The configurational and standard force balances are not always statements of a single law

By Eliot Fried

Department of Theoretical and Applied Mechanics, University of Illinois at Urbana-Champaign, Urbana, IL 61801-2935, USA

By studying the asympototic connection between phase-field and sharp-interface theories for transitions between two phases distinguished only by their constant free-energy densities, we show that the configurational force balance of the sharp-interface theory is completely unrelated to standard force balance. This demonstrates the fallacy of a recently asserted view that the balances for configurational and standard forces are never independent.

Keywords: Configurational forces; defects; phase transitions; sharp-interface theory; phase-field theory.

1. Introduction

The purpose of this paper is to dispel a misconception. Specifically, some workers contend that the configurational force balance is merely a rephrasing of the standard force balance. This view is exemplified by the following statement, written by Maugin (2002) in a review of Gurtin's (2000) book *Configurational Forces as Basic Concepts of Continuum Physics*:

> One reason may be that Gurtin claims an original approach which consists in postulating separately from the start two balance equations of linear momentum, one for physical forces, and the other for configurational forces. However, as shown by other authors during the last twenty years, these two equations are never independent, being two projections of a single equation on two different manifolds. They simply serve different purposes, and they place in evidence different features. In particular, the equation governing configurational forces captures singularities in a most efficient way, hence its role in the construction of phenomenological criteria of progress of these field singularities (crack tips, dislocation and disclination lines, discontinuity surfaces).

Underlying this statement is a viewpoint founded on formal manipulations of the standard force balance (Maugin, 1993). These manipulations allow for continuously distributed material imhomogeneities but not for defects described by geometric structures of dimension lower than three (that is, point defects, line defects, or interfaces). In the absence of any such defects, the configurational force balance is equivalent to the standard force balance. Otherwise, these balances express distinct laws.

Podio-Guidugli (2002) considers the question of whether configurational forces are necessary for the description of lower-dimensional defect structures. Central to his approach is a consideration of the power expended on a migrating referential control volume. If only standard forces are taken into account, the reasonable requirement that this power be invariant under changes of the tangential, and thus extrinsic, component of the velocity that describes the motion of the volume has a consequence that is generally untenable: the standard stress must be a pressure. To avoid this, it is necessary and sufficient to account for power expenditures above and beyond those associated with standard forces. This is accomplished with the introduction of configurational forces.

Configurational forces first arose in the works of Peach and Koehler (1950) and Eshelby (1951, 1956) on lattice defects and of Herring (1951) on the sintering of powders. Beginning with appropriate energy functionals, these works derive configurational forces variationally by considering rearrangements of the relevant defects. The distinction between configurational forces and standard forces is evident from the derivations: whereas standard forces arise from variations in the placement of material particles, configurational forces arise from variations in the arrangement, relative to material particles, of nonmaterial defects. These derivations also show that, when deformation is taken into account, the necessary conditions for equilibrium in a defective medium include not only the Euler–Lagrange equations imposing the balance of standard forces at and away from defects but also an additional Euler–Lagrange equation valid at defects and involving configurational forces. Although the variations leading to these conditions are performed independently, the ensuing equilibrium conditions are generally coupled.

In addition to giving conditions for the description of equilibrium, the variational perspective also provides guidance as to how configurational forces should enter the description of dissipative processes involving defect generation and evolution. Indeed, the conventional generalization of a variationally-based theory for a defective medium involves replacing the relevant Euler–Lagrange equation with a gradient-flow equation requiring that the time-rate of the relevant kinematic descriptor for the defect be proportional to the associated configurational force, with constant of proportionality signed to rule out spurious growth of the underlying energy functional. In this setting, the rate term can be viewed as a configurational drag force that accounts for energy dissipation associated with the motion of defects.

The structure of classical theories of continua allows for a clear distinction to be made between basic laws and constitutive equations. Whereas the basic laws hold for large classes of materials, constitutive equations distinguish between different materials. However, because Euler–Lagrange and gradient-flow equations rest on the provision of constitutive equations, the physical status of these supplemental equations is unclear. Do they represent an additional balance, above and beyond that involving standard forces, or do they simply represent additional constitutive information?

Commencing with a series of papers (Gurtin, 1988; Angenent and Gurtin, 1989; Gurtin and Struthers, 1990) concerning phase transitions, Gurtin advocates the first of these alternative interpretations. These papers take a Gibbsian approach: phase interfaces are modeled as sharp surfaces across which bulk material properties may suffer discontinuities; to account for localized interactions between phases, these surfaces are endowed with excess fields. Briefly, Gurtin's approach hinges on

the treatment of configurational forces as primitive objects that expend power in conjunction with the motion of defects (relative to the underlying material) and are subject to a configurational balance distinct from and supplemental to that involving standard forces. This approach has been applied to the description of defect structures other than interfaces, including cracks (Gurtin and Podio-Guidugli, 1996, 1998; Gurtin and Shvartsman, 1997), edges and junctions (Simha and Bhattacharya, 1998), dislocations (Cermelli and Gurtin, 1999), plasticity (Cermelli, Fried and Sellers, 2001), liquid-crystalline disclinations (Cermelli and Fried, 2002), and epitaxy (Gurtin and Jabbour, 2002; Fried and Gurtin, 2003). A comprehensive treatment of configurational forces and their applications is given in Gurtin's (2000) book.

Within Gurtin's framework, the distinction between the balances for configurational and standard forces is not, as Maugin maintains, merely an efficiency in capturing singularities. To illustrate this point, consider a setting involving a sharp interface $\mathcal{S}$ separating two phases, say α and β. For simplicity, neglect deformation, heat transport, and mass transport. Suppose that the free-energy density of phase $\gamma = \alpha, \beta$ is a constant, say Ψ_γ. Consider the problem of developing a theory that accounts for dependence of the interfacial free-energy density on the interfacial orientation and for dissipation associated with the growth of one phase at the expense of another. As shown by Gurtin (1995, 2000), such a theory involves a single equation governing the evolution of $\mathcal{S}$. Writing $\mathbf{n}$ for the unit orientation of $\mathcal{S}$, directed from the region occupied by phase-α into the region occupied by phase-β, and $V_{\mathcal{S}}$ for the (scalar) normal velocity of $\mathcal{S}$ in the direction of $\mathbf{n}$, this equation is

$$\hat{b}_{\mathcal{S}}(\mathbf{n}, V_{\mathcal{S}})V_{\mathcal{S}} = \left\{\hat{\psi}_{\mathcal{S}}(\mathbf{n})\mathbf{P} + \frac{\partial^2 \hat{\psi}_{\mathcal{S}}(\mathbf{n})}{\partial \mathbf{n}^2}\right\} \cdot \mathbf{L} + [\![\Psi]\!], \tag{1.1}$$

where $\mathbf{P} = \mathbf{1} - \mathbf{n} \otimes \mathbf{n}$ is the interfacial projector, $\mathbf{L} = -\nabla_{\mathcal{S}}\mathbf{n}$ is the interfacial curvature tensor, $\hat{\psi}_{\mathcal{S}}$ is the free-energy per unit interfacial area, $\hat{b}_{\mathcal{S}}$ is the nonnegative kinetic modulus, and $[\![\Psi]\!] = \Psi_\beta - \Psi_\alpha$. Generally, the dependence of $\hat{\psi}_{\mathcal{S}}$ on $\mathbf{n}$ renders certain interfacial orientations more energetically favorable than others. Similarly, the dependence of $\hat{b}_{\mathcal{S}}$ on $\mathbf{n}$ allows for growth at different rates along different orientations. Further, the dependence of $\hat{b}$ on $V_{\mathcal{S}}$ allows for nonlinear growth kinetics. The nonnegativity of $\hat{b}_{\mathcal{S}}$ ensures satisfaction of the second law. If $\hat{\psi}_{\mathcal{S}}(\mathbf{n}) = \psi_{\mathcal{S}}$ and $\hat{b}_{\mathcal{S}}(\mathbf{n}, V_{\mathcal{S}}) = b_{\mathcal{S}}$ with $\psi_{\mathcal{S}}$ and $b_{\mathcal{S}}$ constant, then (1.1) reduces to

$$b_{\mathcal{S}}V_{\mathcal{S}} = \psi_{\mathcal{S}}K_{\mathcal{S}} + [\![\Psi]\!], \tag{1.2}$$

with $K_{\mathcal{S}} = \operatorname{tr}\mathbf{L} = -\operatorname{div}_{\mathcal{S}}\mathbf{n}$ (twice) the mean curvature. When $\Psi_\alpha = \Psi_\beta$, which would be the case for an interface separating two crystal grains, (1.2) reduces to an equation $b_{\mathcal{S}}V_{\mathcal{S}} = \psi_{\mathcal{S}}K_{\mathcal{S}}$, the two-dimensional specialization of which was first proposed by Mullins (1956) as a model for grain-boundary evolution. The two-dimensional version of (1.1), with $b_{\mathcal{S}}$ independent of $V_{\mathcal{S}}$ was proposed by Uhuwa (1987). The general equation (1.1) was first given by Gurtin (1988). A formulation of (1.1) using a variational definition of the curvature term is given by Taylor, Cahn and Handwerker (1992), who provide background and extensive references concerning this equation.

Within Gurtin's theory, (1.2) arises from the normal component of the interfacial configurational force balance

$$\operatorname{div}_{\mathcal{S}}\mathbf{C} + \mathbf{f} + [\![\mathbf{C}]\!]\mathbf{n} = \mathbf{0}, \tag{1.3}$$

in conjunction with the representations

$$\mathbf{C}_\gamma = \Psi_\gamma \mathbf{1} \qquad \text{and} \qquad \mathbf{C} = \psi_{\mathcal{S}} \mathbf{P} - \mathbf{n} \otimes \mathbf{c} \tag{1.4}$$

for the bulk and interfacial configurational stresses and constitutive relations

$$\psi_{\mathcal{S}} = \hat{\psi}_{\mathcal{S}}(\mathbf{n}), \qquad \mathbf{c} = -\frac{\partial \hat{\psi}_{\mathcal{S}}(\mathbf{n})}{\partial \mathbf{n}}, \qquad \text{and} \qquad \mathbf{f} \cdot \mathbf{n} = -\hat{b}_{\mathcal{S}}(\mathbf{n}, V_{\mathcal{S}}) V_{\mathcal{S}}, \tag{1.5}$$

with $\hat{b}_{\mathcal{S}} \geq 0$, that determine the interfacial free-energy density $\psi_{\mathcal{S}}$, the interfacial configurational shear $\mathbf{c}$, and the normal component $\mathbf{f} \cdot \mathbf{n}$ of the internal interfacial configurational body force density $\mathbf{f}$.

Since this theory neglects deformation, the phases are rigid. Thus, the standard stresses in bulk and on the interface stresses are indeterminate and standard force balance is of no importance. It is therefore difficult to conceive of how the interfacial configurational force balance (1.3) or (its consequence) the interfacial evolution equation (1.1) could not be expressions of a law distinct from standard force balance. Nevertheless, the statement quoted at the outset of this paper shows that confusion remains regarding the status of the configurational force balance.

To eliminate this confusion, we consider an alternative approach to deriving the interfacial evolution equation (1.1). This alternative involves considering a theory in which the phases are described by a field φ. In this theory, an interface is not a surface but, rather, a transition layer across which φ varies smoothly. The thickness of such layers is constitutively determined. We consider a version of the phase-field theory that, due to a special choice of constitutive equations and a special scaling, allows us to control the thickness of transition layers. We then investigate the ramifications of shrinking that thickness. The phase-field theory allows for two approaches to deriving sharp-interface equations. We refer to these approaches as 'direct' and 'indirect.' While these yield the same analytical results, the insights that they afford are very different. We illustrate the indirect approach in the simple case where the desired interfacial evolution equation is (1.2). In the indirect approach, this equation arises as a solvability condition imposed on the inner expansion of φ by the Fredholm alternative. This makes it impossible to view (1.2) as an expression of standard force balance but otherwise leaves ambiguous the law underlying (1.2). The direct approach, which involves the configurational force balance of the phase-field theory, yields more insight. Because of the smoothness of the phase field, there is no need to consider configurational forces or their balance. Nevertheless, a configurational force balance can be derived within the phase-field theory and considerations based on this balance prove to be useful. In particular, we work with the component of this balance normal to time-dependent level sets of φ. In the direct aproach, (1.1) arises by expanding and integrating that equation over a layer while shrinking the thickness of the layer to zero. This shows clearly that the interfacial evolution equation (1.1) of the sharp-interface theory is an expression of configurational force balance and, bearing in mind that deformation is neglected, verifies that this equation is unrelated to the standard force balance. Our analysis thus demonstrates that:

> *the configurational and standard force balances are not always statements of a single law.*

The paper is organized as follows. We begin, in Section 2, with a brief overview of the phase-field theory. In so doing, we present both the standard variational derivation, which yields the governing equation for φ as a gradient-flow equation, as well as a less conventional continuum-mechanical derivation due to Fried and Gurtin (1993). Next, in Section 3, we derive the configurational force balance germane to the phase-field theory. Here, again, we consider two approaches. In the first of these, we mimick the formal calculations of Maugin (1993). Specifically, we multiply the evolution equation for φ by $\nabla\varphi$ and arrive at the desired result in a few simple steps. The second approach follows Gurtin's (1995, 2000) general framework for configurational forces. In Section 4, we consider time-dependent level sets of φ and obtain the component of the evolution equation for φ normal to those sets. In Section 5, we specialize the constitutive equations of the phase-field theory to yield an unscaled version of the theory that leads to the simple sharp-interface equation (1.2). Section 6 is concerned with scaling. In Section 7, we discuss expansions. In Sections 8, we obtain asymptotic results for the regions occupied by the bulk phases. In Section 9, we obtain asymptotic results for a generic transition layer. Here, we first take the indirect approach and then take the direct approach. In Section 10, we generalize the constitutive assumptions imposed in Section 4 and derive (1.1) using only the direct approach. Finally, in Section 11, we conclude the paper with a brief dicsussion.

2. Phase-field theory

We present a simple theory for transitions between two phases as described by a dimensionless scalar-valued *phase-field* φ. Intuitively, at an instant when both phases are present, we expect φ to vary smoothly between distinct values associated with each of the phases, manifesting large values of $L\nabla\varphi$ (with L denoting a suitable characteristic length) in any zone connecting those values. Otherwise, at an instant when only one phase is present, we expect φ to be essentially uniform. Thus, φ can be thought of as a regularized characteristic function for one of the phases and phase transitions are embodied in the evolution of the phase distribution as described by φ.

(*a*) *Variational approach*

The conventional approach to developing an equation governing the evolution of φ is variational. Assuming that the free-energy density, say ψ, is determined constitutively as a function $\hat{\psi}$ depending on φ and, to account for energetic contributions from the zones connecting the two phases, on $\nabla\varphi$, the total free-energy of the body $\mathcal{B}$ is given by the functional

$$\mathcal{F}(\varphi) = \int_{\mathcal{B}} \hat{\psi}(\varphi, \nabla\varphi)\, dv. \tag{2.1}$$

The evolution equation for φ then has the form of a gradient-flow equation,

$$\beta(\varphi, \nabla\varphi, \dot{\varphi})\dot{\varphi} = -\frac{\delta\mathcal{F}(\varphi)}{\delta\varphi}, \tag{2.2}$$

with $\beta \geq 0$ a constituively determined *kinetic coefficient* and $\delta\mathcal{F}(\varphi)/\delta\varphi$ defined via the first variation of $\mathcal{F}$, viz.,

$$\frac{\delta\mathcal{F}(\varphi)}{\delta\varphi} = \frac{\partial\hat{\psi}(\varphi,\nabla\varphi)}{\partial\varphi} - \operatorname{div}\left\{\frac{\partial\hat{\psi}(\varphi,\nabla\varphi)}{\partial(\nabla\varphi)}\right\}. \tag{2.3}$$

Tacit to the foregoing is the understanding that, to encompass the existence of two energetically viable phases, the restriction $\hat{\psi}(\cdot,\mathbf{0})$ of $\hat{\psi}$ to homogeneous choices of φ should be a double-well potential.

(*b*) *Alternative formulation*

An alternative to the variational approach shown above is provided by Fried and Gurtin (1993). This alternative hinges on distinguishing between kinematical ingredients, laws of balance and imbalance, and constitutive equations. The phase field φ is the sole kinematical variable of the theory. In recognition that power expenditures should accompany temporal variations of any kinematical descriptor and that such expenditures must involve conjugate forces, a a vector-valued *microstress* $\boldsymbol{\xi}$ and a scalar-valued *internal microforce density* π are introduced. The basic laws of the theory consist of the *balance of microforces* and the *imbalance of free-energy*, which require that for each body-part $\mathcal{P}$, with boundary $\partial\mathcal{P}$ and outward unit normal $\boldsymbol{\nu}$,

$$\int\limits_{\partial\mathcal{P}} \boldsymbol{\xi}\cdot\boldsymbol{\nu}\,da + \int\limits_{\mathcal{P}} \pi\,dv = 0, \tag{2.4}$$

and

$$\dot{\int\limits_{\mathcal{P}} \psi\,dv} \leq \int\limits_{\partial\mathcal{P}} (\boldsymbol{\xi}\cdot\boldsymbol{\nu})\dot{\varphi}\,da. \tag{2.5}$$

The local equivalents of the global laws are the field equation

$$\operatorname{div}\boldsymbol{\xi} + \pi = 0 \tag{2.6}$$

and the free-energy inequality

$$\dot{\psi} + \pi\dot{\varphi} - \boldsymbol{\xi}\cdot\nabla\dot{\varphi} \leq 0. \tag{2.7}$$

Assuming that ψ, $\boldsymbol{\xi}$, and π are determined constitutively by smooth functions of φ, $\nabla\varphi$, and $\dot{\varphi}$ and requiring that these functions be consistent with (2.7) in all processes then gives

$$\psi = \hat{\psi}(\varphi,\nabla\varphi), \quad \boldsymbol{\xi} = \frac{\partial\hat{\psi}(\varphi,\nabla\varphi)}{\partial(\nabla\varphi)}, \quad \text{and} \quad \pi = -\frac{\partial\hat{\psi}(\varphi,\varphi}{\partial\varphi} - \beta(\varphi,\nabla\varphi,\dot{\varphi})\dot{\varphi}, \tag{2.8}$$

with $\beta \geq 0$. Finally, using (2.8) in the local microforce balance (2.6) yields

$$\beta(\varphi,\nabla\varphi,\dot{\varphi})\dot{\varphi} = \operatorname{div}\left\{\frac{\partial\hat{\psi}(\varphi,\nabla\varphi)}{\partial(\nabla\varphi)}\right\} - \frac{\partial\hat{\psi}(\varphi,\nabla\varphi)}{\partial\varphi}, \tag{2.9}$$

which is equivalent to (2.2)–(2.3).

In view of (2.8), the free-energy inequality (2.7) yields an expression

$$\delta = -\beta(\varphi, \nabla\varphi, \dot{\varphi})\dot{\varphi}^2 \tag{2.10}$$

for the rate at which energy is dissipated per unit volume.

3. Configurational forces and their balance

(*a*) *Formal approach*

Consider the evolution equation (2.9). Multiplying each term of that equation by $\nabla\varphi$ and performing a few simple manipulations, one is led to the identity

$$\operatorname{div}\left\{\hat{\psi}(\varphi, \nabla\varphi)\mathbf{1} - \nabla\varphi \otimes \frac{\partial\hat{\psi}(\varphi, \nabla\varphi)}{\partial(\nabla\varphi)}\right\} + \beta(\varphi, \nabla\varphi, \dot{\varphi})\dot{\varphi}\nabla\varphi = \mathbf{0}. \tag{3.1}$$

The tensor

$$\hat{\psi}(\varphi, \nabla\varphi)\mathbf{1} - \nabla\varphi \otimes \frac{\partial\hat{\psi}(\varphi, \nabla\varphi)}{\partial(\nabla\varphi)} \tag{3.2}$$

appearing in (3.1) is immediately recognizable as the *configurational stress tensor* relevant in the present context (Eshelby, 1980). Further, the vector

$$\beta(\varphi, \nabla\varphi, \dot{\varphi})\dot{\varphi}\nabla\varphi \tag{3.3}$$

represents a *configurational body force density*. Thus, the derived identity (3.1) is the *configurational force balance* associated with the evolution equation (2.9). In the absence of defects, which would be associated with irregularities of φ, (3.1) is equivalent to (2.9) whenever $\nabla\varphi$ is nontrivial and, thus, superfluous.

Within the context of the phase-field theory, the configurational force balance (3.1) is a consequence of microforce balance (2.6) and the thermodynamically derived constitutive equations (2.8). In particular, neither standard forces nor their balance enter the derivation. Hence, (3.1) is unrelated to standard force balance.

(*b*) *Alternative approach*

Like the variational derivation of (2.9), the above derivation of (3.1) is predicated on the provision of constitutive equations. An alternative derivation that is free from this restriction is due to Gurtin (1995, 2000). This approach treats configurational forces as basic entities that are associated with the integrity of a body's material structure and expend power in connection with the transfer of material and the evolution of defects. Specifically, a *configurational stress tensor* $\mathbf{C}$ and a *configurational body force density* $\mathbf{f}$ are introduced. These are required to satisfy the *configurational force balance*

$$\int_{\partial\mathcal{P}} \mathbf{C}\boldsymbol{\nu}\, da + \int_{\mathcal{P}} \mathbf{f}\, dv = \mathbf{0} \tag{3.4}$$

for each part $\mathcal{P}$ of $\mathcal{B}$, which is equivalent to the local configurtional force balance

$$\operatorname{div}\mathbf{C}+\mathbf{f}=\mathbf{0}. \tag{3.5}$$

To characterize the manner in which configurational forces expend power, a means of capturing the kinematics associated with the transfer of material is needed. Gurtin (1995, 2000) accomplishes this with the aid of migrating control volumes. The evolution of a migrating control volume $\mathcal{R}$ can be generically described by a time-dependent field $\mathbf{q}$ defined over $\partial\mathcal{R}$ and the configurational traction $\mathbf{C}\boldsymbol{\nu}_{\partial\mathcal{R}}$ is assumed to be power conjugate to $\mathbf{q}$. Further, to properly reckon the power expended by the microtraction $\boldsymbol{\xi}\cdot\boldsymbol{\nu}_{\partial\mathcal{R}}$ on $\mathcal{R}$, it is necessary to consider the convected time-rate $\dot{\varphi}+\nabla\varphi\cdot\mathbf{q}$ of φ following the motion of $\partial\mathcal{R}$. Thus, the net power expended on $\mathcal{R}$ by external agencies can be expressed as

$$\int\limits_{\partial\mathcal{R}}\{(\mathbf{C}+\nabla\varphi\otimes\boldsymbol{\xi})\boldsymbol{\nu}_{\partial\mathcal{R}}\cdot\mathbf{q}+(\boldsymbol{\xi}\cdot\boldsymbol{\nu}_{\partial\mathcal{R}})\dot{\varphi}\}\,da. \tag{3.6}$$

Since the intrinsic motion of $\partial\mathcal{R}$ involves only the normal component $\mathbf{q}\cdot\boldsymbol{\nu}_{\partial\mathcal{R}}$ of $\mathbf{q}$, the net power should be invariant with respect to the choice of the tangential component of $\mathbf{q}$. This requirement implies that $\mathbf{C}+\nabla\varphi\otimes\boldsymbol{\xi}=\alpha\mathbf{1}$ and, thus, that

$$\int\limits_{\partial\mathcal{R}}\{(\mathbf{C}+\nabla\varphi\otimes\boldsymbol{\xi})\boldsymbol{\nu}_{\partial\mathcal{R}}\cdot\mathbf{q}+(\boldsymbol{\xi}\cdot\boldsymbol{\nu}_{\partial\mathcal{R}})\dot{\varphi}\}\,da=\int\limits_{\partial\mathcal{R}}(\alpha\mathbf{q}\cdot\boldsymbol{\nu}_{\partial\mathcal{R}}+(\boldsymbol{\xi}\cdot\boldsymbol{\nu}_{\partial\mathcal{R}})\dot{\varphi})\,da. \tag{3.7}$$

The free-energy imbalance for a migrating control volume $\mathcal{R}$ is simply

$$\dot{\int\limits_{\mathcal{R}}\psi\,dv}\leq\int\limits_{\partial\mathcal{R}}(\alpha\mathbf{q}\cdot\boldsymbol{\nu}_{\partial\mathcal{R}}+(\boldsymbol{\xi}\cdot\boldsymbol{\nu}_{\partial\mathcal{R}})\dot{\varphi})\,da, \tag{3.8}$$

from which it follows that

$$\int\limits_{\mathcal{R}}\dot{\psi}\,dv\leq\int\limits_{\partial\mathcal{R}}(\boldsymbol{\xi}\cdot\boldsymbol{\nu}_{\partial\mathcal{R}})\dot{\varphi}\,da+\int\limits_{\partial\mathcal{R}}(\alpha-\psi)\mathbf{q}\cdot\boldsymbol{\nu}_{\partial\mathcal{R}}\,da. \tag{3.9}$$

Thus, since it is always possible to find another control volume, say $\mathcal{R}'$ which coincides with $\mathcal{R}$ at a given instant but with normal velocity $\mathbf{q}'\cdot\boldsymbol{\nu}_{\partial\mathcal{R}}$ different from $\mathbf{q}\cdot\boldsymbol{\nu}_{\partial\mathcal{R}}$, it follows that $\alpha=\psi$ and that the configurational stress tensor must be of the form

$$\mathbf{C}=\psi\mathbf{1}-\nabla\varphi\otimes\boldsymbol{\xi}. \tag{3.10}$$

Using (3.10) in the local configurational force balance (3.5) yields

$$\operatorname{div}(\psi\mathbf{1}-\nabla\varphi\otimes\boldsymbol{\xi})+\mathbf{f}=\mathbf{0}. \tag{3.11}$$

In the absence of lower-dimensional defect structures, this equation *determines* the configurational body force density $\mathbf{f}=-\operatorname{div}(\psi\mathbf{1}-\nabla\varphi\otimes\boldsymbol{\xi})$. The balance (3.11) stands independent of any particular constitutive assumptions. Only when one invokes (2.8) does it reduce to (3.1), in which case $\mathbf{f}=\beta(\varphi,\nabla\varphi,\dot{\varphi})\dot{\varphi}\nabla\varphi$.

4. Uniformity surfaces. Normal configurational force balance

In the phase-field theory, an interface is a diffuse transition layer and each value that φ takes within such a layer can be thought of as representing a particular state of the material. For this reason the time-dependent level sets

$$\{\mathbf{x} : \varphi(\mathbf{x}, t) = \text{constant}\} \tag{4.1}$$

are important. We refer to such sets as *uniformity surfaces*.

Within transition layers, $\nabla\varphi$ should be nontrivial. Therein:

$$\mathbf{n} = \frac{\nabla\varphi}{|\nabla\varphi|} \tag{4.2}$$

and

$$V = -\frac{\dot{\varphi}}{|\nabla\varphi|} \tag{4.3}$$

represent a unit normal field and a corresponding (scalar) normal velocity field for uniformity surfaces;

$$\mathbf{P} = \mathbf{1} - \mathbf{n} \otimes \mathbf{n} \tag{4.4}$$

projects vector fields onto their components tangent to uniformity surfaces; and

$$\mathbf{L} = -(\nabla\mathbf{n})\mathbf{P} \qquad \text{and} \qquad K = \operatorname{tr}\mathbf{L} = -\operatorname{div}\mathbf{n} \tag{4.5}$$

are the curvature tensor and (twice) the mean curvature of uniformity surfaces.

From (4.2), $|\nabla\varphi|\nabla\mathbf{n} = \mathbf{P}\nabla\nabla\varphi$ and it follows that

$$\mathbf{L} = -\frac{1}{|\nabla\varphi|}\mathbf{P}(\nabla\nabla\varphi)\mathbf{P} \tag{4.6}$$

and

$$K = -\frac{1}{|\nabla\varphi|}(\Delta\varphi - \mathbf{n}\cdot(\nabla\nabla\varphi)\mathbf{n}). \tag{4.7}$$

Assuming that $\nabla\varphi \neq \mathbf{0}$, we may compute the component of the configurational force balance (3.11) in the direction $\mathbf{n}$ normal to uniformity surfaces. Bearing in mind (4.2) and (4.6), this yields the identity

$$\operatorname{div}(\psi\mathbf{n} - |\nabla\varphi|\boldsymbol{\xi}) + \psi K + \mathbf{f}\cdot\mathbf{n} = 0, \tag{4.8}$$

that we refer to as the *normal configurational force balance for uniformity surfaces*. In combination with the constititive equations (2.8), the auxiliary consequence $\mathbf{f} = \beta(\varphi, \nabla\varphi, \dot{\varphi})\dot{\varphi}\nabla\varphi$ of (2.8), and (4.3), (4.8) provides an evolution equation,

$$|\nabla\varphi|^2\beta(\varphi, \nabla\varphi, \dot{\varphi})V = \hat{\psi}(\varphi, \nabla\varphi)K + \operatorname{div}\left\{\hat{\psi}(\varphi, \nabla\varphi)\mathbf{n} - |\nabla\varphi|\frac{\partial\hat{\psi}(\varphi, \nabla\varphi)}{\partial(\nabla\varphi)}\right\}, \tag{4.9}$$

for φ—valid, and equivalent to the evolution equation (2.9), provided $\nabla\varphi \neq \mathbf{0}$. Otherwise, if $\nabla\varphi = \mathbf{0}$, we cannot impose (4.9), which was derived based on the assumption that $\nabla\varphi \neq \mathbf{0}$.

5. Specialization

For simplicity, we suppose that the constitutive relation determining the free-energy density has the simple form

$$\psi = f(\varphi) + \Psi_\alpha(1 - g(\varphi)) + \Psi_\beta g(\varphi) + \tfrac{1}{2}\lambda|\nabla\varphi|^2, \tag{5.1}$$

where: f is a double-well potential with equal minima at $\varphi = \varphi_\alpha$ and $\varphi = \varphi_\beta$, with $\varphi_\alpha < \varphi_\beta$, viz.,

$$0 = f(\varphi_\alpha) = f(\varphi_\beta) < f(\varphi) \qquad \text{for all } \varphi \neq \varphi_\alpha, \varphi_\beta; \tag{5.2}$$

g vanishes for $\varphi \leq \varphi_\alpha$, is equal to unity for $\varphi \geq \varphi_\beta$, and increases monotonically between $\varphi = \varphi_\alpha$ and $\varphi = \varphi_\beta$, viz.,

$$g(\varphi) = \begin{cases} 0 & 0 \leq \varphi_\alpha \\ 1 & \varphi \geq \varphi_\beta \end{cases} \tag{5.3}$$

and

$$g'(\varphi) > 0 \qquad \text{for all } \varphi \in (\varphi_\alpha, \varphi_\beta); \tag{5.4}$$

λ is constant and strictly positive, viz.,

$$\lambda > 0; \tag{5.5}$$

and Ψ_α and Ψ_β are the constant energy densities of the bulk phases α and β. In a body in which φ lies on average between φ_α and φ_β, the double-well structure of f lends energetic preference to distributions of φ consisting of regions with $\varphi = \varphi_\alpha$ and regions with $\varphi = \varphi_\beta$. The term $\frac{1}{2}\lambda|\nabla\varphi|^2$ penalizes sharp transitions between such regions and in so doing facilitates the existence of equilibria in which φ is smooth and $\mathcal{B}$ contains interfacial layers separating regions with φ close to φ_α from regions with φ close to φ_β. Because this term depends only on the magnitude $|\nabla\varphi|$ of $\nabla\varphi$, interfacial layers of all orientations are of equal energetic cost.

Further, we assume that the kinetic modulus β is constant and strictly positive, viz.,

$$\beta(\varphi, \nabla\varphi, \dot{\varphi}) = B > 0. \tag{5.6}$$

With this choice, (2.10) specializes to $\delta = -B\dot{\varphi}^2$; thus, the rate at which energy is dissipated by the growth of either phase at the expense of another is quadratic in $\dot{\varphi}$ and is insensitive to layer orientation.

In view of the specializations (5.1) and (5.6), the evolution equation (2.9) becomes

$$B\dot{\varphi} = \lambda\Delta\varphi - f'(\varphi) - [\![\Psi]\!]g'(\varphi), \tag{5.7}$$

with $[\![\Psi]\!] = \Psi_\beta - \Psi_\alpha$, and the normal configurational force balance (4.9) for uniformity surfaces becomes

$$\begin{aligned} |\nabla\varphi|^2 BV = {} & \big\{f(\varphi) + \Psi_\alpha(1 - g(\varphi)) + \Psi_\beta g(\varphi) + \tfrac{1}{2}\lambda|\nabla\varphi|^2\big\}K \\ & + \operatorname{div}\big\{(f(\varphi) + \Psi_\alpha(1 - g(\varphi)) + \Psi_\beta g(\varphi) - \tfrac{1}{2}\lambda|\nabla\varphi|^2)\mathbf{n}\big\}. \end{aligned} \tag{5.8}$$

We recall that (5.10) is meaningful only if $\nabla\varphi = \mathbf{0}$ and that, (5.10) if it is meaningful, it is equivalent to (5.7). Since

$$\big\{\Psi_\alpha(1-g(\varphi)) + \Psi_\beta g(\varphi)\big\}K + \operatorname{div}\big\{\Psi_\alpha(1-g(\varphi)) + \Psi_\beta g(\varphi)\big\} = [\![\Psi]\!]\mathbf{n}\cdot\nabla g(\varphi), \tag{5.9}$$

(5.8) can be rewritten somewhat more concisely as

$$|\nabla\varphi|^2 BV = \big\{f(\varphi) + \tfrac{1}{2}\lambda|\nabla\varphi|^2\big\}K + \operatorname{div}\big\{(f(\varphi) - \tfrac{1}{2}\lambda|\nabla\varphi|^2)\mathbf{n}\big\} + [\![\Psi]\!]\mathbf{n}\cdot\nabla g(\varphi) \tag{5.10}$$

and we will use this in lieu of (5.8).

6. Scaling

We introduce characteristic measures

$$\mu = \tfrac{1}{2}(\Psi_\alpha + \Psi_\beta) \qquad \text{and} \qquad \nu = \max_{\varphi\in(\varphi_\alpha,\varphi_\beta)} f(\varphi) \tag{6.1}$$

of free energy per unit volume of the bulk phases and of interfacial transition layers and assume that these yield a small dimensionless parameter

$$0 < \epsilon = \frac{\mu}{\nu} \ll 1. \tag{6.2}$$

Then, letting L denote a characteristic length and T a characteristic time and labeling the dimensional (unscaled) fields with asterisks, we introduce the dimensionless independent and dependent variables

$$\mathbf{x} = \frac{\mathbf{x}^*}{L}, \qquad t = \frac{t^*}{T}, \qquad \varphi_\epsilon(\mathbf{x},t) = \varphi^*(\mathbf{x}^*,t^*), \tag{6.3}$$

and constitutive quantities

$$f(\varphi_\epsilon) = \frac{f^*(\varphi^*)}{\nu}, \quad \Psi_\alpha = \frac{\Psi_\alpha^*}{\mu}, \quad \Psi_\beta = \frac{\Psi_\beta^*}{\mu}, \quad \epsilon\lambda = \frac{\lambda^*}{\mu L^2}, \quad \epsilon B = \frac{B^*}{\mu T}, \tag{6.4}$$

where the dependence of the fields on the parameter ϵ has been made explicit and the quantities without asterisks in (6.4) are assumed to be of $O(1)$ in ϵ.

With this scaling, the dimesnionless free-energy density is given by

$$\psi_\epsilon = \frac{\psi}{\mu} = \epsilon^{-1}f(\varphi_\epsilon) + \Psi_\alpha(1-g(\varphi_\epsilon)) + \Psi_\beta g(\varphi_\epsilon) + \tfrac{1}{2}\epsilon\lambda|\nabla\varphi_\epsilon|^2 \tag{6.5}$$

and the governing evolution equation for φ_ϵ becomes

$$\epsilon B\dot{\varphi}_\epsilon = \epsilon\lambda\Delta\varphi_\epsilon - \epsilon^{-1}f'(\varphi_\epsilon) - [\![\Psi]\!]g'(\varphi_\epsilon). \tag{6.6}$$

Further, the normal configurational force balance (5.10) reads

$$\begin{aligned}\epsilon|\nabla\varphi_\epsilon|^2 BV_\epsilon = {}& \big\{\epsilon^{-1}f(\varphi_\epsilon) + \tfrac{1}{2}\epsilon\lambda|\nabla\varphi_\epsilon|^2\big\}K_\epsilon \\ & + \operatorname{div}\Big\{\big\{\epsilon^{-1}f(\varphi_\epsilon) - \tfrac{1}{2}\epsilon\lambda|\nabla\varphi_\epsilon|^2\big\}\mathbf{n}_\epsilon\Big\} + [\![\Psi]\!]\mathbf{n}_\epsilon\cdot\nabla g(\varphi_\epsilon),\end{aligned} \tag{6.7}$$

with (cf. (4.2), (4.3), and (4.7))

$$\mathbf{n}_\epsilon = \frac{\nabla\varphi_\epsilon}{|\nabla\varphi_\epsilon|}, \quad V_\epsilon = -\frac{\dot{\varphi}_\epsilon}{|\nabla\varphi_\epsilon|}, \quad \text{and} \quad K_\epsilon = -\frac{1}{|\nabla\varphi_\epsilon|}(\Delta\varphi_\epsilon - \mathbf{n}_\epsilon\cdot(\nabla\nabla\varphi_\epsilon)\mathbf{n}_\epsilon). \tag{6.8}$$

7. Expansions

Hereafter, we focus on a fixed part $\mathcal{P}$ of $\mathcal{B}$ that, over some time interval, consists of three evolving subregions: $\mathcal{P}_\epsilon^\alpha$, $\mathcal{S}_\epsilon$, and $\mathcal{P}_\epsilon^\beta$. At each time t, $\mathcal{S}_\epsilon(t)$ is a transition layer comprised of points $\mathbf{x}$ in $\mathcal{B}$ with $\varphi_\alpha < \varphi_\epsilon(\mathbf{x},t) < \varphi_\beta$, while $\mathcal{P}_\epsilon^\alpha(t)$ and $\mathcal{P}_\epsilon^\beta(t)$ consist of points $\mathbf{x}$ with $\varphi_\epsilon(\mathbf{x},t) \approx \varphi_\alpha$ and $\varphi_\epsilon(\mathbf{x},t) \approx \varphi_\beta$, respectively. We assume that the limit

$$\mathcal{S} = \lim_{\epsilon\to 0+} \mathcal{S}_\epsilon \tag{7.1}$$

exists, with $\mathcal{S}(t)$ a smoothly evolving surface and with

$$\mathcal{P} = \mathcal{P}^\alpha(t) \cup \mathcal{S}(t) \cup \mathcal{P}^\beta(t), \tag{7.2}$$

with $\mathcal{P}^\gamma(t) = \lim_{\epsilon\to 0} \mathcal{P}_\epsilon^\gamma(t)$ for $\gamma = \alpha, \beta$.

We write $\ell(\mathbf{x},t)$ for the *signed distance* between a point $\mathbf{x}$ in $\mathcal{P}$ and the surface $\mathcal{S}(t)$, with $\ell(\mathbf{x},t) < 0$ in $\mathcal{P}_\epsilon^\alpha(t)$ and $\ell(\mathbf{x},t) > 0$ in $\mathcal{P}_\epsilon^\beta(t)$. Then

$$\mathbf{n}(\mathbf{x},t) = \nabla\ell(\mathbf{x},t) \qquad \text{and} \qquad V_{\mathcal{S}}(\mathbf{x},t) = -\dot{\ell}(\mathbf{x},t) \tag{7.3}$$

represent a unit normal-field and corresponding scalar normal-velocity-field for $\mathcal{S}(t)$. We also assume that $\ell(\mathbf{x},t)$ is smooth within $\mathcal{S}_\epsilon(t)$ and that given any $\mathbf{x}$ on $\mathcal{S}_\epsilon(t)$, there is a unique $\mathbf{z}$ on $\mathcal{S}(t)$ with $\mathbf{z} = \mathbf{x} - \ell(\mathbf{x},t)\mathbf{n}(\mathbf{x},t)$. The mapping $\mathbf{x} \mapsto \big(\ell(\mathbf{x},t), \mathbf{z}(\mathbf{x},t)\big)$ is then one-to-one on $\mathcal{S}_\epsilon(t)$; further, $\mathbf{n}(\mathbf{x},t)$ and $V_{\mathcal{S}}(\mathbf{x},t)$ are well-defined and independent of $\ell(\mathbf{x},t)$ at each $\mathbf{x}$ in $\mathcal{S}_\epsilon(t)$: $\mathbf{n}(\mathbf{x},t) = \mathbf{n}(\mathbf{z},t)$, $V_{\mathcal{S}}(\mathbf{x},t) = V_{\mathcal{S}}(\mathbf{z},t)$. Thus, writing $\nabla_{\mathcal{S}}$ and $\operatorname{div}_{\mathcal{S}}$ for the surface gradient and surface divergence on $\mathcal{S}$, the curvature tensor $\mathbf{L}$ and the total curvature $K_{\mathcal{S}}$ for $\mathcal{S}$,

$$\mathbf{L} = -\nabla_{\mathcal{S}}\mathbf{n} \qquad \text{and} \qquad K_{\mathcal{S}} = \operatorname{tr}\mathbf{L} = -\operatorname{div}_{\mathcal{S}}\mathbf{n} \tag{7.4}$$

are also independent of ℓ: $\mathbf{L}(\mathbf{x},t) = \mathbf{L}(\mathbf{z},t)$, $K_{\mathcal{S}}(\mathbf{x},t) = K_{\mathcal{S}}(\mathbf{z},t)$.

Within $\mathcal{S}_\epsilon(t)$, we stretch the coordinate normal to $\mathcal{S}(t)$ by letting

$$r(\mathbf{x},t) = \epsilon^{-1}\ell(\mathbf{x},t), \tag{7.5}$$

and, in accord with this, we assume that the thickness $h_\epsilon(t)$ of $\mathcal{S}_\epsilon(t)$ tends to zero with ϵ, but at slightly slower rate, viz.,

$$\lim_{\epsilon\to 0} h_\epsilon = 0, \quad \lim_{\epsilon\to 0}(\epsilon^{-1}h_\epsilon) = +\infty, \quad \lim_{\epsilon\to 0}(\epsilon^{-1}h_\epsilon^2) = 0. \tag{7.6}$$

For the phase field φ_ϵ, we introduce an *outer expansion*

$$\varphi_\epsilon(\mathbf{x},t) = \varphi_0^{\text{out}}(\mathbf{x},t) + \epsilon\varphi_1^{\text{out}}(\mathbf{x},t) + O(\epsilon^2), \tag{7.7}$$

assumed valid within the regions $\mathcal{P}_\epsilon^\alpha$ and $\mathcal{P}_\epsilon^\beta$, and an *inner expansion*

$$\varphi_\epsilon(\mathbf{x},t) = \varphi_0^{\text{in}}\big(r(\mathbf{x},t), \mathbf{z}(\mathbf{x},t), t\big) + \epsilon\varphi_1^{\text{in}}\big(r(\mathbf{x},t), \mathbf{z}(\mathbf{x},t), t\big) + O(\epsilon^2) \tag{7.8}$$

assumed valid within the layer; here, $\varphi_0^{\text{out}}(\mathbf{x},t)$, $\varphi_1^{\text{out}}(\mathbf{x},t)$ and $\varphi_0^{\text{in}}(r,\mathbf{z},t)$, $\varphi_1^{\text{in}}(r,\mathbf{z},t)$ are smooth, bounded functions of their arguments. We further assume that these expansions are twice formally differentiable in their arguments in the sense that

$\nabla\varphi_\epsilon = \nabla\varphi_0^{\rm out} + \epsilon\nabla\varphi_1^{\rm out} + O(\epsilon^2)$ for the outer expansion and, on letting $\acute{\varphi}_\epsilon$ denote the partial derivative of φ_ϵ with respect to r, $\acute{\varphi}_\epsilon = \acute{\varphi}_0^{\rm in} + \epsilon\acute{\varphi}_1^{\rm in} + O(\epsilon^2)$ for the inner expansion, and so forth.

Hence, we do not presume that $\mathcal{S}_\epsilon(t)$ is disjoint from $\mathcal{P}_\epsilon^\alpha(t)$ and $\mathcal{P}_\epsilon^\beta(t)$: the regions $\mathcal{S}_\epsilon(t) \cap \big(\mathcal{P}_\epsilon^\alpha(t) \cup \mathcal{P}_\epsilon^\beta(t)\big)$ of overlap represent sets where the outer and inner expansions agree. In particular, we have the matching condition

$$(\varphi_0^{\rm out})^\pm(\mathbf{x},t) = \lim_{d(\mathbf{x},t)\to 0\pm} \varphi_0^{\rm out}(\mathbf{x},t) = \lim_{r\to\pm\infty} \varphi_0^{\rm in}(r,\mathbf{z},t) = (\varphi_0^{\rm in})^\pm(r,\mathbf{z},t) \tag{7.9}$$

relating the $O(1)$ terms of the inner and outer expansions for φ_ϵ within the overlap region.

In terms of the variables $(r,\mathbf{z})$, the derivative with respect to $\mathbf{z}$ holding r fixed may be identified with the gradient $\nabla_{\mathcal{S}}$ on $\mathcal{S}$. Let

$$\mathbf{P} = \mathbf{1} - \mathbf{n}\otimes\mathbf{n}. \tag{7.10}$$

Then, since $\mathbf{z}(\mathbf{x},t) = \mathbf{x} - \ell(\mathbf{x},t)\mathbf{n}(\mathbf{x},t)$, it follows that

$$\nabla\mathbf{z} = \mathbf{P} + \ell\mathbf{M}_\epsilon, \tag{7.11}$$

with

$$\mathbf{M}_\epsilon = -\nabla\mathbf{n}. \tag{7.12}$$

To determine the dependence of $\mathbf{M}_\epsilon$ on ϵ, note that, since $|\ell| \le h_\epsilon = o(1)$ and $\acute{\ell} = \epsilon$, differentiating both sides of the relation $\mathbf{n}(\mathbf{x},t) = \mathbf{n}(\mathbf{z}(\mathbf{x},t),t)$ with respect to $\mathbf{x}$ yields

$$\mathbf{M}_\epsilon = (\mathbf{1} - \ell\mathbf{L})^{-1}\mathbf{L} = \mathbf{L} + o(1). \tag{7.13}$$

Thus, for Φ and $\mathbf{v}$ scalar- and vector-valued fields, we find that

$$\left.\begin{aligned} \nabla\Phi &= \epsilon^{-1}\acute{\Phi}\mathbf{n} + (\mathbf{P}+\ell\mathbf{M}_\epsilon)\nabla_{\mathcal{S}}\Phi = \epsilon^{-1}\acute{\Phi}\mathbf{n} + \big(1+o(1)\big)\nabla_{\mathcal{S}}\Phi, \\ \nabla\mathbf{v} &= \epsilon^{-1}\acute{\mathbf{v}}\otimes\mathbf{n} + (\nabla_{\mathcal{S}}\mathbf{v})(\mathbf{P}+\ell\mathbf{M}_\epsilon) = \epsilon^{-1}\acute{\mathbf{v}}\otimes\mathbf{n} + \big(1+o(1)\big)\nabla_{\mathcal{S}}\mathbf{v}, \end{aligned}\right\} \tag{7.14}$$

so that

$$\begin{aligned} \nabla\nabla\Phi = \epsilon^{-2}\acute{\Phi}\mathbf{n}\otimes\mathbf{n} + \epsilon^{-1}\big(1+o(1)\big)\big(\nabla_{\mathcal{S}}\acute{\Phi}\otimes\mathbf{n} + \mathbf{n}\otimes\nabla_{\mathcal{S}}\acute{\Phi} - \acute{\Phi}\mathbf{L}\big) \\ + (\nabla_{\mathcal{S}}\nabla_{\mathcal{S}}\Phi)O(1) + O(1)\nabla_{\mathcal{S}}\Phi \end{aligned} \tag{7.15}$$

with the $O(1)$ and $o(1)$ estimates in (7.14) and (7.15) of appropriate tensorial order and independent of Φ and $\mathbf{v}$.

As a further consequence of the relation $\mathbf{z}(\mathbf{x},t) = \mathbf{x} - \ell(\mathbf{x},t)\mathbf{n}(\mathbf{x},t)$, it follows that

$$\dot{\mathbf{z}} = V_{\mathcal{S}}\mathbf{n} + \ell\mathbf{v}_\epsilon, \tag{7.16}$$

with

$$\mathbf{v}_\epsilon = -\dot{\mathbf{n}}. \tag{7.17}$$

To determine the dependence of $\mathbf{v}_\epsilon$ on ϵ, note that $\dot{\mathbf{n}} = \nabla\dot{\ell} = -\nabla V_{\mathcal{S}}$. Thus, since $\nabla V_{\mathcal{S}} = (\mathbf{P} + \ell\mathbf{M}_\epsilon)\nabla_{\mathcal{S}} V_{\mathcal{S}}$ and $\mathring{\mathbf{n}} = -\nabla_{\mathcal{S}} V_{\mathcal{S}}$, with $\mathring{\mathbf{n}}$ the time-rate of $\mathbf{n}$ following the normal trajectories of $\mathcal{S}$

$$\mathbf{v}_\epsilon = (\mathbf{P} + \ell\mathbf{M}_\epsilon)\nabla_{\mathcal{S}} V_{\mathcal{S}} = \nabla_{\mathcal{S}} V_{\mathcal{S}} + o(1). \tag{7.18}$$

Thus, for Φ a scalar field,

$$\dot{\Phi} = -\epsilon^{-1} V_{\mathcal{S}} \acute{\Phi} + \ell \nabla_{\mathcal{S}}\Phi \cdot (\mathbf{P} + \ell\mathbf{L})\mathring{\mathbf{n}} + \Phi_t = -\epsilon^{-1} V_{\mathcal{S}} \acute{\Phi} + \Phi_t + o(1), \tag{7.19}$$

where Φ_t denotes the partial time-rate of Φ holding r and $\mathbf{z}$ fixed.

8. Bulk regions

Using the outer expansion (7.7) of φ_ϵ in the scaled evolution equation (6.6) and neglecting terms of $O(1)$ and smaller in ϵ, we find that $f'(\varphi_0^{\text{out}}) = 0$, so that, since f is a double-well potential with equal minima at φ_α and φ_β,

$$\varphi_0^{\text{out}} = \begin{cases} \varphi_\alpha & \text{on } \mathcal{P}_\epsilon^\alpha, \\ \varphi_\beta & \text{on } \mathcal{P}_\epsilon^\beta. \end{cases} \tag{8.1}$$

Further

$$f(\varphi_\epsilon) = o(\epsilon) \quad \text{and} \quad f'(\varphi_\epsilon) = o(1) \quad \text{on} \quad \mathcal{P}_\epsilon^\alpha \cup \mathcal{P}_\epsilon^\beta, \tag{8.2}$$

and

$$\dot{\varphi}_\epsilon, \nabla\varphi_\epsilon, \nabla\dot{\varphi}_\epsilon = O(\epsilon) \qquad \text{on} \qquad \mathcal{P}_\epsilon^\alpha \cup \mathcal{P}_\epsilon^\beta. \tag{8.3}$$

Thus, it follows that

$$\psi_\epsilon = \begin{cases} \Psi_\alpha + O(\epsilon) & \text{on } \mathcal{P}_\epsilon^\alpha, \\ \Psi_\beta + O(\epsilon) & \text{on } \mathcal{P}_\epsilon^\beta. \end{cases} \tag{8.4}$$

9. Transition layer

(*a*) *Basic estimates*

Applying $(7.14)_1$, $(7.14)_2$, and (7.19) to the inner expansion (7.8) of φ_ϵ, we find that

$$\left.\begin{aligned} \nabla\varphi_\epsilon &= \epsilon^{-1}\acute{\varphi}_0^{\text{in}}\mathbf{n} + \nabla_{\mathcal{S}}\varphi_0^{\text{in}} + \acute{\varphi}_1^{\text{in}}\mathbf{n} + O(\epsilon), \\ |\nabla\varphi_\epsilon| &= \epsilon^{-1}\acute{\varphi}_0^{\text{in}} + \acute{\varphi}_1^{\text{in}} + O(\epsilon), \\ \nabla\nabla\varphi_\epsilon &= \epsilon^{-2}\acute{\varphi}_0^{\text{in}}\mathbf{n}\otimes\mathbf{n} \\ &\quad + \epsilon^{-1}(\nabla_{\mathcal{S}}\acute{\varphi}_1^{\text{in}}\otimes\mathbf{n} + \mathbf{n}\otimes\nabla_{\mathcal{S}}\acute{\varphi}_1^{\text{in}} - \acute{\varphi}_0^{\text{in}}\mathbf{L} + \acute{\varphi}_1^{\text{in}}\mathbf{n}\otimes\mathbf{n}) + O(1), \\ \Delta\varphi_\epsilon &= \epsilon^{-2}\acute{\varphi}_0^{\text{in}} - \epsilon^{-1}(K_{\mathcal{S}}\acute{\varphi}_0^{\text{in}} - \acute{\varphi}_1^{\text{in}}) + O(1), \\ \dot{\varphi}_\epsilon &= -\epsilon^{-1}V_{\mathcal{S}}\acute{\varphi}_0^{\text{in}} + O(1), \end{aligned}\right\} \tag{9.1}$$

and, applying these estimates to (6.8), that

$$\mathbf{n}_\epsilon = \mathbf{n} + O(\epsilon), \qquad V_\epsilon = V_{\mathcal{S}} + O(\epsilon), \qquad \text{and} \qquad K_\epsilon = K_{\mathcal{S}} + o(1). \tag{9.2}$$

(*b*) *Equipartion of free-energy density and its consequences*

Using the inner expansion of φ_ϵ and the estimates (9.1) in the scaled evolution equation (6.6) and neglecting terms of $O(1)$ and smaller, we find that $\varphi_0^{\rm in}$ must satisfy the ordinary differential equation

$$\lambda\ddot{\varphi}_0^{\rm in} = f'(\varphi_0^{\rm in}). \tag{9.3}$$

Further, in view of the matching condition (7.9) and the result (8.1) concerning $\varphi_0^{\rm out}$, $\varphi_0^{\rm in}$ must satisfy

$$\varphi_0^{\rm in} \to \begin{cases} \varphi_\alpha & \text{as } r \to -\infty, \\ \varphi_\beta & \text{as } r \to +\infty, \end{cases} \tag{9.4}$$

along with

$$\dot{\varphi}_0^{\rm in} \to 0 \qquad \text{and} \qquad \ddot{\varphi}_0^{\rm in} \to 0 \qquad \text{as } r \to \pm\infty. \tag{9.5}$$

Since f is a double-well potential with equal minima at φ_α and φ_β, the boundary-value problem formed by (9.3) and (9.4) possesses a unique solution $\varphi_0^{\rm in}$ that increases monotonically from the value φ_α at $r = -\infty$ to the value φ_β at $r = +\infty$. Further, $\varphi_0^{\rm in}$ must be independent of $\mathbf{z}$.

Granted the boundary conditions $(9.4)_{2,3}$, the differential equation $(9.3)_1$ possesses a first integral

$$\tfrac{1}{2}\lambda|\dot{\varphi}_0^{\rm in}|^2 = f(\varphi_0^{\rm in}), \tag{9.6}$$

which we interpret as an expression of the equipartition of the free-energy density (to most significant order in ϵ), between the double-well potential f and the gradient energy density $\frac{1}{2}\lambda|\nabla\varphi_\epsilon|^2$, within the layer. Since f and f' vanish at $\varphi = \varphi_\alpha$ and $\varphi = \varphi_\beta$, $\varphi_0^{\rm in}$ must decay according to $\dot{\varphi}_0^{\rm in}(r,\cdot) = O(e^{-c|r|})$ as $|r| \to \infty$, with $c > 0$ independent of r. Hence, $\dot{\varphi}_0^{\rm in}$ is, as a function of r, square-integrable on $(-\infty, +\infty)$. Thus, by (9.6), (9.3), and (9.4),

$$\int_{-\infty}^{+\infty} \sqrt{\lambda}|\dot{\varphi}_0^{\rm in}(r,\cdot)|^2\, dr = \int_{\varphi_\alpha}^{\varphi_\beta} \sqrt{2f(\varphi)}\, d\varphi. \tag{9.7}$$

For convenience, we introduce

$$\psi_{\mathcal{S}} = \sqrt{\lambda}\int_{\varphi_\alpha}^{\varphi_\beta} \sqrt{2f(\varphi)}\, d\varphi \tag{9.8}$$

and note that, if rewritten in terms of dimensional quantities, $\psi_{\mathcal{S}}$ would carry dimensions of free-energy per unit area. Granted (9.8), it follows from (9.7) that

$$\int_{-\infty}^{+\infty} \lambda|\dot{\varphi}_0^{\rm in}(r)|^2\, dr = \psi_{\mathcal{S}}. \tag{9.9}$$

(*c*) *Interfacial evolution equation. Indirect approach*

At $O(1)$, the scaled evolution equation (6.6) yields the linear but inhomogeneous equation

$$\lambda\acute{\varphi}_1^{\rm in} - f''(\varphi_0^{\rm in})\varphi_1^{\rm in} = -\rho, \tag{9.10}$$

with

$$\rho = BV_{\mathcal{S}}\acute{\varphi}_0^{\rm in} - \lambda K_{\mathcal{S}}\acute{\varphi}_0^{\rm in} - [\![\Psi]\!]g'(\varphi_0^{\rm in}). \tag{9.11}$$

On differentiating (9.3) with respect to r, it follows that $\acute{\varphi}_0^{\rm in}$ must satisfy the homogeneous equation $\lambda\acute{\acute{\varphi}}_0^{\rm in} - f''(\varphi_0^{\rm in})\acute{\varphi}_0^{\rm in} = 0$. Thus, by the Fredholm alternative, ρ and $\acute{\varphi}_0^{\rm in}$ must be orthogonal:

$$\int_{-\infty}^{+\infty} \rho\acute{\varphi}_0^{\rm in}\, dr = 0. \tag{9.12}$$

Evaluating the integral on the left side of (9.12), using (9.9), the boundary conditions (9.4), and recalling from (5.3) that g vanishes at $\varphi = \varphi_\alpha$ and is equal to unity at $\varphi = \varphi_\beta$, we find that

$$b_{\mathcal{S}}V_{\mathcal{S}} = \psi_{\mathcal{S}}K_{\mathcal{S}} + [\![\Psi]\!], \tag{9.13}$$

where we have introduced

$$b_{\mathcal{S}} = \frac{B}{\sqrt{\lambda}}\int_{\varphi_\alpha}^{\varphi_\beta} \sqrt{2f(\varphi)}\, d\varphi = \frac{B\psi_{\mathcal{S}}}{\lambda}. \tag{9.14}$$

We note that, if rewritten in terms of dimensional quantities, $b_{\mathcal{S}}$ would carry dimensions of mass per unit time per unit area and would, therefore, represent an interfacial reciprocal mobility.

Granted an appropriate redimensionalization, the equation (9.13) is precisely the interfacial evolution equation (1.2) governing the evolution of a sharp phase interfaces endowed with a constant interfacial free-energy per unit area $\psi_{\mathcal{S}}$ and reciprocal mobility $b_{\mathcal{S}}$ that separates bulk phases α and β with constant free-energy densities Ψ_α and Ψ_β.

(*d*) *Interfacial evolution equation. Direct approach*

Within the layer, $\nabla\varphi_\epsilon$ is generally nontrivial. Thus, it is there permissible to work with the scaled normal configurational force balance (6.7) for uniformity surfaces instead of the scaled evolution equation (6.6). Using the inner expansion of φ_ϵ and the estimates (9.1) and (9.2) in (6.7) and neglecting terms of $O(\epsilon^{-1})$ and smaller, we arrive once again at (9.3) and, bearing in mind (7.9), (8.1), and the properties of f, all the conclusions of Section 9(*b*) follow. Next, at $O(\epsilon^{-1})$, (6.7) yields, in view of the result (9.6) concerning the partition of free-energy density,

$$BV_{\mathcal{S}}|\acute{\varphi}_0^{\rm in}|^2 = \lambda K_{\mathcal{S}}|\acute{\varphi}_0^{\rm in}|^2 + \overline{\{f'(\varphi_0^{\rm in})\acute{\varphi}_1^{\rm in} - \lambda\acute{\varphi}_0^{\rm in}\acute{\varphi}_1^{\rm in}\}} + [\![\Psi]\!]\overline{\acute{g}(\varphi_0^{\rm in})}. \tag{9.15}$$

Integrating the equation (9.15) over r, from $r = -\infty$ to $r = +\infty$, and utilizing the definitions (9.9) and (9.14), the boundary and far-field conditions (9.4) and (9.5), and properties of f and g then yields once again the evolution equation (9.13) obtained in the previous section by the Fredholm alternative. In this sense, (9.13) can be viewed as a consequence of the normal component of the configurational force balance for uniformity surfaces, obtained in passing to the limit $\epsilon \to 0$, a limit that corresponds to collapsing the transition layer to a surface.

We have remarked earlier that, when φ_ϵ is regular, the configurational force balance contains no information beyond that already contained in the evolution equation for φ_ϵ. However, passing to the limit $\epsilon \to 0$ generates surfaces across which φ_ϵ is discontinuous and $\nabla\varphi_\epsilon$ and $\dot{\varphi}_\epsilon$ (as well as other associated derivatives) are undefined. The asymptotic analysis performed here shows that, at such a defect, the normal configurational force balance for uniformity surfaces yields directly information that is only arises indirectly—as a solvability condition imposed by the Fredholm alternative—from the evolution equation for φ_ϵ. In this sense, we view the asymptotically derived interfacial evolution equation as a statement of normal configurational force balance for the interface.

Our asymptotic derivations of the evolution equation (1.2) are predicated on (9.8) and (9.14). We interpret (9.8) and (9.14) as *constitutive connections* between the theories at hand, connections that guarantee that the phase-field theory corresponds asymptotically to the sharp-interface theory.

10. Generalization

To obtain the general evolution equation (1.1) from the phase-field theory, we first modify the constitutive equations (5.1) and (5.6) determining the free-energy density and the kinetic modulus to

$$\psi = f(\varphi) + \Psi_\alpha(1 - g(\varphi)) + \Psi_\beta g(\varphi) + \tfrac{1}{2}\lambda(\mathbf{n})|\nabla\varphi|^2, \tag{10.1}$$

and

$$\beta(\varphi, \nabla\varphi, \dot{\varphi}) = B(\mathbf{n}, V) > 0, \tag{10.2}$$

with $\mathbf{n}$ and V as defined in (4.2) and (4.3).

Scaling as in Section 5(a), we arrive at the evolution equation

$$\epsilon B(\mathbf{n}_\epsilon, V_\epsilon)\dot{\varphi}_\epsilon = \epsilon \mathrm{div}\left\{|\nabla\varphi_\epsilon|\left(\lambda(\mathbf{n}_\epsilon)\mathbf{n}_\epsilon + \frac{1}{2}\frac{\partial\lambda(\mathbf{n}_\epsilon)}{\partial\mathbf{n}_\epsilon}\right)\right\} - \epsilon^{-1}f'(\varphi_\epsilon) - [\![\Psi]\!]g'(\varphi_\epsilon). \tag{10.3}$$

and the normal configurational force balance for uniformity surfaces

$$\begin{aligned}\epsilon|\nabla\varphi_\epsilon|^2 B(\mathbf{n}_\epsilon, V_\epsilon)V_\epsilon &= \left\{\epsilon^{-1}f(\varphi_\epsilon) + \tfrac{1}{2}\epsilon\lambda(\mathbf{n}_\epsilon)|\nabla\varphi_\epsilon|^2\right\}K_\epsilon \\ &+ \mathrm{div}\left\{\left\{\epsilon^{-1}f(\varphi_\epsilon) - \tfrac{1}{2}\epsilon\lambda(\mathbf{n}_\epsilon)|\nabla\varphi_\epsilon|^2\right\}\mathbf{n}_\epsilon - \tfrac{1}{2}\epsilon|\nabla\varphi_\epsilon|^2\frac{\partial\lambda(\mathbf{n}_\epsilon)}{\partial\mathbf{n}_\epsilon}\right\} + [\![\Psi]\!]\mathbf{n}\cdot\nabla g(\varphi_\epsilon),\end{aligned} \tag{10.4}$$

which generalize (6.6) and (6.7).

The results for the bulk regions are unchanged from those presented in Section 8. To study the layer, we follow the approach taken in Section 9(d). Specifically, at $O(\epsilon^{-2})$, (10.4) yields

$$\overline{\{\tfrac{1}{2}\lambda(\mathbf{n})|\acute{\varphi}_0^{\rm in}|^2 - f(\varphi_0^{\rm in})\}} = 0. \tag{10.5}$$

Further, the matching conditions (7.9) and the bulk results (8.1) yield, as before, the far-field conditions (9.4) and (9.5). Combining (10.5), (9.4), and (9.5), we arrive at the first integral

$$\tfrac{1}{2}\lambda(\mathbf{n})|\acute{\varphi}_0^{\rm in}|^2 = f(\varphi_0^{\rm in}) \tag{10.6}$$

and find, in view of the properties of f, once again that, as a function of r, $\acute{\varphi}_0^{\rm in}$ must be square integrable on $(-\infty,+\infty)$. This leads to a generalization

$$\int\limits_{-\infty}^{+\infty} \sqrt{\lambda(\mathbf{n})}|\acute{\varphi}_0^{\rm in}(r,\cdot,\cdot)|^2\,dr = \int\limits_{\varphi_\alpha}^{\varphi_\beta} \sqrt{2f(\varphi)}\,d\varphi. \tag{10.7}$$

of (9.7).

We next introduce analogs

$$\hat{\psi}_{\mathcal{S}}(\mathbf{n}) = \sqrt{\lambda(\mathbf{n})}\int\limits_{\varphi_\alpha}^{\varphi_\beta} \sqrt{2f(\varphi)}\,d\varphi \tag{10.8}$$

and

$$b_{\mathcal{S}}(\mathbf{n},V_{\mathcal{S}}) = \frac{B(\mathbf{n},V_{\mathcal{S}})}{\sqrt{\lambda(\mathbf{n})}}\int\limits_{\varphi_\alpha}^{\varphi_\beta} \sqrt{2f(\varphi)}\,d\varphi = \frac{B(\mathbf{n},V_{\mathcal{S}})\hat{\psi}_{\mathcal{S}}(\mathbf{n})}{\lambda(\mathbf{n})}. \tag{10.9}$$

of the constitutive connections (9.8) and (9.14). Direct consequences of (10.7) and (10.8) are the identities

$$\left.\begin{aligned}
&\int\limits_{-\infty}^{+\infty} \lambda(\mathbf{n})|\acute{\varphi}_0^{\rm in}(r,\cdot,\cdot)|^2\,dr = \hat{\psi}_{\mathcal{S}}(\mathbf{n}),\\
&\int\limits_{-\infty}^{+\infty} \frac{\partial\lambda(\mathbf{n})}{\partial\mathbf{n}}|\acute{\varphi}_0^{\rm in}(r,\cdot,\cdot)|^2\,dr = 2\frac{\partial\hat{\psi}_{\mathcal{S}}(\mathbf{n})}{\partial\mathbf{n}},
\end{aligned}\right\} \tag{10.10}$$

Finally, proceding as in Section 9(d), (10.4) yields at $O(\epsilon^{-1})$

$$\begin{aligned}
|\acute{\varphi}_0^{\rm in}|^2 B(\mathbf{n},V_{\mathcal{S}})V_{\mathcal{S}} &= |\acute{\varphi}_0^{\rm in}|^2\lambda(\mathbf{n})K_{\mathcal{S}} - \operatorname{div}_{\mathcal{S}}\left\{\tfrac{1}{2}|\acute{\varphi}_0^{\rm in}|^2\frac{\partial\lambda(\mathbf{n})}{\partial\mathbf{n}}\right\}\\
&\quad + \overline{\left\{f'(\varphi_0^{\rm in})\varphi_1^{\rm in} - \acute{\varphi}_0^{\rm in}\acute{\varphi}_1^{\rm in}\lambda(\mathbf{n}) - \tfrac{1}{2}\acute{\varphi}_0^{\rm in}\nabla\varphi_0^{\rm in}\cdot\frac{\partial\lambda(\mathbf{n})}{\partial\mathbf{n}}\right\}} + [\![\Psi]\!]\overline{g(\varphi_0^{\rm in})};
\end{aligned} \tag{10.11}$$

integrating (10.11) over r, from $r = -\infty$ to $r = +\infty$, and utilizing the constitutive connections (10.8) and (10.9), the boundary and far-field conditions (9.4) and (9.5), and properties of f and g then yields

$$\hat{b}_{\mathcal{S}}(\mathbf{n}, V_{\mathcal{S}})V_{\mathcal{S}} = \left\{ \hat{\psi}_{\mathcal{S}}(\mathbf{n})\mathbf{P} + \frac{\partial^2 \hat{\psi}_{\mathcal{S}}(\mathbf{n})}{\partial \mathbf{n}^2} \right\} \cdot \mathbf{L} + [\![\Psi]\!], \tag{10.12}$$

which, granted an appropriate redimensionalization, is precisely the general interfacial evolution equation (1.1) of the sharp-interface theory.

11. Discussion

Our conclusions are predicated on the provision of constitutive equations within the phase-field theory and, moreover, upon stipulated connections (10.8) and (10.9) between those constitutive equations and the constitutive equations of the sharp-interface theory. However, because the framework of the phase-field theory is a dynamical one that allows for dissipation, the results of our analysis are more broadly applicable than would be any based on variational methods.

By restricting our attention to a setting where the standard force balance is irrelevant, we leave open the possibility that, once the constraint of rigidity is relaxed and the standard stress is no longer indeterminate, the standard force balance might somehow give rise to the interfacial configurational force balance and, thus, to a law governing the evolution of the interface. However, such an outcome would be at odds with the implications of variationally-based descriptions. Indeed, in considering phase interfaces within the context of the theory of finite elastostatics, Podio-Guidugli (2001) shows that, while both the bulk configurational force balance and the tangential component of the interfacial configurational force balance are implied consequences of standard force balance, the normal component of the interfacial configurational force balance is independent. Moreover, asymptotic analyses of phase-field theories that account for deformation (Fried and Grach, 1997; Fried and Gurtin, 1999) show that the supplemental evolution equation of the sharp-interface theory arises not from the deformational force balance but just as it does in the simple theory considered here—either 'indirectly' from the evolution equation for the phase field or 'directly' from the associated configurational force balance.

References

Angenent, S., Gurtin, M. E., 1989. Multiphase thermodynamics with interfacial structure. 2. Evolution of an isothermal interface. *Archive for Rational Mechanics and Analysis* **108**, 323–391.

Cermelli, P., Fried, E., Sellers, S., 2001. Configurational stress, yield, and flow in rate-independent plasticity. *Proceedings of the Royal Society of London A* **457**, 1447–1467.

Cermelli, P., Fried, E., 2002. The evolution equation for a disclination in a nematic liquid crystal. *Proceedings of the Royal Society of London A* **458**, 1–20.

Cermelli, P., Gurtin, M. E. 1999. The motion of screw disclocations in crystalline materials undergoing antiplane shear: glide, cross-slip, and fine cross-slip. *Archive for Rational Mechanics and Analysis* **148**, 3–52.

Eshelby, J. D., 1951. The force on an elastic singularity. *Philosophical Transactions of the Royal Society of London A* **244**, 87–112.

Eshelby, J. D., 1956. The continuum theory of lattice defects. In *Progress in Solid State Physics 3* (eds. F. Seitz, D. Turnbull), Academic Press, New York.

Eshelby, J. D., 1980. The energy-momentum tensor of complex continua. In *Continuum Models of Discrete Systems* (eds. E. Kröner, K. H. Anthony), University of Waterloo Press, Waterloo.

Fried, E., Grach, G., 1997. An order-parameter based theory as a regularization of a sharp-interface theory for solid-solid phase transitions. *Archive for Rational Mechanics and Analysis* **138**, 355–404.

Fried, E., Gurtin M. E., 1993. Continuum theory of thermally induced phase transitions based on an order parameter. *Physica D* **68**, 326–343.

Fried, E., Gurtin M. E., 1996. A phase-field theory for solidification based on a general anisotropic sharp-interface theory with interfacial energy and entropy. *Physica D* **91**, 143–181.

Fried, E., Gurtin M. E., 1999. Coherent solid-state phase transitions with atomic diffusion: a thermomechanical treatment. *Journal of Statistical Physics* **95**, 1361–1427.

Fried, E., Gurtin, M. E., 2003. The role of configurational force balance in the nonequilibrium epitaxy of films. *Journal of the Mechanics and Physics of Solids* **51**, 487–517.

Gurtin, M. E., Jabbour, M. E., 2002. Interface evolution in three dimensions with curvature-dependent energy and surface diffusion: Interface-controlled evolution, Phase transitions, epitaxial growt of elastic films. *Archive for Rational Mechanics and Analysis* **163**, 171–208.

Gurtin, M. E., 1988. Multiphase thermomechanics with interfacial structure 1. Heat conduction and the capillary balance law. *Archive for Rational Mechanics and Analysis* **104**, 195–221.

Gurtin, M. E., 1995. The nature of configurational forces. *Archive for Rational Mechanics and Analysis* **131**, 67–100.

Gurtin, M. E., 2000. *Configurational Forces as Basic Concepts of Continuum Physics*. Springer, New York.

Gurtin, M. E., Podio-Guidugli. P., 1996. Configurational forces and the basic laws for crack propagation, *Journal of the Mechanics and Physics of Solids* **44**, 905–927.

Gurtin, M. E., Podio-Guidugli. P., 1998. Configurational forces and a constitutive theory for crack propagation that allows for curving and kinking. *Journal of the Mechanics and Physics of Solids* **46**, 1343–1378.

Gurtin, M. E., Struthers, A., 1990. Multiphase thermomechanics with interfacial structure 3. Evolving phase boundaries in the presence of bulk deformation. *Archive for Rational Mechanics and Analysis* **112**, 97–160.

Gurtin, M. E., Shvartsman, M., 1997. Configurational forces and the dynamics of planar cracks in three-dimensional bodies. *Journal of Elasticity* **48**, 167–191.

Herring, C., 1951. Surface tension as a motivation for sintering. In *The Physics of Powder Metallurgy* (ed. W. E. Kingston), McGraw-Hill, New York.

Maugin, G. A., 2002. *Mathematical Reviews* **2002f:74001**.

Maugin, G. A., 1993. *Material Inhomogeneities in Elasticity*. Chapman and Hall, London.

Peach, M. O., Koehler, J. S., 1950. The forces exerted on dislocations and the stress fields produced by them. *Physical Review* **80**, 436–439.

Podio-Guidugli, P., 2001. Configurational balances via variational arguments. *Interfaces and Free Boundaries* **3**, 223–232.

Podio-Guidugli, P., 2002. Configurational forces: are they needed? *Mechanics Research Communications* **29**, 513–519.

Simha, N. K., Bhattacharya, K., 1998. Kinetics of phase boundaries with edges. *Journal of the Mechanics and Physics of Solids* **46**, 2323–2359.

Taylor, J., Cahn, J. W., Handwerker, C. A.., 1992. Geometrical models of crystal growth. *Acta Metallurgica* **40**, 1443–1474.

Uhuwa, M., 1987. Asymptotic growth shapes developed from two-dimensional nuclei. *Journal of Crystal Growth* **80**, 84–90.

List of Recent TAM Reports

No.	Authors	Title	Date
938	Bagchi, P., and S. Balachandar	Linearly varying ambient flow past a sphere at finite Reynolds number—Part 1: Wake structure and forces in steady straining flow	Apr. 2000
939	Gioia, G., A. DeSimone, M. Ortiz, and A. M. Cuitiño	Folding energetics in thin-film diaphragms—*Proceedings of the Royal Society of London A* **458**, 1223–1229 (2002)	Apr. 2000
940	Chaïeb, S., and G. H. McKinley	Mixing immiscible fluids: Drainage induced cusp formation	May 2000
941	Thoroddsen, S. T., and A. Q. Shen	Granular jets—*Physics of Fluids* **13**, 4–6 (2001)	May 2000
942	Riahi, D. N.	Non-axisymmetric chimney convection in a mushy layer under a high-gravity environment—In *Centrifugal Materials Processing* (L. L. Regel and W. R. Wilcox, eds.), 295–302 (2001)	May 2000
943	Christensen, K. T., S. M. Soloff, and R. J. Adrian	PIV Sleuth: Integrated particle image velocimetry interrogation/validation software	May 2000
944	Wang, J., N. R. Sottos, and R. L. Weaver	Laser induced thin film spallation—*Experimental Mechanics* (submitted)	May 2000
945	Riahi, D. N.	Magnetohydrodynamic effects in high gravity convection during alloy solidification—In *Centrifugal Materials Processing* (L. L. Regel and W. R. Wilcox, eds.), 317–324 (2001)	June 2000
946	Gioia, G., Y. Wang, and A. M. Cuitiño	The energetics of heterogeneous deformation in open-cell solid foams—*Proceedings of the Royal Society of London A* **457**, 1079–1096 (2001)	June 2000
947	Kessler, M. R., and S. R. White	Self-activated healing of delamination damage in woven composites—*Composites A: Applied Science and Manufacturing* **32**, 683–699 (2001)	June 2000
948	Phillips, W. R. C.	On the pseudomomentum and generalized Stokes drift in a spectrum of rotational waves—*Journal of Fluid Mechanics* **430**, 209–229 (2001)	July 2000
949	Hsui, A. T., and D. N. Riahi	Does the Earth's nonuniform gravitational field affect its mantle convection?—*Physics of the Earth and Planetary Interiors* (submitted)	July 2000
950	Phillips, J. W.	Abstract Book, 20th International Congress of Theoretical and Applied Mechanics (27 August – 2 September, 2000, Chicago)	July 2000
951	Vainchtein, D. L., and H. Aref	Morphological transition in compressible foam—*Physics of Fluids* **13**, 2152–2160 (2001)	July 2000
952	Chaïeb, S., E. Sato-Matsuo, and T. Tanaka	Shrinking-induced instabilities in gels	July 2000
953	Riahi, D. N., and A. T. Hsui	A theoretical investigation of high Rayleigh number convection in a nonuniform gravitational field—*International Journal of Pure and Applied Mathematics*, in press (2003)	Aug. 2000
954	Riahi, D. N.	Effects of centrifugal and Coriolis forces on a hydromagnetic chimney convection in a mushy layer—*Journal of Crystal Growth* **226**, 393–405 (2001)	Aug. 2000
955	Fried, E.	An elementary molecular-statistical basis for the Mooney and Rivlin–Saunders theories of rubber-elasticity—*Journal of the Mechanics and Physics of Solids* **50**, 571–582 (2002)	Sept. 2000
956	Phillips, W. R. C.	On an instability to Langmuir circulations and the role of Prandtl and Richardson numbers—*Journal of Fluid Mechanics* **442**, 335–358 (2001)	Sept. 2000
957	Chaïeb, S., and J. Sutin	Growth of myelin figures made of water soluble surfactant—Proceedings of the 1st Annual International IEEE–EMBS Conference on Microtechnologies in Medicine and Biology (October 2000, Lyon, France), 345–348	Oct. 2000
958	Christensen, K. T., and R. J. Adrian	Statistical evidence of hairpin vortex packets in wall turbulence—*Journal of Fluid Mechanics* **431**, 433–443 (2001)	Oct. 2000

List of Recent TAM Reports (cont'd)

No.	*Authors*	*Title*	*Date*
959	Kuznetsov, I. R., and D. S. Stewart	Modeling the thermal expansion boundary layer during the combustion of energetic materials—*Combustion and Flame*, in press (2001)	Oct. 2000
960	Zhang, S., K. J. Hsia, and A. J. Pearlstein	Potential flow model of cavitation-induced interfacial fracture in a confined ductile layer—*Journal of the Mechanics and Physics of Solids*, **50**, 549–569 (2002)	Nov. 2000
961	Sharp, K. V., R. J. Adrian, J. G. Santiago, and J. I. Molho	Liquid flows in microchannels—Chapter 6 of *CRC Handbook of MEMS* (M. Gad-el-Hak, ed.) (2001)	Nov. 2000
962	Harris, J. G.	Rayleigh wave propagation in curved waveguides—*Wave Motion* **36**, 425–441 (2002)	Jan. 2001
963	Dong, F., A. T. Hsui, and D. N. Riahi	A stability analysis and some numerical computations for thermal convection with a variable buoyancy factor—*Journal of Theoretical and Applied Mechanics* **2**, 19–46 (2002)	Jan. 2001
964	Phillips, W. R. C.	Langmuir circulations beneath growing or decaying surface waves—*Journal of Fluid Mechanics* (submitted)	Jan. 2001
965	Bdzil, J. B., D. S. Stewart, and T. L. Jackson	Program burn algorithms based on detonation shock dynamics—*Journal of Computational Physics* (submitted)	Jan. 2001
966	Bagchi, P., and S. Balachandar	Linearly varying ambient flow past a sphere at finite Reynolds number: Part 2—Equation of motion—*Journal of Fluid Mechanics* (submitted)	Feb. 2001
967	Cermelli, P., and E. Fried	The evolution equation for a disclination in a nematic fluid—*Proceedings of the Royal Society A* **458**, 1–20 (2002)	Apr. 2001
968	Riahi, D. N.	Effects of rotation on convection in a porous layer during alloy solidification—Chapter 12 in *Transport Phenomena in Porous Media* (D. B. Ingham and I. Pop, eds.), 316–340 (2002)	Apr. 2001
969	Damljanovic, V., and R. L. Weaver	Elastic waves in cylindrical waveguides of arbitrary cross section—*Journal of Sound and Vibration* (submitted)	May 2001
970	Gioia, G., and A. M. Cuitiño	Two-phase densification of cohesive granular aggregates—*Physical Review Letters* **88**, 204302 (2002) (in extended form and with added co-authors S. Zheng and T. Uribe)	May 2001
971	Subramanian, S. J., and P. Sofronis	Calculation of a constitutive potential for isostatic powder compaction—*International Journal of Mechanical Sciences* (submitted)	June 2001
972	Sofronis, P., and I. M. Robertson	Atomistic scale experimental observations and micromechanical/continuum models for the effect of hydrogen on the mechanical behavior of metals—*Philosophical Magazine* (submitted)	June 2001
973	Pushkin, D. O., and H. Aref	Self-similarity theory of stationary coagulation—*Physics of Fluids* **14**, 694–703 (2002)	July 2001
974	Lian, L., and N. R. Sottos	Stress effects in ferroelectric thin films—*Journal of the Mechanics and Physics of Solids* (submitted)	Aug. 2001
975	Fried, E., and R. E. Todres	Prediction of disclinations in nematic elastomers—*Proceedings of the National Academy of Sciences* **98**, 14773–14777 (2001)	Aug. 2001
976	Fried, E., and V. A. Korchagin	Striping of nematic elastomers—*International Journal of Solids and Structures* **39**, 3451–3467 (2002)	Aug. 2001
977	Riahi, D. N.	On nonlinear convection in mushy layers: Part I. Oscillatory modes of convection—*Journal of Fluid Mechanics* **467**, 331–359 (2002)	Sept. 2001
978	Sofronis, P., I. M. Robertson, Y. Liang, D. F. Teter, and N. Aravas	Recent advances in the study of hydrogen embrittlement at the University of Illinois—Invited paper, Hydrogen–Corrosion Deformation Interactions (Sept. 16–21, 2001, Jackson Lake Lodge, Wyo.)	Sept. 2001
979	Fried, E., M. E. Gurtin, and K. Hutter	A void-based description of compaction and segregation in flowing granular materials—*Proceedings of the Royal Society of London A* (submitted)	Sept. 2001

List of Recent TAM Reports (cont'd)

No.	Authors	Title	Date
980	Adrian, R. J., S. Balachandar, and Z.-C. Liu	Spanwise growth of vortex structure in wall turbulence—*Korean Society of Mechanical Engineers International Journal* **15**, 1741–1749 (2001)	Sept. 2001
981	Adrian, R. J.	Information and the study of turbulence and complex flow—*Japanese Society of Mechanical Engineers Journal B*, in press (2002)	Oct. 2001
982	Adrian, R. J., and Z.-C. Liu	Observation of vortex packets in direct numerical simulation of fully turbulent channel flow—*Journal of Visualization*, in press (2002)	Oct. 2001
983	Fried, E., and R. E. Todres	Disclinated states in nematic elastomers—*Journal of the Mechanics and Physics of Solids* **50**, 2691–2716 (2002)	Oct. 2001
984	Stewart, D. S.	Towards the miniaturization of explosive technology—Proceedings of the 23rd International Conference on Shock Waves (2001)	Oct. 2001
985	Kasimov, A. R., and Stewart, D. S.	Spinning instability of gaseous detonations—*Journal of Fluid Mechanics* (submitted)	Oct. 2001
986	Brown, E. N., N. R. Sottos, and S. R. White	Fracture testing of a self-healing polymer composite—*Experimental Mechanics* (submitted)	Nov. 2001
987	Phillips, W. R. C.	Langmuir circulations—*Surface Waves* (J. C. R. Hunt and S. Sajjadi, eds.), in press (2002)	Nov. 2001
988	Gioia, G., and F. A. Bombardelli	Scaling and similarity in rough channel flows—*Physical Review Letters* **88**, 014501 (2002)	Nov. 2001
989	Riahi, D. N.	On stationary and oscillatory modes of flow instabilities in a rotating porous layer during alloy solidification—*Journal of Porous Media*, in press (2002)	Nov. 2001
990	Okhuysen, B. S., and D. N. Riahi	Effect of Coriolis force on instabilities of liquid and mushy regions during alloy solidification—*Physics of Fluids* (submitted)	Dec. 2001
991	Christensen, K. T., and R. J. Adrian	Measurement of instantaneous Eulerian acceleration fields by particle-image accelerometry: Method and accuracy—*Experimental Fluids* (submitted)	Dec. 2001
992	Liu, M., and K. J. Hsia	Interfacial cracks between piezoelectric and elastic materials under in-plane electric loading—*Journal of the Mechanics and Physics of Solids* **51**, 921–944 (2003)	Dec. 2001
993	Panat, R. P., S. Zhang, and K. J. Hsia	Bond coat surface rumpling in thermal barrier coatings—*Acta Materialia* **51**, 239–249 (2003)	Jan. 2002
994	Aref, H.	A transformation of the point vortex equations—*Physics of Fluids* **14**, 2395–2401 (2002)	Jan. 2002
995	Saif, M. T. A, S. Zhang, A. Haque, and K. J. Hsia	Effect of native Al_2O_3 on the elastic response of nanoscale aluminum films—*Acta Materialia* **50**, 2779–2786 (2002)	Jan. 2002
996	Fried, E., and M. E. Gurtin	A nonequilibrium theory of epitaxial growth that accounts for surface stress and surface diffusion—*Journal of the Mechanics and Physics of Solids*, in press (2002)	Jan. 2002
997	Aref, H.	The development of chaotic advection—*Physics of Fluids* **14**, 1315–1325 (2002); see also *Virtual Journal of Nanoscale Science and Technology*, 11 March 2002	Jan. 2002
998	Christensen, K. T., and R. J. Adrian	The velocity and acceleration signatures of small-scale vortices in turbulent channel flow—*Journal of Turbulence*, in press (2002)	Jan. 2002
999	Riahi, D. N.	Flow instabilities in a horizontal dendrite layer rotating about an inclined axis—*Proceedings of the Royal Society of London A* (submitted)	Feb. 2002
1000	Kessler, M. R., and S. R. White	Cure kinetics of ring-opening metathesis polymerization of dicyclopentadiene—*Journal of Polymer Science A* **40**, 2373–2383 (2002)	Feb. 2002
1001	Dolbow, J. E., E. Fried, and A. Q. Shen	Point defects in nematic gels: The case for hedgehogs—*Proceedings of the National Academy of Sciences* (submitted)	Feb. 2002
1002	Riahi, D. N.	Nonlinear steady convection in rotating mushy layers—*Journal of Fluid Mechanics*, in press (2003)	Mar. 2002

List of Recent TAM Reports (cont'd)

No.	*Authors*	*Title*	*Date*
1003	Carlson, D. E., E. Fried, and S. Sellers	The totality of soft-states in a neo-classical nematic elastomer—*Proceedings of the Royal Society A* (submitted)	Mar. 2002
1004	Fried, E., and R. E. Todres	Normal-stress differences and the detection of disclinations in nematic elastomers—*Journal of Polymer Science B: Polymer Physics* **40**, 2098–2106 (2002)	June 2002
1005	Fried, E., and B. C. Roy	Gravity-induced segregation of cohesionless granular mixtures—*Lecture Notes in Mechanics*, in press (2002)	July 2002
1006	Tomkins, C. D., and R. J. Adrian	Spanwise structure and scale growth in turbulent boundary layers—*Journal of Fluid Mechanics* (submitted)	Aug. 2002
1007	Riahi, D. N.	On nonlinear convection in mushy layers: Part 2. Mixed oscillatory and stationary modes of convection—*Journal of Fluid Mechanics* (submitted)	Sept. 2002
1008	Aref, H., P. K. Newton, M. A. Stremler, T. Tokieda, and D. L. Vainchtein	Vortex crystals—*Advances in Applied Mathematics* **39**, in press (2002)	Oct. 2002
1009	Bagchi, P., and S. Balachandar	Effect of turbulence on the drag and lift of a particle—*Physics of Fluids* (submitted)	Oct. 2002
1010	Zhang, S., R. Panat, and K. J. Hsia	Influence of surface morphology on the adhesive strength of aluminum/epoxy interfaces—*Journal of Adhesion Science and Technology* (submitted)	Oct. 2002
1011	Carlson, D. E., E. Fried, and D. A. Tortorelli	On internal constraints in continuum mechanics—*Journal of Elasticity* (submitted)	Oct. 2002
1012	Boyland, P. L., M. A. Stremler, and H. Aref	Topological fluid mechanics of point vortex motions—*Physica D* **175**, 69–95 (2002)	Oct. 2002
1013	Bhattacharjee, P., and D. N. Riahi	Computational studies of the effect of rotation on convection during protein crystallization—*Journal of Crystal Growth* (submitted)	Feb. 2003
1014	Brown, E. N., M. R. Kessler, N. R. Sottos, and S. R. White	*In situ* poly(urea-formaldehyde) microencapsulation of dicyclopentadiene—*Journal of Microencapsulation* (submitted)	Feb. 2003
1015	Brown, E. N., S. R. White, and N. R. Sottos	Microcapsule induced toughening in a self-healing polymer composite—*Journal of Materials Science* (submitted)	Feb. 2003
1016	Kuznetsov, I. R., and D. S. Stewart	Burning rate of energetic materials with thermal expansion—*Combustion and Flame* (submitted)	Mar. 2003
1017	Dolbow, J., E. Fried, and H. Ji	Chemically induced swelling of hydrogels—*Journal of the Mechanics and Physics of Solids* (submitted)	Mar. 2003
1018	Costello, G. A.	Mechanics of wire rope—Mordica Lecture, Interwire 2003, Wire Association International, Atlanta, Georgia, May 12, 2003	Mar. 2003
1019	Wang, J., N. R. Sottos, and R. L. Weaver	Thin film adhesion measurement by laser induced stress waves—*Journal of the Mechanics and Physics of Solids* (submitted)	Apr. 2003
1020	Bhattacharjee, P., and D. N. Riahi	Effect of rotation on surface tension driven flow during protein crystallization—*Microgravity Science and Technology* (submitted)	Apr. 2003
1021	Fried, E.	The configurational and standard force balances are not always statements of a single law—*Proceedings of the Royal Society* (submitted)	Apr. 2003