences), but they also directly apply some of the very concepts, such as that of adaptivity, that parody the "kinetic laws"

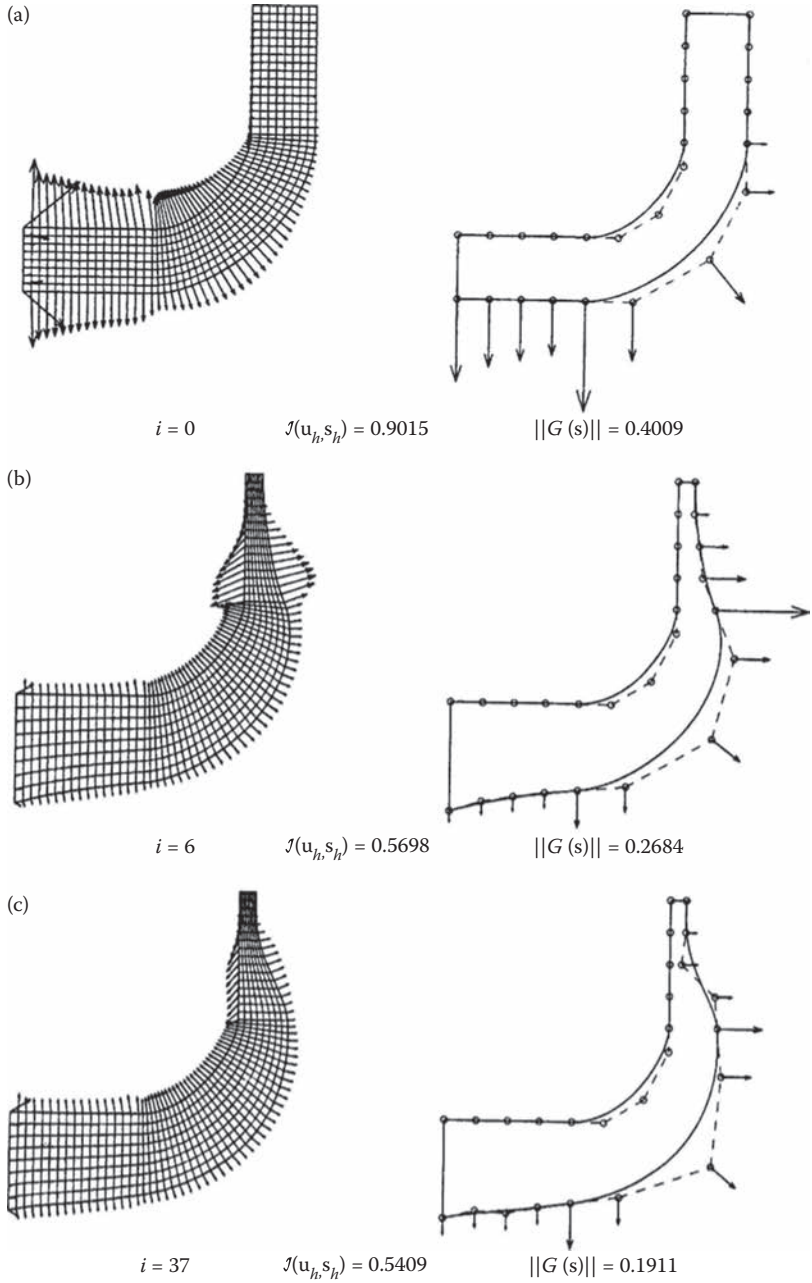


**FIGURE 13.27**
Three steps of iteration of a problem of topological optimization: Shape optimization of a "hook" of most efficient material distribution with respect to the overall stiffness of the structure with a constraint of constant volume exhibiting material forces along the boundary. (Courtesy of Materna, D., and Barthold, F.J., *Int. J. Fract.*, 147, 133–55, 2007.)

of physical processes. This is the most surprising development, which shows the application of notions originating from mathematical physics (invariances and Noether's theorem) not only to practical problems—which constitutes a normal spinoff of theoretical concepts—but also to the improvement of the numerical techniques themselves.

To conclude on an engineering note and pay a tribute to the scientist who did much, although without much fuss, in the application of the concept of material forces to engineering design and the FEM we may illustrate our point with the problem of optimization of a truss, following M. Braun (Braun, 2005, 2007): Figure 13.28a shows the basic structure in its reference

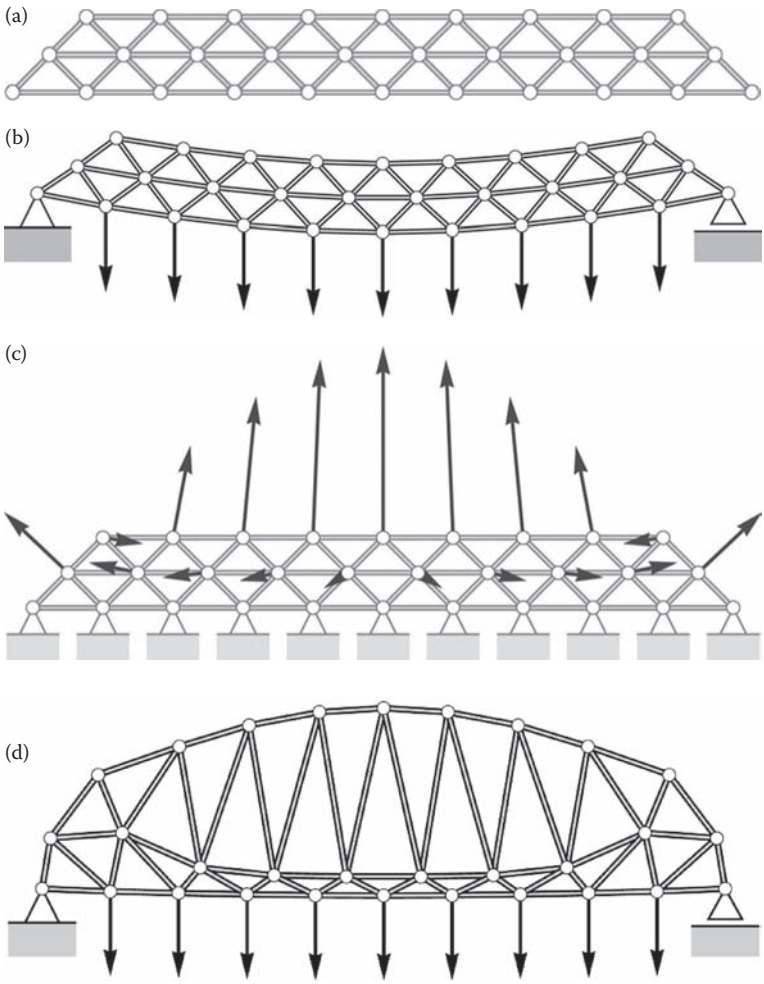


**FIGURE 13.28**
Optimization of a truss exploiting configurational forces. (Courtesy of Prof. M. Braun, Duisburg, Germany, who prepared this exemplary figure especially for the present book.)

configuration $K_R$. Figure 13.28b shows the same structure, in its actual configuration $K_t$, supported and with its actual (physical) loading. Figure 13.28c shows the same basic structure but back in its reference configuration after loading. Configurational supports are introduced at the bottom to keep the bottom row (boundary) fixed in $K_R$, while the computation by material pull back of material forces at the other joints from the physical force distribution found in Figure 13.28b yields the indicated arrows. Finally—in Figure 13.28c—relocatable nodes are moved, resulting in an optimized structure (Figure 13.28d) supported and loaded, in the actual configuration, with practically vanishing configurational forces at these nodes. The strain energy is reduced by more than 80% compared to the basic structure under the same load as depicted in Figure 13.28b. Then we recognize the good old railroad bridges as designed by smart civil engineers in the nineteenth century.

# 14

# *More on Eshelby-Like Problems and Solutions*

### Object of the Chapter

Where we see once more that it is not so much the notion of energy and its invariance that matters but the existence of something akin to a potential and some basic mathematical properties discovered a long time ago by Cauchy and Riemann.

## 14.1 Introduction

In this short concluding chapter we discover that contour integrals exist in other theories than solid mechanics and electromagnetics, including in heat and electricity conductions and in classical problems of aerodynamics. Such a general framework that favors analogies useful in problem solving in different disciplines concurs with the existence of a true world of material-configurational forces and their overwhelming importance in many problems of mechanics, physics, and materials science.

## 14.2 Analogy: Path-Independent Integrals in Heat and Electricity Conductions

In contemporary continuum mechanics (see Chapter 1, but also Maugin, 1992, 1999), for example, in elastoplasticity, it is often admitted that the whole constitutive theory may be based on the considerations of two potentials—potential-like scalars sometimes referred to as pseudopotentials, for instance, the free energy density $W$ often considered in preceding chapters, and a (pseudo) potential of dissipation, say $D$, from which one derives the thermodynamically

reversible and irreversible parts of the constitutive behavior, respectively. The notion of dissipation potential goes back to Lord Rayleigh. If this is the case, then many reasonings made concerning the free energy, insofar as the theories of material inhomogeneity and fracture are concerned, also apply to the dissipation potential. The essential operations then are the computation of the material gradients of both $W$ and $D$ while accounting for the classical equations (e.g., balance of momentum and energy), and the integration over a material region including a singularity of the relevant field. To illustrate this viewpoint, we consider such coupled electric–heat conductions as may occur in good conductors such as metals. Although we keep the same notation as before, deformation is discarded to alleviate the formulation.

In the absence of body heat and electric-charge sources, at each regular point in the material body we have the following quasistatic equations that govern temperature and electric potential, respectively:

$$\nabla.\mathbf{S} = 0, \quad \nabla.\mathbf{J} = 0, \tag{14.1}$$

where $\mathbf{S}$ is the entropy flux and $\mathbf{J}$ is the conduction electric current. These two fields jointly satisfy the remaining entropy inequality

$$\Phi := \mathbf{J}.\mathbf{E} - \mathbf{S}.\nabla\theta \geq 0\,, \tag{14.2}$$

where $\mathbf{E}$ is the electric field. In quasistatics $\mathbf{E} = -\nabla\varphi$, so that (14.2) takes a more symmetric form in electric and heat conductions:

$$-\Phi = \mathbf{J}.\nabla\varphi + \mathbf{S}.\nabla\theta \leq 0. \tag{14.3}$$

This analogy between electric and heat conduction has been known since the 1840s thanks to W. Thomson (later Lord Kelvin). The inequality (14.3) is at the basis of a discussion of coupled conduction effects. Following old ideas of Rayleigh and Maxwell but also modern continuum mechanics (H. Ziegler, P. Germain), consider the case where the dissipative phenomena contributing to (14.2) or (14.3) are derivable from a potential of dissipation. For instance, assume the existence of a nonnegative potential $D(\mathbf{E}, \nabla\theta, \theta, \mathbf{X})$, convex in $\mathbf{E}$ and $\nabla\theta$, homogeneous of degree $n$, where the homogeneity property holds for the first two arguments, such that

$$\mathbf{J} = \frac{\partial D}{\partial \mathbf{E}}, \quad \mathbf{S} = -\frac{\partial D}{\partial(\nabla\theta)}. \tag{14.4}$$

Then (14.3) is automatically fulfilled. It is intentional that we let $D$ depend explicitly on the temperature field $\theta$ and the material point $\mathbf{X}$, the latter indicating that the body is materially inhomogeneous from the point of view of heat and electricity conductions. The equations (14.4) are general statements of conduction laws. In particular, they are indeed Ohm's and Fourier's laws when $D$ is a homogeneous function of degree two in $\mathbf{E}$ and $\nabla\theta$.

To place the role of material inhomogeneities in evidence, it is natural to compute the gradient of $D$. We let the reader check that the result of this operation, on account of the field equations (14.1), reads as a covectorial "conservation" law (Maugin, 1996):

$$\mathrm{div}_R\mathbf{d} + \mathbf{h}^{\mathrm{inh}} + \mathbf{h}^{\mathrm{th}} = \mathbf{0}, \tag{14.5}$$

in which we have defined the following mixed material tensor $\mathbf{d}$ and two covectors:

$$\mathbf{d} = D\mathbf{1} + \mathbf{S}\otimes\nabla\theta + \mathbf{J}\otimes\nabla\varphi = D\mathbf{1} - \frac{\partial D}{\partial(\nabla\theta)}\otimes\nabla\theta - \frac{\partial D}{\partial(\nabla\varphi)}\otimes\nabla\varphi, \tag{14.6}$$

$$\mathbf{h}^{\mathrm{inh}} := -\left.\frac{\partial D}{\partial \mathbf{X}}\right|_{\mathrm{expl}}, \tag{14.7}$$

$$\mathbf{h}^{\mathrm{th}} := R\nabla\theta, \quad R := -\frac{\partial D}{\partial\theta}. \tag{14.8}$$

Of course we realize immediately that (14.5) and the definitions are perfectly analogous to the quantities defined in the balance of material momentum in its quasistatic form in the presence of temperature effects. The tensor $\mathbf{d}$ may be referred to as the *Eshelby dissipation-momentum tensor* (Maugin, 1996) or *the material conduction (stress) tensor* (Epstein, 1992) in the absence of electric conduction and inhomogeneity; that is, when (14.5) and (14.6) reduce to

$$\mathrm{div}_R\mathbf{d} + \mathbf{h}^{\mathrm{th}} = \mathbf{0}, \quad \mathbf{d} = D\mathbf{1} + \mathbf{S}\otimes\nabla\theta. \tag{14.9}$$

Epstein (1992) derived this equation by the method introduced in the theory of material uniformity.

Now, applying a direct analogy with what we did for mechanical fields, we can characterize field singularities in temperature or electric potential by the tool just constructed. For instance, in heat conduction governed by Fourier's law in isotropic bodies, the standard singularity of heat-conduction problems is that of the Laplacian, and therefore the same order of singularity as that of the 2D elasticity problem (cf. brittle fracture in Maugin, 1992). Hence the components of the covector $\mathrm{div}_R\,\mathbf{d}$ are not integrable at the tip $A$ of a straight-through crack; that is, $\theta$ behaves like $\sqrt{r}$ in local polar coordinates centered at $A$. Accordingly, the quantity defined by

$$T = \lim \mathbf{e}_1 . \int_V (\mathrm{div}_R\mathbf{d})\,dV \neq 0 \quad \text{as} \quad V \to A, \tag{14.10}$$

where $\mathbf{e}_1$ is a unit vector in the direction of extension of the crack, can be used as an indicator of the singularity of the temperature field. It plays the same role in heat conduction as the *J*-integral in mechanics. For an isotropic body with a linear conduction behavior, we have

$$D = \frac{1}{2}\chi\nabla\theta.\nabla\theta, \quad \mathbf{S} = -\chi\nabla\theta, \quad \chi \geq 0, \tag{14.11}$$

from which there follows from (14.10) a contour integral in the ($X_1$, $X_2$) plane:

$$T = \frac{\chi}{2}\int_{\Gamma}\left(\|\nabla\theta\|^2 N_1 - 2\frac{\partial\theta}{\partial X_1}\frac{\partial\theta}{\partial N}\right)d\Gamma, \tag{14.12}$$

where $N_1 = \mathbf{N}.\mathbf{e}_1$ along the contour Γ. This can alternately be expressed in terms of **S** or **Q**.

The same reasoning can be performed with electricity conduction where the physical meaning of the resulting expression is perhaps more transparent. In this case the starting point is the conservation of charge equation $(14.1)_2$. For a pure electric conductor that is materially homogeneous, the preceding formulation reduces to

$$\mathrm{div}_R\mathbf{d} = \mathbf{0}, \quad \mathbf{d} := D\mathbf{1} - \mathbf{J}\otimes\mathbf{E}, \tag{14.13}$$

since $\mathbf{E} = -\nabla\varphi$. For a linear isotropic electric conductor, we naturally take

$$D = \frac{1}{2}\sigma\mathbf{E}^2 = \frac{\mathbf{J}^2}{2\sigma}, \quad \mathbf{J} = \sigma\mathbf{E}, \quad \mathbf{E} = R\mathbf{J}, \quad (R = \sigma^{-1}). \tag{14.14}$$

The field singularity at the tip *A* of the crack *C* is that of the Laplacian; that is, φ behaves like $\sqrt{r}$ and the components of **E** like $1/\sqrt{r}$. We call *B* the contour integral given by

$$B = \int_{\Gamma}\left(DN_1 - (\mathbf{N}.\mathbf{J})(\mathbf{E}.\mathbf{e}_1)\right)d\Gamma \tag{14.15}$$

in the 2D problem as it presents itself in a thin conducting plate (cf. Mukherjee et al., 1982; Huy and Ruina, 1985). Equation 14.15 can be expressed either in terms of the current **J** or in terms of the electrostatic potential via its gradient (i.e., the voltage or difference of potential). In terms of currents, it reads

$$B = \frac{1}{2\sigma}\int_{\Gamma}\left(\mathbf{J}^2 N_1 - 2QJ_1\right)d\Gamma, \tag{14.16}$$

where $Q = \mathbf{N}.\mathbf{J}$ is a time rate of surface charge at $\Gamma$. By analogy with the technical use of the *J*-integral of fracture, the expression (14.16) could be used as a critical quantity relating to the breakage (sudden rupture in conduction at a critical level) of conductors, hence the symbolism *B* for the contour integral of interest. This idea is presented by Parton and Kudryavtsev (1988, Section 8.4, p. 494 on) although the introduction of such a critical quantity by these authors has nothing to do with the theory of inhomogeneities outlined in the preceding. The same authors in fact also propose an expression equivalent to (14.12) for heat conduction by mere analogy (see their Equations 54.10 or 52.10), that is,

$$T = \int_{\Gamma} \left( \frac{\mathbf{S}^2}{2\chi} N_1 - \frac{S_1}{\chi} (\mathbf{N}.\mathbf{S}) \right) d\Gamma. \tag{14.17}$$

They in fact follow the formal analogies between path-independent integrals of elasticity (*J*-integral) and the electrostatics of conductors and heat conduction that were apparently first noticed by Hoening (1984) and Saka and Abe (1985), whereas we based the reasoning on the canonical covectorial conservation equation (14.5) in the general spirit of the present book.

## 14.3 The Eshelbian Nature of Aerodynamic Forces

Following Atilgan (1997), we consider the irrotational steady flow of a perfect fluid past a rigid body of arbitrary cylindrical shape. The body *S* has regular boundary *C* orthogonally to the cylindrical direction $\mathbf{e}_3$. As a matter of fact the body is translated with constant velocity $V_\infty$. The total fluid force acting on the body is given by the surface integral

$$\mathbf{F} = \int_S \mathbf{n}.\sigma dA, \tag{14.18}$$

where the Cauchy stress $\sigma$ is due to the local pressure *p*, that is, $\sigma = -p\mathbf{1}$, and (14.18) is a Newtonian type of force given by

$$\mathbf{F} = -\int_S p\mathbf{n} dA. \tag{14.19}$$

This stress flux, called *total traction*, will vanish in the limit as *S* shrinks to zero. In this form, therefore, it is not a good indicator of the presence of a singularity that is normally created by the rigid body in the fluid. But we can call for the Bernoulli theorem between a point at infinity upstream and

a local point at $S$, that is, for steady flows (see any book on fluid mechanics such as the classic one by Karamcheti [1966/1980])

$$p(\mathbf{x} \in S) = p_\infty - \rho \mathbf{V}_\infty . \mathbf{q} - \frac{1}{2}\rho \mathbf{q}^2, \tag{14.20}$$

where the velocity field has been written as $\mathbf{v} = \mathbf{V}_\infty + \mathbf{q}$ and, because of irrotationality, the perturbing velocity $\mathbf{q}$ is such that $\mathbf{q} = \nabla\varphi$, where $\varphi$ is a potential. At $S$, the boundary condition $\mathbf{v}.\mathbf{n} = 0$ holds true. On substituting from (14.20) and keeping only the relevant terms we obtain the following expression orthogonally to the direction of motion of the solid $S$ (equivalently, the direction of $\mathbf{V}_\infty$ chosen as axis $\mathbf{e}_1$):

$$F = \int_C \left( K - (\rho V_\infty) \frac{\partial \varphi}{\partial X_1} \right) n_2 dC, \tag{14.21}$$

which is a contour integral in which $n_2 = \mathbf{n}.\mathbf{e}_2$ and $K = \rho\mathbf{q}^2/2 = \rho(\nabla\varphi)^2/2$; it is written per unit length of the cylinder (one would say per unit *span* in airfoil theory). The expression (14.21) reminds us of the $J$-integral if $K$, $\varphi$, and the flux $\rho V_\infty$ are replaced (one-to-one correspondence!) by the quadratic elastic potential energy, the elastic displacement, and the traction, respectively. This provides the analogy of the force $F_1$ with a configurational force such as the integral of fracture. Furthermore, in fluid mechanics (cf. Karamcheti, 1966/1980), introducing the *circulation* $\Gamma$ by

$$\Gamma = \oint_C \mathbf{v}.d\mathbf{s}, \tag{14.22}$$

it is shown that (14.21) reads in vectorial form

$$\mathbf{F} = -\rho \mathbf{V}_\infty \times \Gamma \mathbf{e}_3 = \rho V_\infty \Gamma \mathbf{e}_2, \tag{14.23}$$

which is along $\mathbf{e}_2$ for $\mathbf{V}_\infty$ set along $\mathbf{e}_1$. Accordingly, to have a nonzero force, the circulation must not vanish as we would shrink $C$ to zero. This, obviously, calls for a *singular* flow field, which is none other than a vortex, while we note that the value obtained via (14.21) is unaltered inasmuch as the contour includes the body. Therefore, two aspects, path-independence and the existence of a singular field, are shared by the fluid-mechanics integral (14.21) and path-independent integrals of fracture. Cherepanov (1977) first emphasized this analogy and reported on useful invariant integrals in hydrodynamics.

The analogy can be pursued between vortex distributions in aerodynamics and dislocation distributions in defect solid mechanics. To show this we consider a flat plate (infinite in the direction $\mathbf{e}_3$) at small incidence angle $\alpha$ (on axis $\mathbf{e}_1$) in a uniform flow. The fluid disturbance field due to the presence of

the plate is represented by a vortex distribution $\gamma(x_1)$, which is a circulation per unit length of the plate of width $2c$ and thus may be called a circulation density (cf. Karamcheti, 1966/1980, Chapter 17 on thin airfoil theory). This is located at $x_2 = 0$ on the interval $x_1 \in [-c, +c]$. The kinematic boundary condition at the plate requires the total velocity field (sum of the uniform flow velocity and the perturbance contributed by the vortices) to have vanishing normal component at the plate. This condition provides a celebrated integral equation in the form (see (17.69) in Karamcheti [1966/1980], with a change in notation)

$$\frac{1}{2\pi}\int_{-c}^{+c}\frac{\gamma(x_1)}{x_1-\xi}d\xi = -v(x_1, 0_{\pm}) = -V_{\infty}\alpha. \tag{14.24}$$

Such an integral equation is completely analogous to an integral equation given by Bilby and Eshelby (1968) in a modeling that determines a dislocation density in fracture mechanics. The analogy is established by replacing the vortex line by a dislocation line, the circulation density by the dislocation density, and the uniform flow by the transverse stress. The solution of (14.24), which originally provided a dislocation density but now is applied to the circulation density, is given by Bilby and Eshelby (1968) as

$$\gamma(x_1) = \frac{1}{\pi\sqrt{c^2 - x_1^2}}\left\{K + 2V_{\infty}\alpha\int_{-c}^{+c}\frac{\sqrt{c^2-\xi^2}}{x_1-\xi}d\xi\right\}, \tag{14.25}$$

and the total circulation is obtained by summing over the circulation density, that is,

$$\Gamma = \int_{-c}^{+c}\gamma(\xi)d\xi = K. \tag{14.26}$$

The total fluid force acting on the thin plate is now determined by applying the formula (14.23), and the result is obviously orthogonal to $\mathbf{V}_{\infty}$, and this mathematically explains the mystery of lift in aeronautics! But then two questions remain, the answers to which also have analogies in fracture mechanics. These questions are (i) where is the point of application of the force (14.23), and (ii) what is the magnitude of this Eshelbian-like force? In the preceding example one has to determine the constant $K$. For this we would need the value of the circulation density at the end points of the interval of integration. Equation 14.25 implies that this should be either infinite or zero. The condition of uniform flow around the "airfoil" (our flat plate) is satisfied only if the shape of the cross section is rounded with a vertical slope at the

end point or is flat (zero slope) like a cusp. The same conclusion is reached for the geometric representation of cracks in fracture mechanics. In this case there may exist large short-range but nonlocal forces at the crack tip (cf. the Barenblatt model in Maugin, 1992) giving rise to barriers, while in the fluid case the velocity vanishes, implying an equilibrium distribution for $\gamma(x_1)$. Accordingly, one can choose to fix one end point, say $x_1 = -c$ with $\gamma(-c) = 0$, and then deduce the value of $K$ by applying (14.25). This is known as applying the so-called *Kutta condition* in ideal-fluid aerodynamics (potential-flow theory). The result of this computation is

$$K = 2V_\infty \alpha \int_{-c}^{+c} \left( \frac{c-\xi}{c+\xi} \right)^{1/2} d\xi = \pi V_\infty \alpha, \tag{14.27}$$

from which there follows the remarkably simple formula

$$F = (\rho V_\infty^2)\pi\alpha. \tag{14.28}$$

This derivation shows that the magnitude of the force exerted by the fluid on the "airfoil" can be determined only by "locking" (Atilgan's expression) the point vortex at the end point. In turn, this suggests that the application point of the said force is at the fixed vortex point, in the same way as the force on a crack is located at the tip (crack end) where the crack is sucked in the material. This interpretation, where the force acting on a fixed singularity provides the lift of the airfoil, is in contradiction with the standard interpretation, where the lift is applied at the aerodynamic center (the center of pressure; cf. Karamcheti, 1966/1980, pp. 515–516).

We may conclude this section by noting another integral equation that intervenes in both fracture mechanics and aerodynamics. In evaluating the so-called stress-intensity factor at the crack tip in a celebrated work by Westergaard (1939), which exploits the complex-variable technique, one has to solve the integral equation (cf. Maugin, 1992, p. 317, with change in notation)

$$-g(x) = \frac{1}{\pi\sqrt{x^2 - c^2}} \int_{-c}^{+c} \frac{g(\xi)\sqrt{c^2 - \xi^2}}{x - \xi} d\xi, \tag{14.29}$$

where $2c$ is the width of a straight crack set along the $x$-axis and the crack is acted on by a normal symmetric load such that $\sigma_{22}^{+} = \sigma_{22}^{-} = -g(x)$ for $|x| \le c$, $y = 0^{\pm}$, and zero otherwise. The integral (14.29) is extended to the complex plane ($x$ is replaced by $z$), and one has to find a solution that is sufficiently regular outside the crack segment, vanishes at infinity, and provides a real

part that is none other than $g(x)$. The integral equation (14.29) with complex $z$ was introduced by Sedov (1934) in an airfoil problem. Recently, Ben Amar and Rice (2002) have returned to the question of contour integrals in fluid mechanics in their study of the growth of fingers and the problem of electromigration (see also references therein).

## 14.4 The World of Configurational Forces

It is time to conclude after such a long excursion in what we may really call the *world* of configurational forces. What mechanicians would call Eshelbian mechanics or the theory of material and configurational forces appears to be a systematic application of the concepts of invariance or lack of invariance under groups of transformations that concern essentially, for a mechanician, the parametrization in space and time. In this framework, material homogeneity is the main material property that is given its proper importance at a moment of development in materials science where this is duly taken into account because of a concomitant development of techniques of measurement and observation. We can thus say that the conjunction between this interest and the development of Eshelby's ideas is spot on. This is achieved pragmatically without the shadows of mystery that have sometimes blurred the subject matter. In a previous book (Maugin, 1993), we tried to delineate the obvious differences between standard Newtonian forces and so-called Eshelbian forces, the main actors on the present stage. Some authors, not fully realizing the efficiency of the concepts, have emitted doubts about their reality and their usefulness, playing Cassandras. In this line we may cite authors in fluid mechanics (Andrew and McIntyre, 1978; McIntyre, 1981), thermodynamics (Mueller, 1999; Buratti et al., 2003), and solid mechanics (Podio-Guidugli, 2002). Some inquisitive physicists have rightly questioned the nature of pseudomomentum (our material or canonical momentum)—see Peierls (1979, 1985, 1991)—and we answered those in Maugin (1997) in a nontechnical format.

But it is now clear that all concepts such as those of Eshelby stress and wave momentum acquire a precise mathematical definition when a good space–time parametrization is employed (that of modern continuum mechanics, even in relativistic continuum mechanics). A great scientist like Peierls would have realized at once the community of thought between his own reasoning and Eshelby's, had he known the original papers of Eshelby in mechanics and the theory of defects. Witness of this is the typical argument (thought experiment) envisioned by Peierls in his examination of wave momentum in transparent media, which practically is a paraphrase of Eshelby's reasoning exposed on Chapter 3 here ("the system is still invariant under the following transformation: (a) displace the flow pattern as above, (b) displace the immersed object by some amount, (c) displace the fluid around the object so

as to clear the space into which the object has moved, and to fill the void it has left"). This is the intellectual reconstruction of the Jones–Richard experiment as reported by Peierls (1985, pp. 243–244). Quite symmetrically, the lack of interest of many (if not all) engineers in the modern bases of physics (principles of invariance, variational principles, Noether's theorem, the systematic reasoning in both space and time) has delayed a true understanding of the matter and its now rapidly developing range of applications. In their classical book inspired by Hilbert, Morse and Feshbach (1953) had remarked on some additional conservation laws in the theory of one-dimensional structural members, but we had to await the works of Herrmann, Kienzler, and Braun to exploit these in useful engineering situations. Even so, a modern book like Gurtin's (1999) does not touch this matter of invariance and, in spite of an attractive and ambitious title, does not fulfill its program by restricting the applications essentially to fracture and the propagation of interfaces, not acknowledging the role of canonical conservation laws in the whole of physics at the usual ontological level of the first principle of thermodynamics. What we gather from the lengthy exposition in the present book is that many properties and fields of interest cover the whole of phenomenological physics but in a necessarily modern guise, and we retain in a pragmatic vision free of any mysticism the following rich and enlightening features:

- The conceptual and applicative differences between classical balance laws and additional conservation laws.
- The fact that the new conservation laws concern, like energy, the *whole* physical system under consideration and not only degrees of freedom separately.
- The deep relationship with the notion of local structural rearrangement.
- The theoretical equivalence of standard material inhomogeneities with mathematical "inhomogeneities" (singularities) and pseudo-inhomogeneities (in particular large classes of dissipative behaviors that deviate from pure elasticity and pure Eulerian fluidity).
- The role played by the newly introduced entities in the design of criteria of progress (motion of dislocation, extension of fracture, propagation of phase-transition fronts, growth of damage and plasticity zones and of living material; breakage of electric conductors); and criteria of accuracy in numerical schemes (in finite elements, finite differences, etc.).

The last point mentioned, that dealing with *criteria*, is of utmost importance. In effect, many problems in engineering and phenomenological physics may now be solved by means of numerical tools, given the impossibility of reaching analytical solutions. But the practitioner must know when to stop or continue the computation at each point or globally, and such a criterion

that yields a definite *decision* can be based only on these conservation laws, which have not yet been exploited to obtain the momentaneous solution, which itself is based on the solution of the more traditional balance laws in the form of boundary-value problems often expressed in a weak variational form. In a less engineering-like vision, the intimate relationship of the present approach with the theory of structural defects (because of the third and fourth points listed) need not be emphasized. This mixes arguments of both analysis (singularity problems) and geometry (choice of the most representative manifold), which gives a modern but difficult touch to the theory. We limited ourselves to applications in solid-like materials, avoiding nonclassical (i.e., quantum) effects. But we have remarked on analogies between singularity problems and their approaches in various sciences (defects in materials science, flow defects—vortices—in fluid mechanics), so that we note in conclusion the natural extension of the concepts of conservation laws such as those of canonical momentum, energy, and spin to more recently formulated theories, such as that of vortices in nonlinear fields (cf. Pismen, 1999).

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## Chapter 1


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