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The Nature of Configurational Forces

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Contents

1. Introduction

The standard forces associated with continua arise as a response to the motion of material points. That additional, *configurational*[1] forces may be needed to describe the internal structure of the material is clear from ESHELBY's work on lattice defects[2] and is at least intimated by GIBBS[3] in his discussion of multiphase equilibria. These studies are statical, based on variational arguments, with the configurational forces *defined* as derivatives of the energy. I take a different point of view. Although variational derivations may point the way toward a correct statement of basic laws, such derivations obscure the fundamental nature of balance laws in any general framework that includes dissipation. While I am not in favor of the capricious introduction of "fundamental physical laws", I do believe that *configurational forces should be viewed as basic primitive objects consistent with their own force balance*, rather than as variational constructs.[4]

My objective here is to demonstrate the role of configurational force balances in the study of dynamical phase transitions. In the standard theories of

(i) Stefan-type solidification,
(ii) interface motion neglecting bulk behavior,
(iii) solid-solid phase transitions

an *extra* interface condition — over and above those that follow from standard balance laws — is needed:

- for (i), the extra condition is the classical Stefan condition, temperature equals melting temperature, or a more general relation between temperature, curvature, and normal velocity;
- for (ii), the condition is the motion-by-curvature equation of BURKE & TURNBULL [1952] and MULLINS [1956], or a more general relation of that type;

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[1] I use the adjective "*configurational*" to differentiate these forces from the standard forces, which I refer to as "*deformational*". In the past I used the term "accretive" rather than "configurational", but I now use "accretive" to describe the addition or removal of material.

[2] Cf. [1951, 1970]. ESHELBY [1951] remarks that the idea of a force on a lattice defect goes back to "an interesting paper" of BURTON [1892].

[3] GIBBS's discussion [1878, pp. 314–331] is paraphrased by CAHN [1980] as follows: "solid surfaces can have their physical area changed in two ways, either by creating or destroying surface without changing surface structure and properties per unit area, or by an elastic strain . . . along the surface keeping the number of surface lattice sites constant . . . ." The creation of surface involves configurational forces, while stretching the surface involves more standard deformational forces.

See also NOZIERES [1989, p. 26], who uses the term "chemical" rather than "configurational" and writes: "Such a concept of 'chemical stresses', although somewhat misleading, is often useful in asessing equilibrium shapes."

[4] It is difficult to imagine distinct force systems acting concurrently at each point of a body, which is perhaps why configurational forces have never been more than just variational constructs. Here I am reminded of opposition to the use of standard forces more than half a century after the publication of NEWTON's *Principia*: as TRUESDELL [1966] writes, "D'Alembert spoke of Newtonian forces as 'obscure and metaphysical beings, capable of nothing but spreading darkness over a science clear by itself.'"

- for (iii), (in the absence of interfacial stress) the condition is a kinetic relation of the type proposed by TRUSKINOVSKY [1987, 1991] and ABEYARATNE & KNOWLES [1990, 1991].

There are, I believe, three compelling arguments in support of configurational forces:

(i) Configurational forces provide a conceptual unification, *as each of these extra conditions is a consequence of the configurational force balance applied across the interface.*
(ii) Configurational forces lead to new results, an example being a weak formulation of the supercooled Stefan problem.
(iii) Configurational forces provide a valuable tool in the framing of new theories.[5]

The general configurational force balance upon which I base the theory is[6]

$$\int_{\partial R} \boldsymbol{C}\boldsymbol{m}\, da + \int_{R} \boldsymbol{f}\, da + \int_{\partial \mathscr{G}} \mathbf{C}\mathbf{v}\, ds + \int_{\mathscr{G}} \mathbf{e}\, da = 0, \tag{1.1}$$

with R a control volume that intersects the phase interface, $\boldsymbol{m}$ the outward unit normal to ∂R, $\mathscr{G}$ the portion of the interface in R, and $\mathbf{v}$ the outward unit normal to the boundary curve $\partial\mathscr{G}$ (Figure 1). The configurational fields appearing in (1.1) have the following interpretation: $\boldsymbol{C}$ is a bulk stress that acts in response to the exchange of material at the boundary of R; $\mathbf{C}$, a generalization of surface tension, is a stress within the interface that acts in response to increases in interfacial area as well as to changes in the orientation of the interface; $\mathbf{e}$ represents internal forces distributed over the interface; $\boldsymbol{f}$ represents internal forces distributed over the bulk volume. In the theories discussed here $\boldsymbol{f}$ is generally unimportant, but $\mathbf{e}$ is essential, as it represents dissipative forces associated with the kinetics of the interface.

Configurational forces are irrelevant when discussing defect-free single-phase materials, but their inclusion gives insight into the relation between $\boldsymbol{C}$, the bulk free energy Ψ, the standard bulk deformational-stress $\boldsymbol{S}$, and the deformation gradient $\boldsymbol{F}$. Here, to capture the mechanics associated with the addition and deletion of material points at the boundary of a portion of the body, *I use referential control volumes $R = R(t)$ whose boundaries evolve within the reference configuration.* Their use, which requires generalizations of the basic physical laws, leads to an important expression, $\boldsymbol{C} = \Psi\mathbf{1} - \boldsymbol{F}^T\boldsymbol{S}$, discovered by ESHELBY [1951, 1970]. My derivation of the Eshelby relation is accomplished without recourse to constitutive equations or to a variational principle;[7] the derivation is based on a version of the second law appropriate to a mechanical theory in conjunction with a requirement that this law be invariant under changes in the time-dependent parametrization of $\partial R(t)$.

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[5] Cf. CERMELLI & GURTIN [1994].

[6] GURTIN [1994a, eq. (4.3)]. A less specific version appears in GURTIN [1988, eq. (3.2)] and GURTIN & STRUTHERS [1990, eq. (7.9)], where the balance is applied directly to the interface with the effects of $\boldsymbol{C}$ and $\mathbf{e}$ combined.

[7] And is hence applicable to theories, such as plasticity and viscoelasticity, for which memory effects render variational derivations inappropriate.

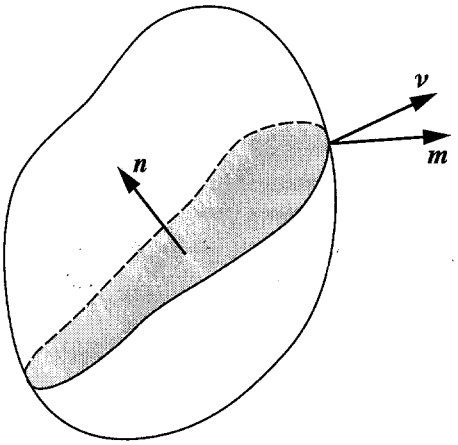

Figure 1. The portion $\mathscr{G}$ (shaded) of the interface contained in the control volume R; $\boldsymbol{m}$ is the outward unit normal to ∂R; $\boldsymbol{n}$ is the unit normal to the interface; $\boldsymbol{v}$ (tangent to the interface) is the outward unit normal to the boundary curve $\partial\mathscr{G}$.

The theories I discuss utilize the method of COLEMAN & NOLL [1963] to restrict constitutive equations. This procedure is based on the premise that the second law be satisfied in all conceivable processes; its rational application requires external fields (heat supplies, body forces, etc.) that ensure satisfaction of the underlying balance laws in all processes. Here, for convenience, I omit all mention of external fields, although the dissipation inequalities I use to reduce constitutive equations are the same as those that would occur were such fields present. I refer the reader to GURTIN [1988, 1993b], ANGENENT & GURTIN [1989], and GURTIN & STRUTHERS [1990] for statements fo the basic laws with external fields.

Notation. I use notation standard in continuum mechanics (cf. GURTIN [1981]). The body B is identified with the region of $\mathbb{R}^3$ it occupies in a fixed reference configuration; terms such as "referential volume" and "undeformed volume" are used interchangeably; $\boldsymbol{X}$ designates an arbitrary material point (point of B); fields Φ are described materially (as functions of $(\boldsymbol{X}, t)$); $\dot{\Phi}$ denotes the material time-derivative of Φ (with respect to t holding $\boldsymbol{X}$ fixed), ∇ and div denote the material gradient and divergence (with respect to $\boldsymbol{X}$ holding t fixed).

2. Variational definition of configurational forces

To better understand the nature of configurational forces, I begin with a standard variational derivation for a coherent two-phase elastic solid, neglecting thermal and compositional variations as well as interfacial energy. I consider a body B whose phases α and β occupy closed complementary subregions B_α and B_β of B, with the interface $\mathscr{S} = B_\alpha \cap B_\beta$ a smooth, oriented surface whose continuous unit normal field $\boldsymbol{n}$ points outward from B_α (Figure 2). A *deformation* $\boldsymbol{y}$ of B is

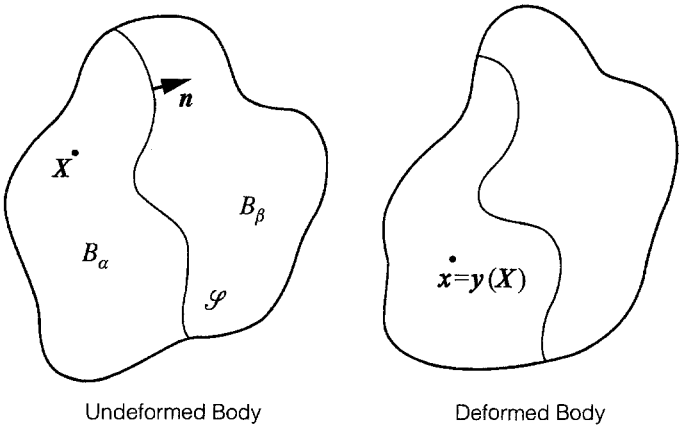

Figure 2. The regions B_α and B_β occupied by the phases α and β in the underformed body.

then a continuous function that assigns to each material point $\boldsymbol{X}$ in B a point $\boldsymbol{x} = \boldsymbol{y}(\boldsymbol{X})$ of space, has *deformation gradient*

$$\boldsymbol{F} = \nabla \boldsymbol{y} \tag{2.1}$$

continuous up to the interface from either side, and has $\det \boldsymbol{F} > 0$.

I restrict attention to deformations $\boldsymbol{y}$ that obey a given boundary condition on ∂B. Then, for equilibrium, the position of the interface and the deformation minimize the total energy

$$E(\mathscr{S},\boldsymbol{y}) = \int_{B_\alpha} \Psi \, dv + \int_{B_\beta} \Psi \, dv, \tag{2.2}$$

where the bulk energy $\psi(\boldsymbol{X})$, per unit volume, is given by constitutive equations

$$\Psi(\boldsymbol{X}) = \Psi_\alpha(\boldsymbol{F}(\boldsymbol{X})) \text{ in } B_\alpha, \quad \Psi(\boldsymbol{X}) = \Psi_\beta(\boldsymbol{F}(\boldsymbol{X})) \text{ in } B_\beta. \tag{2.3}$$

To formally compute the first variation $\delta E(\mathscr{S},\boldsymbol{y})$, which must vanish, the compatibility condition and the identity

$$[\delta \boldsymbol{y}] = -(\delta \mathscr{S})[\mathbf{F}]\boldsymbol{n}, \quad [fg] = \langle f \rangle [g] + \langle g \rangle [f] \tag{2.4}$$

are useful. Here $\delta \boldsymbol{y}$ (with $\delta \boldsymbol{y} = \boldsymbol{0}$ on ∂B) is the variation of $\boldsymbol{y}$; $\delta \mathscr{S}$, a scalar field, is the normal variation of $\mathscr{S}$; $[f]$ denotes the jump in a field f across the interface (limit from β minus that form α); and $\langle f \rangle$ denotes the average of the interfacial limits of f. (Less formally, by considering time-dependent departures $(\mathscr{S}(t),\boldsymbol{y}(t))$ from $(\mathscr{S},\boldsymbol{y})$, the variations $\delta E(\mathscr{S},\boldsymbol{y})$, $\delta \boldsymbol{y}$, and $\delta \mathscr{S}$ may be identified with $E(\mathscr{S},\boldsymbol{y})^{\cdot}$, $\boldsymbol{y}^{\cdot}$, and the normal velocity V of $\mathscr{S}(t)$.) The requirement $\delta E(\mathscr{S},\boldsymbol{y}) = 0$, (2.4), and the divergence theorem yield the expression

$$\int_{B_\alpha} \operatorname{div} \boldsymbol{S}_\alpha \cdot \delta \boldsymbol{y} \, dv + \int_{B_\beta} \operatorname{div} \boldsymbol{S}_\beta \cdot \delta \boldsymbol{y} \, dv + \int_{\mathscr{S}} \{ [\boldsymbol{S}]\boldsymbol{n} \cdot \langle \delta \boldsymbol{y} \rangle + ([\Psi] - \langle \mathbf{Sn} \rangle \cdot [\boldsymbol{F}\boldsymbol{n}]) \delta \mathscr{S} \} \, da = 0, \tag{2.5}$$

where $\boldsymbol{S}(\boldsymbol{X})$ is the bulk stress, here defined as the derivative of the energy:

$$\boldsymbol{S} = \partial_{\boldsymbol{F}} \Psi_\alpha(\boldsymbol{F}) \text{ in } B_\alpha, \quad \boldsymbol{S} = \partial_{\boldsymbol{F}} \Psi_\beta(\boldsymbol{F}) \text{ in } B_\beta. \tag{2.6}$$

Since $\delta \boldsymbol{y}$ can be specified arbitrarily away from $\mathscr{S}$, and since $\langle \delta \mathbf{y} \rangle$ and $\delta \mathscr{S}$ can be specified arbitrarily on $\mathscr{S}$, (2.5) yields the standard equilibrium equations

$$\operatorname{div} \boldsymbol{S} = \boldsymbol{0} \quad \text{in bulk} \tag{2.7}$$

(that is, in B_α and in B_β), the standard force balance

$$[\boldsymbol{S}]\boldsymbol{n} = \boldsymbol{0} \quad \text{on the interface,} \tag{2.8}$$

and an additional condition[8]

$$[\Psi] = [\boldsymbol{F}\boldsymbol{n} \cdot \boldsymbol{S}\boldsymbol{n}] \quad \text{on the interface,} \tag{2.9}$$

often referred to as the Maxwell relation.

Since (2.9) cannot be derived from balance of force alone, this leads to the question of whether the Maxwell relation represents an additional "force balance". In fact it does. To see this, consider the "stress tensor"

$$\boldsymbol{C} = \Psi \boldsymbol{1} - \boldsymbol{F}^T \boldsymbol{S} \tag{2.10}$$

introduced by ESHELBY in his discussion of defects.[9] In terms of the Eshelby tensor, the Maxwell relation has the simple form $\boldsymbol{n} \cdot [\boldsymbol{C}]\boldsymbol{n} = 0$. Further, the continuity of $\boldsymbol{y}$ across the interface implies that $[\boldsymbol{F}]\boldsymbol{t} = 0$ for any vector $\boldsymbol{t}$ tangent to the interface, so that (2.8) yields $\boldsymbol{t} \cdot [\boldsymbol{C}]\boldsymbol{n} = 0$. Thus[10]

$$[\boldsymbol{C}]\boldsymbol{n} = \boldsymbol{0} \quad \text{on the interface,} \tag{2.11}$$

implying continuity of the Eshelby traction across the interface. Further, a computation based on (2.6) and (2.7) yields the conclusion[11]

$$\operatorname{div} \boldsymbol{C} = \boldsymbol{0} \quad \text{in bulk,} \tag{2.12}$$

so that the force system corresponding to the Eshelby tensor satisfies a balance law; in fact, (2.11) and (2.12) together imply the more standard integral balance

$$\int_{\partial R} \boldsymbol{C}\boldsymbol{m}\, da = 0 \tag{2.13}$$

for every subregion R of B, where $\boldsymbol{m}$ is the outward unit normal to ∂R.

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[8] Cf. ESHELBY [1970], ROBIN [1974], LARCHÉ & CAHN [1978], GRINFELD [1981], JAMES [1981], GURTIN [1983].

[9] GRINFELD [1981] refers to $\boldsymbol{C}/\rho$ as a chemical-potential tensor.

[10] Cf. KAGANOVA & ROITBURD [1988].

[11] $\operatorname{div} \boldsymbol{C} = \boldsymbol{0} \Leftrightarrow \operatorname{div} \boldsymbol{S} = \boldsymbol{0}$ in bulk, an equivalence not carried over to the interface conditions (2.8) and (2.11).

I henceforth use the term *deformational balance* for balances such as (2.7) and (2.8) involving the standard (Piola-Kirchhoff) stress $\boldsymbol{S}$, as opposed to the term *configurational balance*, which I reserve for balances of the form (2.13) involving the Eshelby tensor $\boldsymbol{C}$.

This analysis leads to the questions:

- Is there a formulation in which $\boldsymbol{C}$ is a primitive quantity, consistent with a force balance of the type (2.13), and in which the Eshelby relation (2.10) follows as a natural consequence?
- Aside from a possible better understanding of the underlying physics, does the introduction of configurational force lead to new results?

In what follows I attempt to answer these questions.

3. Basic ideas. Configurational forces in a single-phase material[12]

Configurational forces are irrelevant to the theory of single-phase continua without defects, but their study within that context provides essential information regarding their nature.

a. Referential control volumes that evolve with time

Let B be a single-phase body, and let $\boldsymbol{y}$ be a motion of B, so that $\boldsymbol{y}(\boldsymbol{X},t)$ is a deformation for each fixed t, with deformation gradient $\boldsymbol{F}(\boldsymbol{X},t)$ and material velocity $\boldsymbol{y}^{\cdot}(\boldsymbol{X},t)$ smooth functions.

As is standard, I formulate balance laws using referential control volumes (subregions of B). But as is not standard, I capture the mechanics associated with the addition and deletion of material points at the boundary of a portion of the body by using *referential control volumes whose boundaries evolve within the reference configuration.* Given such a control volume $R(t)$, I write $\mathscr{V}(\boldsymbol{X},t)$ for the normal velocity of $\partial R(t)$ in the direction of the outward unit normal $\boldsymbol{m}(\boldsymbol{X},t)$. Then for $\Phi(\boldsymbol{X},t)$ a smooth field,

$$\frac{d}{dt}\left\{\int_R \Phi\right\} = \int_R \Phi^{\cdot}\, dv + \int_{\partial R} \Phi \mathscr{V}\, da, \tag{3.1}$$

where

$$\frac{d}{dt}\left\{\int_R \Phi\, dv\right\} \quad \text{denotes} \quad \frac{d}{dt}\left\{\int_{R(t)} \Phi(\boldsymbol{X},t)\, dv(\boldsymbol{X})\right\}. \tag{3.2}$$

The evolving surface $\partial R(t)$ may be parametrized in a sufficiently small time interval and in a neighborhood of any of its points by a function of the form

[12] GURTIN [1994a].

$\boldsymbol{X} = \hat{\boldsymbol{X}}(u_1, u_2, t)$; the field

$$\upsilon(\boldsymbol{X}, t) = \frac{\partial \hat{\boldsymbol{X}}(u_1, u_2, t)}{\partial t} \tag{3.3}$$

then represents a velocity field for $\partial R(t)$ in that neighborhood. It is possible to use such parametrizations to construct a *velocity field* υ for ∂R; that is, a smooth field $\upsilon(\boldsymbol{X}, t)$ defined for all $\boldsymbol{X}$ on $\partial R(t)$ and *all* t in any (sufficiently small) time interval. A field υ so constructed depends on the choice of local parametrizations, but its normal component is intrinsic:

$$\upsilon \cdot \boldsymbol{m} = \mathscr{V}. \tag{3.4}$$

Under the motion $\boldsymbol{y}$, $R(t)$ deforms to a region $\mathscr{R}(t) = \boldsymbol{y}(R(t), t)$, and each local parametrization $\boldsymbol{X} = \hat{\boldsymbol{X}}(u_1, u_2, t)$ induces a corresponding local parametrization $\boldsymbol{x} = \hat{\boldsymbol{x}}(u_1, u_2, t) = \boldsymbol{y}(\hat{\boldsymbol{X}}(u_1, u_2, t), t)$ for $\partial \mathscr{R}(t)$; the corresponding velocity field

$$\bar{\upsilon}(X, t) = \frac{\partial \hat{\boldsymbol{x}}(u_1, u_2, t)}{\partial t} \tag{3.5}$$

for $\partial \mathscr{R}(t)$ is related to υ through the relation

$$\bar{\upsilon} = \boldsymbol{y}^{\cdot} + \boldsymbol{F}\upsilon; \tag{3.6}$$

$\bar{\upsilon}$ is referred to as the *velocity field for* $\partial \mathscr{R}$ *induced by* υ (Figure 3).

b. *Classical deformational forces. Mechanical version of the second law*

Let $\boldsymbol{S}$ denote the standard stress that arises in response to deformation, with $\boldsymbol{S}$ measured per unit referential area, and let ρ denote the reference density. Then,

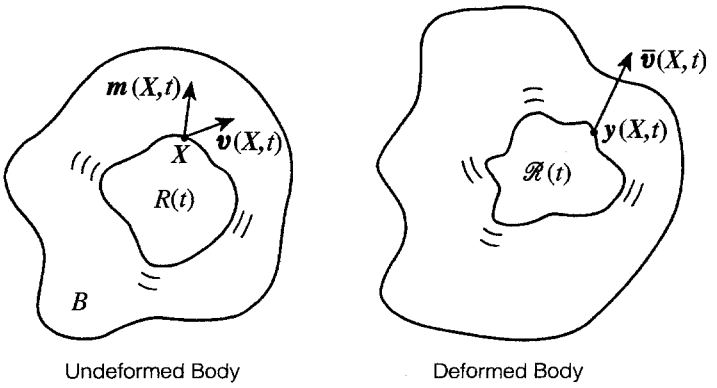

Figure 3. The time-dependent control volume $R(t)$, which deforms to $\mathscr{R}(t)$, with $\upsilon(\mathbf{X}, t)$ a velocity field for $\partial R(t)$ and $\bar{\upsilon}(\mathbf{X}, t)$ a corresponding velocity field for $\partial \mathscr{R}(t)$.

representing inertia through the body force

$$\boldsymbol{b} = -\rho \boldsymbol{y}^{\cdot\cdot}, \tag{3.7}$$

but neglecting other external forces, I write the standard balance laws for forces and moments in the form

$$\int_{\partial R} \boldsymbol{S}\boldsymbol{m}\, da + \int_R \boldsymbol{b}\, dv = \boldsymbol{0}, \quad \int_{\partial R} \boldsymbol{y} \times \boldsymbol{S}\boldsymbol{m}\, da + \int_R \boldsymbol{y} \times \boldsymbol{b}\, dv = \boldsymbol{0} \tag{3.8}$$

for each referential control volume R, with $\boldsymbol{m}$ the outward unit normal to ∂R. Since R is arbitrary, a standard argument[13] yields the local relations

$$\operatorname{div} \boldsymbol{S} + \boldsymbol{b} = \boldsymbol{0}, \quad \boldsymbol{S}\boldsymbol{F}^T = \boldsymbol{F}\boldsymbol{S}^T. \tag{3.9}$$

In the absence of thermal and compositional effects the classical theory may be based on a "second law" that utilizes time-independent control volumes R and has the form[14]

$$\frac{d}{dt}\left\{\int_R \Psi\, dv\right\} \leqq \int_{\partial R} \boldsymbol{S}\boldsymbol{m} \cdot \boldsymbol{y}^{\cdot}\, da + \int_R \boldsymbol{b} \cdot \boldsymbol{y}^{\cdot}\, dv \tag{3.10}$$

with Ψ the *free energy*, per unit referential volume. For an *evolving* control volume $R(t)$ the standard generalization of (3.10) would include the term

$$\text{energy flow} = \int_{\partial R} \Psi \mathscr{V}\, da \tag{3.11}$$

on the right side. My discussion of configurational forces will be based on what I believe to be a more fundamental version of the second law.

c. Configurational stress. A version of the second law that accounts for accretion

I consider the dependence of $R(t)$ on t as representing the addition of material to — or the removal of material from — the boundary $\partial R(t)$. A standard precept of continuum mechanics is that when writing basic laws for $R(t)$ the material outside of $R(t)$ may be accounted for by the action of forces on $\partial R(t)$. I believe that — consistent with this — an accounting of the work required to add or remove material precludes an (explicit) accounting of the flow of energy into $R(t)$. In this spirit I base the mechanical theory on a "second law" of the form

$$\frac{d}{dt}\{\text{energy of } R(t)\} \leqq \{\text{rate at which work is performed on } R(t)\}. \tag{3.12}$$

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[13] Cf. e.g., GURTIN [1981, p. 179].

[14] (3.10) (with Ψ the free energy) follows from standard statements of the first two laws (cf. GURTIN [1991]).

The view expressed above requires a careful treatment of the kinematics and mechanics of *accretion*, the term I use to describe the addition and removal of material. Kinematically, accretion is independent of the motion $\boldsymbol{y}$, and since independent kinematical processes generally give rise to independent force systems, it seems reasonable to introduce additional forces that perform work during accretion. I therefore consider a tensor field $\boldsymbol{C}$, the *configurational stress*, whose working accompanies the evolution of ∂R. More precisely, I choose local parametrizations $\boldsymbol{X} = \hat{\boldsymbol{X}}(u_1, u_2, t)$ for $\partial R(t)$, define a velocity field v for ∂R through (3.3), and assume that $\boldsymbol{C}\boldsymbol{m} \cdot v$ represents the corresponding working, per unit area.

The working of the deformational stress $\boldsymbol{S}$ must also be taken into account. The motion of the deformed boundary $\partial \mathscr{R}(t) = \boldsymbol{y}(\partial R(t), t)$ — for R independent of time — is described by the material velocity $\boldsymbol{y}^{\cdot}$, and $\boldsymbol{S}\boldsymbol{m} \cdot \boldsymbol{y}^{\cdot}$ gives the required working. But when $R(t)$ depends on t, there is no intrinsic material description of $\partial \mathscr{R}(t)$, as material is continually being added and removed, and it would seem appropriate to use, as a velocity for $\partial \mathscr{R}(t)$, the derivative $\bar{v}(\boldsymbol{X}, t)$ of $\boldsymbol{y}(\hat{\boldsymbol{X}}(u_1, u_2, t), t)$ with respect to t holding the surface parameters (u_1, u_2) fixed; for that reason I write the working of $\boldsymbol{S}$ in the form $\boldsymbol{S}\boldsymbol{m} \cdot \bar{v}$.

I therefore take as an appropriate form of the second law the inequality

$$\frac{d}{dt}\left\{\int_R \Psi \, dv\right\} \leqq \int_{\partial R} (\boldsymbol{S}\boldsymbol{m} \cdot \bar{v} + \boldsymbol{C}\boldsymbol{m} \cdot v) \, da + \int_R \boldsymbol{b} \cdot \boldsymbol{y}^{\cdot} \, dv \tag{3.13}$$

with v a velocity field for $\partial R = \partial R(t)$ and $\bar{v}$ the corresponding induced velocity field for $\partial \mathscr{R}$. (Note that the deformational working $\boldsymbol{S}\boldsymbol{m} \cdot \bar{v}$ is a classical term $\boldsymbol{S}\boldsymbol{m} \cdot \boldsymbol{y}^{\cdot}$ plus a term $\boldsymbol{S}\boldsymbol{m} \cdot \boldsymbol{F}v$ that accounts for the addition of deformed material to ∂R.) To ensure that the resulting theory be independent of local parametrizations, I require that (3.13) hold for any choice of the velocity field v for ∂R. This requirement of *invariance under reparametrization* has important consequences.

d. Bulk tension. Derivation of the Eshelby relation

Invariance of (3.13) under reparametrization is equivalent to invariance of the *working*

$$\mathscr{W}(R) = \int_{\partial R} (\boldsymbol{S}\boldsymbol{m} \cdot \bar{v} + \boldsymbol{C}\boldsymbol{m} \cdot v) \, da + \int_R \boldsymbol{b} \cdot \boldsymbol{y}^{\cdot} \, dv \tag{3.14}$$

$$= \int_{\partial R} \{\boldsymbol{S}\boldsymbol{m} \cdot \boldsymbol{y}^{\cdot} + (\boldsymbol{F}^T\boldsymbol{S}\boldsymbol{m} + \boldsymbol{C}\boldsymbol{m}) \cdot v\} \, da + \int_R \boldsymbol{b} \cdot \boldsymbol{y}^{\cdot} \, dv. \tag{3.15}$$

Because of (3.4), changes in parametrization affect the tangential component of v, but leave the normal component unaltered. In fact, invariance of (3.15) under reparametrization is equivalent to the requirement that $(\boldsymbol{F}^T\boldsymbol{S}\boldsymbol{m} + \boldsymbol{C}\boldsymbol{m}) \cdot \boldsymbol{t} = 0$ on ∂R for all tangential vector fields $\boldsymbol{t}$ on ∂R; thus, since R is arbitrary, $(\boldsymbol{F}^T\boldsymbol{S} + \boldsymbol{C})\boldsymbol{m}$ must be parallel to $\boldsymbol{m}$ for all $\boldsymbol{m}$, so that

$$\boldsymbol{C} + \boldsymbol{F}^T\boldsymbol{S} = \pi \boldsymbol{1} \tag{3.16}$$

and, by (3.4), the working has the intrinsic form

$$\mathscr{W}(R) = \int_{\partial R} \boldsymbol{Sm}\cdot\boldsymbol{y}^{\cdot}\, da + \int_{R} \boldsymbol{b}\cdot\boldsymbol{y}^{\cdot}\, dv + \int_{\partial R} \pi\mathscr{V}\, da. \tag{3.17}$$

The scalar field π is a *bulk tension* that works to increase the volume of R through the addition of material at its boundary. If we refer to the final term in (3.17) as the *configurational working*, then (3.17) may be written more suggestively as

$$\{\text{working}\} = \{\text{mechanical working}\} + \{\text{configurational working}\}. \tag{3.18}$$

Note that the configurational working $\pi\mathscr{V}$ is not due solely to the action of the configurational stress $\boldsymbol{C}$; the deformational stress contributes also through the term $(\boldsymbol{Sm}\cdot\boldsymbol{Fm})\mathscr{V}$.

My next step is to relate π to the free energy Ψ. Using (3.1) and (3.17), I write the inequality (3.13) as

$$\int_{R} \Psi^{\cdot}\, dv \leqq \int_{\partial R} \{\boldsymbol{Sm}\cdot\boldsymbol{y}^{\cdot} + (\pi - \Psi)\mathscr{V}\}\, da + \int_{R} \boldsymbol{b}\cdot\boldsymbol{y}^{\cdot}\, dv. \tag{3.19}$$

Given a time τ, it is possible to find a second referential control volume $R'(t)$ with $R'(\tau) = R(\tau)$, but with $\mathscr{V}'(\boldsymbol{X}, \tau)$, the normal velocity of $\partial R'(\tau)$, an *arbitrary* scalar field on $\partial R'(\tau)$; satisfaction of (3.19) for all such $\mathscr{V}'$ implies

$$\pi = \Psi. \tag{3.20}$$

Bulk tension therefore coincides with bulk free-energy, a result analogous to the coincidence of surface tension and surface free-energy; but what is more important, (3.16) and (3.20) yield the Eshelby relation

$$\boldsymbol{C} = \Psi\boldsymbol{1} - \boldsymbol{F}^{T}\boldsymbol{S}. \tag{3.21}$$

This derivation of the Eshelby relation was accomplished without recourse to constitutive equations or to a variational principle; the derivation was based on a version of the second law appropriate to referential control volumes whose boundaries evolve with time. This observation is not simply of pedagogical interest; it establishes the Eshelby relation as appropriate to theories, such as plasticity and viscoelasticity, for which memory effects render variational derivations inappropriate.

The result (3.16) is a consequence of the invariance of $\mathscr{W}(R)$ under reparametrization; it is independent of the particular form chosen for the second law and is hence more basic than (3.21). In fact, the identification of π with a "grand canonical potential" such as the free energy depends on whether or not there are associated transport processes; (3.16) is independent of such considerations.

Finally, in the notation of (3.11) and (3.18),

$$\{\text{configurational working}\} = \{\text{energy flow}\}, \tag{3.22}$$

at least in this purely mechanical context, establishing consistency of the "second law" (3.13) with the more standard inequality (3.10) modified by (3.11).

e. The configurational force balance

In addition to the configurational stress $\boldsymbol{C}$, I allow for *internal configurational (body) forces* $\boldsymbol{f}$, which, being internal, contribute neither to the working (3.14) nor to the "second law" (3.13). As a second point of departure from the classical theory, I postulate a *configurational force balance*

$$\int_{\partial R} \boldsymbol{C}\boldsymbol{m}\, da + \int_R \boldsymbol{f}\, dv = \boldsymbol{0} \tag{3.23}$$

for each R, or equivalently,

$$\operatorname{div} \boldsymbol{C} + \boldsymbol{f} = \boldsymbol{0}. \tag{3.24}$$

$\boldsymbol{C}$ performs work when material is added to R through the motion of ∂R. Material is neither added nor removed from the interior of R. In fact, each material point $\boldsymbol{X}$ is constrained to a given position in the reference configuration for all time. Consequently, the force $\boldsymbol{f}$, which acts interior to R, performs no work (an observation consistent with its omission from (3.14)). I therefore consider $\boldsymbol{f}$ to be *indeterminate*,[15] in fact, as defined by the configurational balance (3.24).

Assume, for the moment, that the material is *elastic* and *homogeneous* with constitutive equations giving the stress $\boldsymbol{S}$ as the derivative of the free energy Ψ:

$$\Psi = \hat{\Psi}(\boldsymbol{F}), \quad \boldsymbol{S} = \partial_{\boldsymbol{F}} \hat{\Psi}(\boldsymbol{F}). \tag{3.25}$$

Then (3.21) yields an auxiliary relation giving $\boldsymbol{C}$ as a function of $\boldsymbol{F}$, and (3.9), (3.21), (3.24), and (3.25) yield $\boldsymbol{f} = \boldsymbol{F}^T \boldsymbol{b}$. If $\boldsymbol{b} = \boldsymbol{0}$ (equilibrium), then the internal configurational force vanishes. This is a direct consequence of *homogeneity*; for an *inhomogeneous* material with energy $\hat{\Psi}(\boldsymbol{F},\boldsymbol{X})$ and stress $\boldsymbol{S} = \partial_{\boldsymbol{F}} \hat{\Psi}(\boldsymbol{F},\boldsymbol{X})$,

$$\boldsymbol{f} = -\partial_{\boldsymbol{X}} \hat{\Psi} \tag{3.26}$$

and internal configurational forces are present (even though $\boldsymbol{b} = \boldsymbol{0}$). A one-dimensional cartoon giving an intuitive description of the configurational force system for homogeneous and inhomogeneous reference configurations is given in Figure 4.

Thus *for a single-phase elastic material the theory is equivalent to the classical theory* based on (3.9) with (3.24) and (3.21) considered as defining relations for $\boldsymbol{f}$ and $\boldsymbol{C}$; configurational forces play no role. On the other hand, for a two-phase system configurational forces play a pivotal role in the evolution of the *interface*, since it is at the interface that the material structure undergoes change.

In subsequent sections I demonstrate the role played by configurational forces in the study of evolving phase interfaces. But this does not seem the only circumstance in which this concept could be useful: configurational forces might form a basis for the systematic study of time-dependent defect structures such as dislocations and cracks.[16].

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[15] That is, not specified constitutively (cf. TRUESDELL & NOLL [1965, p. 70]).

[16] An idea due to PAOLO PODIO-GUIDUGLI (private communication).

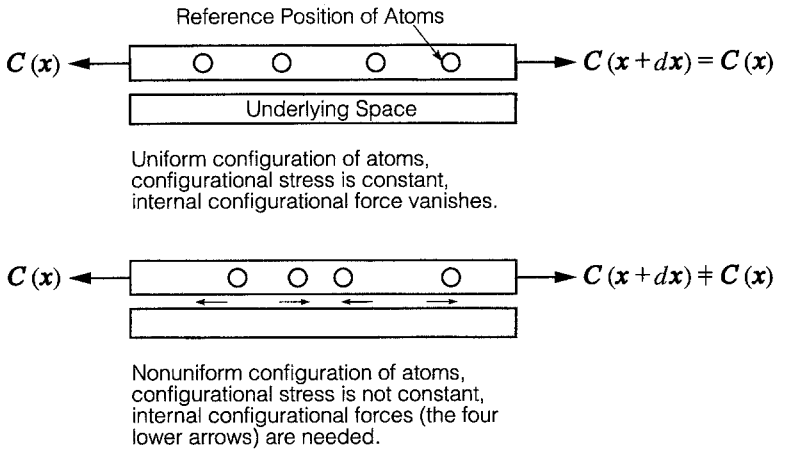

Figure 4. Cartoon showing why internal configurational forces respond to the inhomogeniety of the reference configuration.

4. Configurational forces for an evolving interface, neglecting bulk behavior

There are situations of physical interest in which the motion of a phase interface is effectively independent of deformational and transport processes in the bulk material;[17] here the underlying balance law is a configurational balance for the interface. I now turn toward a characterization of such situations.

a. Configurational force balance. Working

I consider two phases separated by a smoothly evolving surface $\mathscr{S}(t)$. I assume that $\mathscr{S}$ is oriented by a choice of unit normal field $\boldsymbol{n}$ and write V for the normal velocity, $\mathbf{L}$ for the curvature tensor, K for the total curvature (twice the mean curvature), and $\nabla_{\mathscr{S}}$ and $\mathrm{div}_{\mathscr{S}}$ for the surface gradient and surface divergence. (Cf. the Appendix for a discussion of evolving surfaces.)

I restrict attention to a configurational force system described by the fields:

$\boldsymbol{C}$ *bulk stress*
$\mathbf{C}$ *surface stress*
$\boldsymbol{f}$ *internal bulk force*
$\mathbf{e}$ *internal surface force*

$\boldsymbol{C}$ and $\boldsymbol{f}$ are as discussed in Section 3. The superficial vector field $\mathbf{e}$ represents internal forces distributed over the interface, while $\mathbf{C}$, a superficial tensor field on

[17] Cf. the Introduction of TAYLOR, CAHN & HANDWERKER [1992].

$\mathscr{S}$, generalizes surface tension. Given a referential control volume $R(t)$, let

$$\mathscr{G}(t) = \mathscr{S}(t) \cap R(t)$$

denote the portion of the interface in $R(t)$ with $\boldsymbol{v}(\boldsymbol{X}, t)$ (a tangential field on $\mathscr{S}(t)$) the outward unit normal to $\partial\mathscr{G}(t)$ (Figure 1); then $\mathbf{C}\boldsymbol{v}$ represents configurational forces within the interface applied to R across $\partial\mathscr{G}$.

The *configurational force balance* now takes the form

$$\int_{\partial R} \boldsymbol{C}\boldsymbol{m}\, da + \int_{R} \boldsymbol{f}\, da + \int_{\partial\mathscr{G}} \mathbf{C}\boldsymbol{v}\, ds + \int_{\mathscr{G}} \mathbf{e}\, da = 0, \tag{4.1}$$

with $R(t)$ a control volume and $\boldsymbol{m}$ the outward unit normal to ∂R. Shrinking R to the interface gives

$$\int_{\mathscr{G}} ([\boldsymbol{C}]\boldsymbol{n} + \mathbf{e})\, da + \int_{\partial\mathscr{G}} \mathbf{C}\boldsymbol{v}\, ds = \mathbf{0},$$

which, by virtue of the surface divergence theorem (A9), yields the *interfacial force balance*

$$[\boldsymbol{C}]\boldsymbol{n} + \mathbf{e} + \operatorname{div}_{\mathscr{S}} \mathbf{C} = \mathbf{0}. \tag{4.2}$$

On the other hand, restricting attention to R in (4.1) that do not interest the interface yields the bulk relation (3.24).

The motion of the curve $\partial\mathscr{G}(t)$ is characterized intrinsically by the velocity field $V\boldsymbol{n} + V_{\partial\mathscr{G}}\mathbf{v}$, where $V_{\partial\mathscr{G}}$, the tangential edge velocity of $\mathscr{G}$, is the velocity of $\partial\mathscr{G}$ in the direction of the normal $\mathbf{v}$. Alternatively, $\partial\mathscr{G}(t)$ may be parametrized locally by functions $\boldsymbol{X} = \boldsymbol{r}(u, t)$, which may be used to generate a *velocity field*

$$\boldsymbol{w}(\boldsymbol{X}, t) = \frac{\partial \boldsymbol{r}(u, t)}{\partial t} \tag{4.3}$$

for $\partial\mathscr{G}(t)$. Then

$$\boldsymbol{w} \cdot \boldsymbol{n} = V, \quad \boldsymbol{w} \cdot \boldsymbol{v} = V_{\partial\mathscr{G}}, \tag{4.4}$$

but the component of $\boldsymbol{w}$ tangent to $\partial\mathscr{G}$ depends on the choice of local parametrizations.

Guided by the discussion leading to (3.14), I define the working $\mathscr{W}(R)$ by

$$\mathscr{W}(R) = \int_{\partial R} \boldsymbol{C}\boldsymbol{m} \cdot \boldsymbol{v}\, da + \int_{\partial\mathscr{G}} \mathbf{C}\boldsymbol{v} \cdot \boldsymbol{w}\, ds, \tag{4.5}$$

with the stipulation that $\mathscr{W}(R)$ *be independent of the particular local parametrizations* $\boldsymbol{X} = \hat{\boldsymbol{X}}(u_1, u_2, t)$ *and* $\boldsymbol{X} = \boldsymbol{r}(u, t)$ *used to determine the velocity fields* $\boldsymbol{v}(\boldsymbol{X}, t)$ *and* $\boldsymbol{w}(\boldsymbol{X}, t)$ *for* $\partial R(t)$ *and* $\partial\mathscr{G}(t)$. The argument leading to (3.16) then reduces $\boldsymbol{C}$ to a bulk tension:

$$\boldsymbol{C} = \pi \mathbf{1}. \tag{4.6}$$

Invariance under changes in parametrization for $\partial\mathscr{G}(t)$ has an equally stringent consequence. Because of (4.4), such changes effect the component of $\boldsymbol{w}$ tangential to $\partial\mathscr{G}$, but leave $\boldsymbol{w}$ otherwise unaltered. In fact, invariance of $\mathscr{W}(R)$ under changes in parametrization for $\partial\mathscr{G}$ is equivalent to the requirement that

$$\int_{\partial\mathscr{G}} \mathbf{C}\boldsymbol{v}\cdot\boldsymbol{t}\,ds = 0 \tag{4.7}$$

for every vector field $\boldsymbol{t}$ tangential to $\partial\mathscr{G}$. Since R and hence $\partial\mathscr{G}$ are arbitrary, it follows[18] that the tangential part of $\mathbf{C}$ is a surface tension:

$$\mathbf{C}_{\tan} = \sigma\boldsymbol{P} \tag{4.8}$$

(cf. (A3)) with σ the *surface tension*. Thus, by (A4),

$$\mathbf{C} = \sigma\boldsymbol{P} + \boldsymbol{n}\otimes\mathbf{c}, \tag{4.9}$$

where $\mathbf{c}$, the *surface shear*, is a tangential vector field that represents forces within $\mathscr{S}$ whose action is normal to $\mathscr{S}$.[19]

A computation, based on (A1), (A7), (A8), and (4.9), yields

$$\operatorname{div}_{\mathscr{S}}\mathbf{C} = (\sigma K + \operatorname{div}_{\mathscr{S}}\mathbf{c})\boldsymbol{n} + \nabla_{\mathscr{S}}\sigma - \mathbf{L}\mathbf{c}, \tag{4.10}$$

and since $\nabla_{\mathscr{S}}\sigma$ and $\mathbf{L}\mathbf{c}$ are tangential, (4.2) and (4.6) yield the *normal force balance*

$$\sigma K + \operatorname{div}_{\mathscr{S}}\mathbf{c} + [\![\pi]\!] + e = 0 \tag{4.11}$$

with

$$e = \mathbf{e}\cdot\boldsymbol{n} \tag{4.12}$$

the *normal internal force*.

Next, by (3.4), (4.4), (4.5), (4.6), and (4.9),

$$\mathscr{W}(R) = \int_{\partial\mathscr{G}} (\sigma V_{\partial\mathscr{G}} + V\mathbf{c}\cdot\boldsymbol{v})\,ds + \int_{\partial R} \pi\mathscr{V}\,da, \tag{4.13}$$

and hence (A9), (A10), and (4.11) yield[20]

$$\mathscr{W}(R) = -\int_{\mathscr{G}} \{\sigma K V + \mathbf{c}\cdot\boldsymbol{n}^{\circ} + ([\![\pi]\!] + e)V\}\,ds + \int_{\partial\mathscr{G}} \sigma V_{\partial\mathscr{G}}\,ds + \int_{\partial R} \pi\mathscr{V}\,da, \tag{4.14}$$

---

[18] GURTIN & STRUTHERS [1990, eq. (7.4)].

[19] GURTIN & STRUTHERS [1990, eq. (7.5)] (cf. GURTIN [1988]). For statics an essentially equivalent relation was derived by HERRING [1951], HOFFMAN & CAHN [1972], and CAHN & HOFFMAN [1974] by using variational arguments based on a constitutive equation $\psi = \hat{\psi}(\boldsymbol{n})$ for the interfacial energy, with σ and $\mathbf{c}$ defined by (4.19) and (4.22). The derivation given above is independent of constitutive equations.

[20] GURTIN [1988], GURTIN & STRUTHERS [1990].

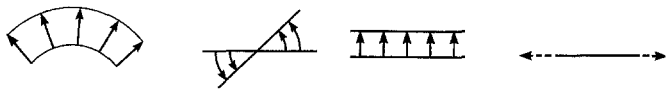

Figure 5. Contributions to the working at a phase interface.

where $(\ldots)^{\circ}$ denotes the time derivative following the normal trajectories of the interface. The right side of this relation catalogs the manner in which configurational forces perform work (Figure 5):

- The surface tension σ works to increase the area of $\mathscr{G}$: at internal points through $-\sigma KV$, at its boundary through $\sigma V_{\partial\mathscr{G}}$.
- The surface shear $\mathbf{c}$ works to change the orientation of $\mathscr{G}$.
- The jump $[\pi]$ in bulk tension and the normal internal force e work to advance the interface.
- The bulk tension works over ∂R to increase the volume of R.

Note that there is no expenditure of work associated with "tangential motion" of the interface (cf. the paragraph following (3.24)). Consistent with a "constraint" of this type, I leave as *indeterminate* the tangential component $\boldsymbol{Pe}$ of the internal force, an assumption that allows me to restrict attention to the normal balance (4.11).

b. The second law neglecting variations in temperature and composition

As before, I allow for a *bulk free-energy* Ψ, but, in accord with the physical assumptions underlying the current development, I assume that Ψ is constant in each phase and write

$$U = [\Psi] \ (= \text{constant}). \tag{4.15}$$

In addition, I now allow for an *interfacial free-energy* $\psi(\boldsymbol{X},t)$, per unit area, and write the second law in the form (3.12):

$$\frac{d}{dt}\left\{\int_R \Psi\, dv + \int_{\mathscr{G}} \psi\, ds\right\} \leqq \mathscr{W}(R) \tag{4.16}$$

for every evolving control volume $R(t)$, with $\mathscr{G}(t) = \mathscr{S}(t)\cap R(t)$.

The argument leading to (3.20) is valid here also. Further, by (4.15),

$$\frac{d}{dt}\left\{\int_R \Psi\, dv\right\} = -\int_{\mathscr{G}} UV\, da + \int_{\partial R} \Psi\mathscr{V}\, da, \tag{4.17}$$

so that, by (3.20), (4.14), and (A13), (4.16) becomes

$$\int_{\mathscr{G}} (\psi^\circ - \psi KV)\, da + \int_{\partial\mathscr{G}} \psi V_{\partial\mathscr{G}}\, ds \leqq -\int_{\mathscr{G}} \{\sigma KV + \mathbf{c}\cdot\boldsymbol{n}^\circ + Ve\}\, ds + \int_{\partial\mathscr{G}} \sigma V_{\partial\mathscr{G}}\, ds. \quad (4.18)$$

Given a time τ, it is possible to find a second referential control volume $R'(t)$ with $R'(\tau) = R(\tau)$, but with $V_{\partial\mathscr{G}'}(\boldsymbol{X}, \tau)$, the normal velocity of $\partial\mathscr{G}'(\tau)$, an *arbitrary* scalar field on $\partial\mathscr{G}'(\tau)$; satisfaction of (4.18) for all such $V_{\partial\mathscr{G}'}$ implies

$$\sigma = \psi \quad (4.19)$$

and the surface tension and surface free-energy coincide.[21] Thus, since $\mathscr{G}$ is arbitrary, what remains is the *interfacial dissipation inequality*

$$\psi^\circ + \mathbf{c}\cdot\boldsymbol{n}^\circ + eV \leqq 0. \quad (4.20)$$

At this point it is worth noting the similarities between the bulk tension π and the surface tension σ:

- Bulk tension works to increase the volume of bulk material, surface tension works to increase the area of the interface.
- The configurational stresses $\boldsymbol{C} = \pi\mathbf{1}$ and $\mathbf{C}_{\tan} = \sigma\boldsymbol{P}$ have isotropic forms; these are not consequences of material symmetry, but follow instead from invariance under reparametrization.
- Both π and σ are related to energy: π to bulk free-energy, σ to interfacial free-energy.

c. Constitutive equations

Guided by the dissipation inequality (4.20), I consider constitutive equations for the interface giving the free energy ψ, the surface shear $\mathbf{c}$, and the normal internal force e as functions of the orientation $\boldsymbol{n}$ and the normal velocity V:

$$\psi = \hat{\psi}(\boldsymbol{n}, V), \quad \mathbf{c} = \hat{\mathbf{c}}(\boldsymbol{n}, V), \quad e = \hat{e}(\boldsymbol{n}, V). \quad (4.21)$$

I view the second law as a restriction on constitutive relations;[22] more precisely, granted (4.21), I require that the dissipation inequality (4.20) be satisfied in all motions of the interface:

$$\partial_V \hat{\psi}(\boldsymbol{n}, V) V^\circ + \{\partial_{\boldsymbol{n}} \hat{\psi}(\boldsymbol{n}, V) + \hat{\mathbf{c}}(\boldsymbol{n}, V)\}\cdot\boldsymbol{n}^\circ + \hat{e}(\boldsymbol{n}, V) V \leqq 0$$

---

[21] GURTIN & STRUTHERS [1990] (cf. GURTIN [1991]).

[22] This use of the second law is due to COLEMAN & NOLL [1963], who study single-phase thermoelastic materials; the extension to two-phase materials is given by GURTIN [1988] (cf. ANGENENT & GURTIN [1989], GURTIN [1993a]). An interesting feature of this procedure is that the local dissipation inequality generally suggests which fields should be given constitutive descriptions, a use of the second law that seems to lead — in all classical continuum theories — to the "correct" set of constitutive variables. This contrasts the standard formalism of studying balance laws to see where a lack of field equations may be compensated for by the introduction of constitutive relations.

in all such motions. It is possible to construct a motion of the interface for which $\boldsymbol{n}$, $\boldsymbol{n}^\circ$, V, and V° have arbitrarily assigned values at some given point and time, an observation that leads to the following constitutive restrictions: the free energy must be independent of the velocity V; the shear must be the negative of the derivative of the energy with respect to $\boldsymbol{n}$,

$$\mathbf{c} = -\partial_n \hat{\psi}(\boldsymbol{n}); \tag{4.22}$$

the relation $e = \hat{e}(\boldsymbol{n}, V)$ for the normal internal force must have the form

$$e = -b(\boldsymbol{n}, V)V, \quad b(\boldsymbol{n}, V) \geqq 0, \tag{4.23}$$

with $b(\boldsymbol{n}, V)$ a constitutive quantity called the kinetic modulus.[23] These are the most general constitutive equations of the form (4.21) that are consistent with (4.20).

Anisotropy of the interface manifests itself in a nontrivial dependence of $\hat{\psi}(\boldsymbol{n})$ on $\boldsymbol{n}$; for an isotropic interface ψ is constant. An interesting consequence of (4.22) is that *for an anisotropic interface the surface shear cannot generally vanish.* This demonstrates the nonintuitive nature of configurational forces: the interface is presumed to be infinitesimally thin, yet it supports shear; thus the danger inherent in visualizing the interface as a membrane.

The surface shear must be balanced by couples exerted by the bulk material, although such couples, being indeterminate, need not be made explicit.[24] This furnishes an additional argument in support of the separate treatment of configurational forces when discussing deformation. If the variational treatment of Section 2, for an elastic material, is generalized to include an anisotropic interfacial energy, then the resulting Euler-Lagrange equations *in bulk* remain (2.7). Since these classical equations support neither bulk internal-couples nor bulk couple-stresses, a configurational system is needed to balance the couples induced by surface-shear.

d. Evolution equation for the interface

The evolution equation for the interface follows from the normal force-balance (4.11), (4.15), the tension-energy relations (3.20) and (4.19), the reduced constitutive relations (4.22) and (4.23), and the identity (A15):[25]

$$b(\boldsymbol{n}, V)V = \{\hat{\psi}(\boldsymbol{n})1 + \partial_n \partial_n \hat{\psi}(\boldsymbol{n})\} \cdot \mathbf{L} + U. \tag{4.24}$$

---

[23] For $b(\boldsymbol{n}, V)$ independent of V, $b(\boldsymbol{n})^{-1}$ is referred to as the mobility of the interface.

[24] GURTIN [1988, Remark 3.2].

[25] Proposed by UWAHA [1987, eq. (2)] in ($\mathbb{R}^2$ with $b = b(\boldsymbol{n})$) and independently by GURTIN [1988, eq. (8.3)]. Evolution according to (4.24) with $b = b(\boldsymbol{n})$ is studied by ANGENENT [1991], CHEN, GIGA & GOTO [1991], and SONER [1993]. The special case $V = -b(\boldsymbol{n})^{-1}U$ was introduced by FRANK [1958]. A formulation of (4.24) using a variational definition of the curvature term (TAYLOR [1992]) is given by TAYLOR, CAHN & HANDWERKER [1992], who give extensive references.

For an isotropic material with b independent of V and $U = 0$, (4.24), after a rescaling, reduces to the curve-shortening equation, $V = K$.[26] In (4.24) the derivatives must respect the constraint $|\boldsymbol{n}| = 1$. A simpler form of the equation follows if $\hat{\psi}(\boldsymbol{n})$ is extended from the unit sphere to $\mathbb{R}^3$ by defining $\tilde{\psi}(z) = |z|\hat{\psi}(z/|z|)$, for then the term $\{\ldots\}$ reduces to $\{\partial_z\partial_z\tilde{\psi}(z)\}$ at $z = \boldsymbol{n}$. Finally, the analogous relation for evolution in $\mathbb{R}^2$, with $\boldsymbol{n}$ replaced by the counterclockwise angle φ from a fixed axis to $\boldsymbol{n}$, is[27]

$$b(\varphi, V)V = \{\hat{\psi}(\varphi) + \hat{\psi}''(\varphi)\}K + U. \tag{4.25}$$

The expression (4.24) represents the normal part of the configurational force balance (4.2). The indeterminancy of the tangential part of $\mathbf{e}$ renders the tangential part of (4.2) unimportant. Interestingly, a computation using $(A15)_1$, (4.6), (4.10), (4.19), and (4.22) shows the tangential balances to be satisfied automatically with $\boldsymbol{P}\mathbf{e} = \mathbf{0}$, so that $\mathbf{e} = e\boldsymbol{n}$.

For *nonsmooth* interfaces — which are possible when $\tilde{\psi}(z)$ is nonconvex — the evolution equation (4.24) is not, by itself, sufficient to describe the motion of the interface: the weaker form (4.1) must be used, for example across curves defined by a jump in the interface normal $\boldsymbol{n}$.[28]

5. Two-phase theory with deformation[29]

a. Theory neglecting interfacial energy

I now consider a coherent two-phase elastic solid, neglecting interfacial energy, interfacial stress, and, as before, thermal and compositional variations. The body B is presumed independent of time, but the subregions $B_\alpha(t)$ and $B_\beta(t)$ occupied by α and β as well as the interface $\mathscr{S}(t)$ depend on t. Coherency requires that motions $\boldsymbol{y}$ of B be continuous across the interface, with deformation gradient $\boldsymbol{F}$ and material velocity $\boldsymbol{y}^\cdot$ continuous up to the interface from either side, a constraint that yields the compatibility conditions

$$[\![\boldsymbol{y}^\cdot]\!] = -V[\![\boldsymbol{F}]\!]\boldsymbol{n}, \quad [\![\boldsymbol{F}]\!]\boldsymbol{P} = \mathbf{0}, \tag{5.1}$$

with $\boldsymbol{n}$ the unit normal to $\mathscr{S}$ directed outward from B_α and V the normal velocity of $\mathscr{S}$.

---

[26] BURKE & TURNBULL [1952] and MULLINS [1956] introduced $V = K$ to study the motion of grain boundaries. Evolution according to this equation is discussed by many authors (cf. GURTIN [1993a, Footnote 12]).

[27] Derived using a thermomechanical argument by ANGENENT & GURTIN [1989], although the configurational force system is somewhat different (cf. GURTIN [1993a]).

[28] Cf. ANGENENT & GURTIN [1989] and GURTIN [1993a] for discussions of this issue in $\mathbb{R}^2$.

[29] GURTIN [1993b, 1994a].

While inertia is easily included, I neglect it to simplify the presentation. The basic balance laws are as discussed in Section 3 for single-phase materials, but with the interface accounted for by internal configurational forces with density $\mathbf{e}$ distributed over $\mathscr{S}$. The deformational and configurational balances thus take the form

$$\int_{\partial R} \boldsymbol{S}\boldsymbol{m}\, da = \mathbf{0}, \quad \int_{\partial R} \boldsymbol{y}\times\boldsymbol{S}\boldsymbol{m}\, da = \mathbf{0}, \tag{5.2}$$

$$\int_{\partial R} \boldsymbol{C}\boldsymbol{m}\, da + \int_R \boldsymbol{f}\, da + \int_{\mathscr{G}} \mathbf{e}\, da = \mathbf{0}, \tag{5.3}$$

where $R(t)$ is an arbitrary referential control volume with $\mathscr{G}(t) = \mathscr{S}(t)\cap R(t)$ the portion of the interface in $R(t)$.

The local force-balances now consist of bulk equations and interface conditions; the bulk equations remain (3.9) (with $\boldsymbol{b} = \mathbf{0}$) and (3.24), while the interface conditions are

$$[\boldsymbol{S}]\boldsymbol{n} = \mathbf{0}, \quad [\boldsymbol{C}]\boldsymbol{n} + \mathbf{e} = 0. \tag{5.4}$$

The working still has the form (3.14) (with $\boldsymbol{b} = \mathbf{0}$); there is no contribution of $\mathbf{e}$, as it acts internally. Restricting $R(t)$ to not intersect the interface leads to the relation (3.16) for the configurational stress. Further, since interfacial energy as well as variations in temperature and composition are neglected, the second law takes the form (3.13) and leads again to the bulk Eshelby relation (3.21).

To derive an expression for the second law at the interface, I restrict attention to time-independent control volumes that intersect the interface; granted this, (3.13) reduces to

$$\frac{d}{dt}\left\{\int_R \Psi\, dv\right\} \leqq \int_{\partial R} \boldsymbol{S}\boldsymbol{m}\cdot\boldsymbol{y}^{\cdot}\, da. \tag{5.5}$$

But

$$\frac{d}{dt}\left\{\int_R \Psi\, dv\right\} = -\int_{\mathscr{G}} [\Psi]\, V\, da + \int_R \Psi^{\cdot}\, dv. \tag{5.6}$$

Thus shrinking R to the interface yields the jump condition $[\Psi]V + [Sn\cdot y^{\cdot}] \geqq 0$, so that, by (5.1) and the first of (5.4), $([\Psi] - [\boldsymbol{F}\boldsymbol{n}\cdot\boldsymbol{S}\boldsymbol{n}])V \geqq 0$, or equivalently, by using (3.21) and the second of (5.4),

$$eV \leqq 0, \tag{5.7}$$

with $e = \mathbf{e}\cdot\boldsymbol{n}$ the normal internal force.

I consider bulk constitutive equations of the form (3.25) for each phase. (These are the most general constitutive equations — consistent with (5.5) — for ψ and $\boldsymbol{S}$ as functions of $\boldsymbol{F}$.) In addition, I consider a constitutive equation for the interface giving e as a function of V and a list $\boldsymbol{z}$ of fields such as $\boldsymbol{n}$ and the interfacial limits of

$\boldsymbol{F}$; the requirement that (5.7) hold in all motions then yields the reduced constitutive relation

$$e = -bV, \quad b = b(z, V) \geqq 0, \tag{5.8}$$

with $b(z, V)$ a constitutive modulus.

The relations (3.21), (5.4), and (5.8) yield final interface conditions

$$[\![\boldsymbol{S}]\!]\boldsymbol{n} = \boldsymbol{0}, \quad \boldsymbol{n}\cdot[\![\Psi\mathbf{1} - \boldsymbol{F}^T\boldsymbol{S}]\!]\boldsymbol{n} = bV, \tag{5.9}$$

which are replaced by

$$[\![\boldsymbol{S}]\!]\boldsymbol{n} = -\rho[\![\boldsymbol{y}^{\cdot}]\!]V, \quad \boldsymbol{n}\cdot[\![\Psi\mathbf{1} - \boldsymbol{F}^T\boldsymbol{S}]\!]\boldsymbol{n} = -\mathcal{k} + bV, \tag{5.10}$$

when inertia is included. Here $\mathcal{k} = (\rho/2)[\![|\boldsymbol{F}\boldsymbol{n}|^2]\!]V^2$.

The kinetic relation $(5.10)_2$ was derived by TRUSKINOVSKY [1987, 1991] and ABEYARATNE & KNOWLES [1990, 1991] on the basis of an argument that does not require the introduction of configurational forces. They note that the second law yields the inequality $([\![\Psi]\!] - [\![\boldsymbol{F}\boldsymbol{n}\cdot\boldsymbol{S}\boldsymbol{n}]\!] + \mathcal{k})V \geqq 0$, which they use to motivate a constitutive relation for the "driving traction" $f = -[\![\Psi]\!] + [\![\boldsymbol{F}\boldsymbol{n}\cdot\boldsymbol{S}\boldsymbol{n}]\!] - \mathcal{k}$ of the form $f = -bV$, $b \geqq 0$. This argument is simpler than the one I have given, since it does not involve a configurational force balance, but I believe it to be unsound: $\mathcal{k}$ is a known function of $\boldsymbol{F}$, $\boldsymbol{n}$, and V, while Ψ and $\boldsymbol{S}$ are prescribed as functions of $\boldsymbol{F}$ through constitutive relations; therefore postulating an additional relation for $[\![\Psi]\!] - [\![\boldsymbol{F}\boldsymbol{n}\cdot\boldsymbol{S}\boldsymbol{n}]\!] + \mathcal{k}$ seems both superfluous and arbitrary. I know of no other example from continuum mechanics in which fields specified by constitutive relations are presumed related by yet another such relation.

b. Theory with interfacial energy and stress

I now generalize the theory of Section 5a to include interfacial structure, but I merely sketch the analysis, as it is complicated. The inclusion of interfacial stress characterized by the superficial tensor fields

S *deformational surface stress*
C *configurational surface stress*

necessitates modification of (5.2) and (5.3) as follows: let $\boldsymbol{\nu}$ denote the outward unit normal to $\partial\mathscr{G}$; then the terms

$$\int_{\partial\mathscr{G}} \mathbf{S}\boldsymbol{\nu}\, ds, \quad \int_{\partial\mathscr{G}} \boldsymbol{y}\times\mathbf{S}\boldsymbol{\nu}\, ds, \quad \int_{\partial\mathscr{G}} \mathbf{C}\boldsymbol{\nu}\, ds,$$

respectively, should be added to the left sides of the deformational force and moment balances and the left side of the configurational balance. This yields

$$[\![\boldsymbol{S}]\!]\boldsymbol{n} + \mathrm{div}_{\mathscr{S}}\mathbf{S} = \boldsymbol{0}, \quad \mathbf{S}\mathbf{F}^T = \mathbf{F}\mathbf{S}^T, \quad [\![\boldsymbol{C}]\!]\boldsymbol{n} + \mathbf{e} + \mathrm{div}_{\mathscr{S}}\mathbf{C} = \boldsymbol{0}, \tag{5.11}$$

with

$$\mathbf{F} = \boldsymbol{F}_\alpha \boldsymbol{P} = \boldsymbol{F}_\beta \boldsymbol{P} \tag{5.12}$$

the tangential deformation gradient (cf. $(5.1)_2$).

In addition to the bulk free-energy Ψ, there is an interfacial free-energy ψ, and the inequality representing the second law takes the form

$$\frac{d}{dt}\left\{\int_R \Psi\, dv + \int_{\mathscr{G}} \psi\, da\right\} \leqq \mathscr{W}(R) \tag{5.13}$$

for all $R(t)$, where $\mathscr{W}(R)$ now includes working of the surface forces:

$$\mathscr{W}(R) = \int_{\partial R} (\boldsymbol{S}\boldsymbol{m}\cdot\bar{\boldsymbol{v}} + \boldsymbol{C}\boldsymbol{m}\cdot\boldsymbol{v})\, da + \int_{\partial\mathscr{G}} (\mathbf{C}\boldsymbol{v}\cdot\boldsymbol{w} + \mathbf{S}\boldsymbol{v}\cdot\bar{\boldsymbol{w}})\, ds. \tag{5.14}$$

Here $\boldsymbol{v}$ is a velocity field for ∂R with $\bar{\boldsymbol{v}}$ the corresponding induced velocity field for $\partial\mathscr{R}$, while $\boldsymbol{w}$ is a velocity field for the curve $\partial\mathscr{G}(t)$ with $\bar{\boldsymbol{w}}$ the corresponding induced velocity field for the deformed curve $\boldsymbol{y}(\partial\mathscr{G}(t), t)$; that is, $\boldsymbol{w}(\boldsymbol{X}, t)$ is computed using time-dependent parametrizations (4.3) for $\partial\mathscr{G}(t)$ and $\bar{\boldsymbol{w}} = \boldsymbol{y}^{\cdot} + \boldsymbol{F}\boldsymbol{w}$.

Invariance under reparametrization for $\partial R(t)$ then yields the Eshelby relation (3.21), while invariance under reparametrization for $\partial\mathscr{G}(t)$ yields an Eshelby relation for the interface:

$$\mathbf{C}_{\tan} = \psi \boldsymbol{P} - \mathbf{F}^T\mathbf{S}. \tag{5.15}$$

The resulting interfacial dissipation inequality, which generalizes (4.20), is

$$\psi^\circ + (\mathbf{c} + \mathbf{S}^T\boldsymbol{E}\boldsymbol{n})\cdot\boldsymbol{n}^\circ - \mathbf{S}\cdot\boldsymbol{E}^\circ + eV \leqq 0, \tag{5.16}$$

with $\mathbf{c}$ the configurational shear and $\boldsymbol{E}$ the average of the interfacial limits $\boldsymbol{F}_\alpha$ and $\boldsymbol{F}_\beta$ of $\boldsymbol{F}$:

$$\mathbf{c} = \mathbf{C}^T\boldsymbol{n}, \quad \boldsymbol{E} = \langle \boldsymbol{F} \rangle. \tag{5.17}$$

As constitutive equations for the interface I allow ψ, $\mathbf{S}$, $\mathbf{c}$, and e to depend on $\boldsymbol{n}$, V, $\boldsymbol{F}_\alpha$, and $\boldsymbol{F}_\beta$. A consequence of (5.16) is that ψ, $\mathbf{S}$, and $\mathbf{c}$ are independent of V and depend on $\boldsymbol{F}_\alpha$ and $\boldsymbol{F}_\beta$ through their average $\boldsymbol{E}$. In fact, the energy $\psi = \hat{\psi}(\boldsymbol{E}, \boldsymbol{n})$ determines $\mathbf{S}$ and $\mathbf{c}$ through the relations

$$\mathbf{S} = \partial_{\boldsymbol{E}}\hat{\psi}(\boldsymbol{E}, \boldsymbol{n}), \quad \mathbf{c} + \mathbf{S}^T\boldsymbol{E}\boldsymbol{n} = -\partial_{\boldsymbol{n}}\hat{\psi}(\boldsymbol{E}, \boldsymbol{n}), \tag{5.18}$$

$$e = -bV, \quad b = b(\boldsymbol{F}_\alpha, \boldsymbol{F}_\beta, \boldsymbol{n}, V) \geqq 0. \tag{5.19}$$

The final interface conditions consist of the compatibility condition (5.1) and the force balances[30]

$$[\boldsymbol{S}]\boldsymbol{n} = -\operatorname{div}_{\mathscr{G}}\mathbf{S}, \quad \boldsymbol{n}\cdot[\Psi\mathbf{1} - \boldsymbol{F}^T\boldsymbol{S}]\boldsymbol{n} + (\psi\boldsymbol{P} - \mathbf{F}^T\boldsymbol{S})\cdot\mathbf{L} + \operatorname{div}_{\mathscr{G}}\mathbf{c} = bV \tag{5.20}$$

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[30] GURTIN & STRUTHERS [1990], GURTIN [1993b, 1994a]. See also LUSK [1992]. For statics $(5.20)_1$ was derived by GURTIN & MURDOCH [1974] from a force balance, while $(5.20)_2$ was derived by LEO & SEKERKA [1989] as an Euler-Lagrange equation for stable equilibria (cf. ALEXANDER & JOHNSON [1985], JOHNSON & ALEXANDER [1986], and FONSECA [1989]).

supplemented by the constitutive equations (5.18) and (5.19) as well as those for the bulk material. Note that $(5.20)_2$, which represents the normal configurational force balance, may be written in the form[31]

$$\boldsymbol{n}\cdot[\text{bulk Eshelby tensor}]\boldsymbol{n} + (\text{interfacial Eshelby tensor})\cdot\mathbf{L} + \operatorname{div}_{\mathscr{S}}\mathbf{c} = bV. \tag{5.21}$$

6. Solidification. The Stefan and Gibbs-Thompson conditions as consequences of the configurational force balance

To demonstrate the role of configurational forces in situations that are not purely mechanical, I turn now to two-phase heat flow, neglecting deformation. Paralleling (3.12), I write the first two laws for a control volume $R(t)$ as

$$\frac{d}{dt}\{\text{internal energy}\} = \{\text{heating}\} + \{\text{working}\},$$

$$\frac{d}{dt}\{\text{internal entropy}\} \geqq \{\text{entropy flux induced by heating}\}$$

in which the right sides include an accounting of the work and *heat* required to add or remove material, but make no explicit mention of flows of internal energy and internal entropy across ∂R.

a. Single-phase theory

To the classical fields

ε *internal energy*
η *internal entropy*
ϑ *absolute temperature*
$\boldsymbol{q}$ *heat flux vector*

I add three configurational fields

$\boldsymbol{C}$ *stress*
$\boldsymbol{f}$ *internal force*
Q *heating*

where Q is a scalar field, while $\boldsymbol{C}$ and $\boldsymbol{f}$ are as discussed previously, and I define the free energy through

$$\Psi = \varepsilon - \vartheta\eta. \tag{6.1}$$

---

[31] The insight afforded by the use of bulk and interfacial Eshelby tensors was pointed out to me by P. PODIO-GUIDUGLI (private communication).

For $R(t)$ an evolving control volume, with $\mathscr{V}$ the normal velocity of ∂R,

$$\int_{\partial R} Q\mathscr{V}\, da, \quad \int_{\partial R} \frac{Q}{\vartheta}\mathscr{V}\, da$$

represent flows of heat and entropy into R associated with the motion of ∂R.

The basic laws, for each evolving control volume $R(t)$, are *balance of energy*

$$\frac{d}{dt}\left\{\int_R \varepsilon\, dv\right\} = -\int_{\partial R} \boldsymbol{q}\cdot\boldsymbol{m}\, da + \int_{\partial R} Q\mathscr{V}\, da + \int_{\partial R} \boldsymbol{C}\boldsymbol{m}\cdot\boldsymbol{v}\, da, \tag{6.2}$$

growth of entropy

$$\frac{d}{dt}\left\{\int_R \eta\, dv\right\} \geqq -\int_{\partial R} \frac{\boldsymbol{q}}{\vartheta}\cdot\boldsymbol{m}\, da + \int_{\partial R} \frac{Q}{\vartheta}\mathscr{V}\, da, \tag{6.3}$$

and *balance of configurational forces*

$$\int_{\partial R} \boldsymbol{C}\boldsymbol{m}\, da + \int_R \boldsymbol{f}\, dv = 0, \tag{6.4}$$

with $\boldsymbol{m}$ the outward unit normal to ∂R, and with the stipulation that *balance of energy be independent of the particular local parametrizations used to determine the velocity field* $\boldsymbol{v}$ *for* ∂R. For R stationary (6.2) and (6.3) become

$$\frac{d}{dt}\left\{\int_R \varepsilon\, dv\right\} = -\int_{\partial R} \boldsymbol{q}\cdot\boldsymbol{m}\, da, \qquad \frac{d}{dt}\left\{\int_R \eta\, dv\right\} \geqq -\int_{\partial R} \frac{\boldsymbol{q}}{\vartheta}\cdot\boldsymbol{m}\, da, \tag{6.5}$$

again demonstrating consistency with more standard ideas.

As before, invariance under changes in reparametrization for $\partial R(t)$ yields the conclusion that $\boldsymbol{C}$ is a pure tension π, as in (4.6); therefore, by (3.1) applied to ε in (6.2) and η in (6.3),

$$\varepsilon = \pi + Q, \quad \eta = \frac{Q}{\vartheta}, \tag{6.6}$$

relations that, when multiplied by $\mathscr{V}$, express balance of energy and entropy associated with the addition of material to R. A trivial but important corollary of these relations is that, once again, bulk tension and bulk free energy coincide: $\pi = \Psi$. Thus

$$\boldsymbol{C} = \Psi\boldsymbol{1}. \tag{6.7}$$

Finally, restricting attention to stationary control volumes, and using (6.1) and the energy balance to rewrite the entropy inequality yields the local relations

$$\varepsilon^{\cdot} = -\operatorname{div}\boldsymbol{q}, \tag{6.8}$$

$$\Psi^{\cdot} + \eta\vartheta^{\cdot} + \vartheta^{-1}\boldsymbol{q}\cdot\nabla\vartheta \leqq 0. \tag{6.9}$$

The standard constitutive equations consist of a relation between free energy and temperature, a relation giving the entropy as the negative of the derivative of the free energy with respect to temperature, and a Fourier law for heat conduction,[32]

$$\Psi = \hat{\Psi}(\vartheta), \quad \eta = -\hat{\Psi}'(\vartheta), \quad \boldsymbol{q} = -K(\vartheta)\nabla\vartheta, \tag{6.10}$$

with $\boldsymbol{K}(\vartheta)$, the conductivity tensor, assumed positive definite. Granted these, the dissipation inequality (6.9) is satisfied identically. By (6.1) and (6.10), there is an auxiliary relation for the internal energy:

$$\varepsilon = \hat{\Psi}(\vartheta) - \vartheta\hat{\Psi}'(\vartheta). \tag{6.11}$$

The basic partial differential equation of the theory is given by balance of energy supplemented by $(6.10)_3$ and (6.11).

Note that, by the local form (3.24) of (6.4) and the equations (6.7) and (6.10),

$$\boldsymbol{f} = \eta\nabla\vartheta, \tag{6.12}$$

which I take as a defining relation for $\boldsymbol{f}$.

b. The classical two-phase theory revisited. The Stefan condition as a consequence of the configurational force balance

I now consider two phases, α and β, with $\Psi_\alpha(\vartheta)$ and $\Psi_\beta(\vartheta)$, and $\boldsymbol{K}_\alpha(\vartheta)$ and $\boldsymbol{K}_\beta(\vartheta)$ the corresponding free energies and conductivity tensors, and with resulting constitutive relations of the form (6.10). I assume further that there is a unique temperature, the *melting temperature* ϑ_M, at which the free energies of the individual phases coincide:

$$\Psi_\alpha(\vartheta_M) = \Psi_\beta(\vartheta_M). \tag{6.13}$$

I neglect interfacial structure, so that the basic laws remain (6.2)–(6.4). Further, I assume that the *temperature is continuous*, but allow the other fields to suffer jump discontinuities across the interface.

Balance of energy then yields the interfacial balance

$$[\![\varepsilon]\!]V = [\![\boldsymbol{q}]\!]\cdot\boldsymbol{n}, \tag{6.14}$$

which is the first of the classical interface conditions for the Stefan problem.

Next, the configurational balance (6.4) yields

$$[\![\boldsymbol{C}]\!]\boldsymbol{n} = \boldsymbol{0}, \tag{6.15}$$

---

[32] These are consequences of (7.9) in conjunction with constitutive equations giving Ψ, η, and $\boldsymbol{q}$ as functions of θ and $\nabla\theta$ with $\boldsymbol{q}$ linear in $\nabla\theta$.

which, by (6.7), has the alternative form

$$[\Psi] = 0, \tag{6.16}$$

or, in view of the hypothesis ending in (6.13),

$$\vartheta = \vartheta_M \quad \text{on the interface.} \tag{6.17}$$

Thus *the classical Stefan condition equating the temperature at the interface to the melting temperature is equivalent to the configurational balance applied across the interface.*[33]

c. *Weak form of the two-phase problem using the configurational balance*

Not only does the configurational balance allow for a derivation of the classical Stefan condition, it allows for a weak formulation of the Stefan problem by replacing the condition $\vartheta = \vartheta_M$ on the interface, which is local and inappropriate to a weak formulation, with a partial differential equation. In particular, (6.5) and the configurational balance $\operatorname{div} \boldsymbol{C} = -\boldsymbol{f}$ with $\boldsymbol{C}$ given by (6.7) and $\boldsymbol{f}$ by (6.12) yield partial differential equations

$$\varepsilon^{\cdot} = -\operatorname{div} \boldsymbol{q}, \quad \nabla\Psi = -\eta\nabla\vartheta, \quad \eta^{\cdot} \geqq -\operatorname{div}\frac{\boldsymbol{q}}{\vartheta} \tag{6.18}$$

to be interpreted in a weak sense, for example in the sense of distributions. The distributional form of $(6.18)_1$ gives that partial differential equation classically in bulk and the balance (6.14) at the interface. The configurational balance $(6.18)_2$ is satisfied automatically in bulk; its only contribution is at the interface, where $\nabla\Psi$ is a distribution, as Ψ suffers a jump discontinuity ($\eta\nabla\vartheta$ does not contribute, as η and $\nabla\vartheta$ are bounded). In fact, $(6.18)_2$ formally yields (6.16) and hence the Stefan condition (6.17). Finally, $(6.18)_3$ is satisfied automatically in bulk as well as across the interface. To verify the latter assertion, note that $(6.18)_3$ yields $\vartheta[\eta]V \leqq [\boldsymbol{q}]\cdot\boldsymbol{n}$, or equivalently, by (6.1) and (6.14), $[\Psi]V \geqq 0$, an inequality satisfied by virtue of (6.16). It might therefore appear that the entropy inequality $(6.18)_3$ is superfluous, which is true when the interface moves smoothly, but there are situations involving large amounts of supercooling or superheating in which the interface moves "infinitely fast" resulting in an instantaneous change in phase for entire subregions of the body;[34] the entropy inequality is then needed to ensure that such instantaneous changes be consistent with the second law.[35]

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[33] GURTIN [1988]. To this point the *assumption* of continuity of temperature across the interface is not needed; however, it is basic to Sections 6c and 6d.

[34] SHERMAN [1970], FASANO & PRIMICERIO [1977], GÖTZ & ZALTSMAN [1993], GURTIN [1994b].

[35] GURTIN [1994b].

d. The two-phase theory with surface structure. The Gibbs-Thompson condition as a consequence of the configurational balance[36]

I now generalize the theory to include surface structure by considering the basic laws for each evolving control volume $R(t)$ in the form

$$\frac{d}{dt}\left\{\int_R \varepsilon\, dv + \int_{\mathscr{G}} \bar{\varepsilon}\, da\right\} = -\int_{\partial R} \boldsymbol{q}\cdot\boldsymbol{m}\, da + \int_{\partial R} Q\mathscr{V}\, da + \int_{\partial\mathscr{G}} \bar{Q} V_{\partial\mathscr{G}}\, ds + \mathscr{W}(R), \tag{6.19}$$

$$\frac{d}{dt}\left\{\int_R \eta\, dv + \int_{\mathscr{G}} \bar{\eta}\, da\right\} \geqq -\int_{\partial R} \frac{\boldsymbol{q}}{\vartheta}\cdot\boldsymbol{m}\, da + \int_{\partial R} \frac{Q}{\vartheta}\mathscr{V}\, da + \int_{\partial\mathscr{G}} \frac{\bar{Q}}{\vartheta} V_{\partial\mathscr{G}}\, ds, \tag{6.20}$$

$$\int_{\partial R} \boldsymbol{C}\boldsymbol{m}\, da + \int_R \boldsymbol{f}\, da + \int_{\partial\mathscr{G}} \mathbf{C}\mathbf{v}\, ds + \int_{\mathscr{G}} \mathbf{e}\, da = \mathbf{0}, \tag{6.21}$$

where $\mathscr{W}(R)$ is given by (4.5), $\mathbf{C}$, $\mathbf{e}$ and Q are as discussed before, $\bar{\varepsilon}$ is the interfacial energy, $\bar{\eta}$ is the interfacial entropy, and $\bar{Q}$, a configurational heating, is an analog of Q in the sense that

$$\int_{\partial\mathscr{G}} \bar{Q} V_{\partial\mathscr{G}}\, ds, \quad \int_{\partial\mathscr{G}} \frac{\bar{Q}}{\vartheta} V_{\partial\mathscr{G}}\, ds$$

represent flows of heat and entropy into $\mathscr{G}$ induced by the motion of the boundary curve $\partial\mathscr{G}$.

The arguments used before then yield the bulk relations discussed in the paragraph containing (6.7), the interface relations

$$\bar{\eta} = \frac{\bar{Q}}{\vartheta}, \quad \sigma = \psi, \tag{6.22}$$

and the results (4.9) and (4.19) with the interfacial free-energy given by

$$\psi = \bar{\varepsilon} - \vartheta\bar{\eta}. \tag{6.23}$$

The configurational balance remains (4.11), but the remaining interface conditions are more complicated than before: balance of energy has the form

$$[\varepsilon]V = [\boldsymbol{q}]\cdot\boldsymbol{n} + \bar{\varepsilon}^\circ - \bar{\varepsilon}KV - \mathrm{div}_{\mathscr{S}}(V\mathbf{c}) \tag{6.24}$$

(cf. (A13), (4.13), (6.6), (6.22), (6.23)), an analogous inequality for the entropy follows from (6.20), and this inequality, (4.11), and (6.24) yield the interfacial dissipation inequality

$$\psi^\circ + \bar{\eta}\vartheta^\circ + \mathbf{c}\cdot\boldsymbol{n}^\circ + eV \leqq 0. \tag{6.25}$$

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[36] This section, which represents a major improvement of my work [1988], is based on ideas introduced in GURTIN & STRUTHERS [1990] and GURTIN [1993, 1994a].

Guided by this inequality, I consider constitutive equations of the form (4.21), but with $(\vartheta, \boldsymbol{n}, V)$ as independent variables and with an additional constitutive equation, of the same form, for the entropy $\bar{\eta}$. The most general constitutive equations of this form consistent with the dissipation inequality (6.25) are

$$\psi = \hat{\psi}(\vartheta, \boldsymbol{n}), \quad \bar{\eta} = -\partial_\vartheta \hat{\psi}(\vartheta, \boldsymbol{n}), \quad \mathbf{c} = -\partial_{\boldsymbol{n}} \hat{\psi}(\vartheta, \boldsymbol{n}), \quad e = -b(\vartheta, \boldsymbol{n}, V)V, \tag{6.26}$$

with $b(\vartheta, \boldsymbol{n}, V) \geqq 0$. I henceforth assume that b is independent of V.

The resulting interface conditions consist of the energy balance (6.24) and the configurational balance (4.11) with $\pi = \Psi$, $\sigma = \psi$:

$$[\![\Psi]\!] = -\psi K - \operatorname{div}_{\mathscr{S}} \mathbf{c} - e. \tag{6.27}$$

These interface conditions supplemented by the constitutive equations are the basic free-boundary conditions of the theory; the condition (6.27) replaces the classical Stefan condition.

The interface conditions (6.24) and (6.27) are complicated. In [1988] I formally derived an approximate theory appropriate to an interface whose free energy, internal energy, and kinetic coefficient are small, with the latter independent of V. Let

$$\begin{gathered} u = \frac{(\vartheta - \vartheta_M)}{\vartheta_M}, \quad l = \varepsilon_\beta(\vartheta_M) - \varepsilon_\alpha(\vartheta_M), \\ \psi_M(\boldsymbol{n}) = \hat{\psi}(\vartheta_M, \boldsymbol{n}), \quad b_M(\boldsymbol{n}) = b(\vartheta_M, \boldsymbol{n}), \end{gathered} \tag{6.28}$$

where $\varepsilon_\alpha(\vartheta)$ and $\varepsilon_\beta(\vartheta)$ are the constitutive functions for the internal energy computed from the free energies $\Psi_\alpha(\vartheta)$ and $\Psi_\beta(\vartheta)$ via (6.11), so that l is the latent heat. Then the approximate interface conditions consist of an energy balance

$$lV = [\![\boldsymbol{q}]\!] \cdot \boldsymbol{n} \tag{6.29}$$

and a generalized Stefan condition

$$lu = \{\psi_M(\boldsymbol{n})\mathbf{1} + \partial_{\boldsymbol{n}} \partial_{\boldsymbol{n}} \psi_M(\boldsymbol{n})\} \cdot \mathbf{L} - b_M(\boldsymbol{n})V, \tag{6.30}$$

which includes the effects of curvature and kinetics. For an isotropic material ψ_M and b_M are constants, which I write as ψ and b, and (6.30) reduces to[37]

$$lu = \psi K - bV, \tag{6.31}$$

which is the Gibbs-Thompson condition $lu = \psi K$ augmented by the term bV, which accounts for interface kinetics.

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[37] $lu = -b(\boldsymbol{n})V$ was introduced by FRANK [1958] and used by CHERNOV [1963, 1964]; $lu = \psi K$ was introduced by MULLINS [1960] (in the context of mass transport) and used by MULLINS & SEKERA [1963, 1964]; $lu = \psi K - bV$ was used by VORONKOV [1964]. Cf. GURTIN [1993a, Footnote 84] for additional references.

Appendix on evolving surfaces

a. Surfaces

Let $\mathscr{S}$ be a smooth closed surface oriented by a choice of unit normal field $\boldsymbol{n}(\boldsymbol{X})$. The space $\boldsymbol{n}(\boldsymbol{X})^{\perp}$ of all vectors perpendicular to $\boldsymbol{n}(\boldsymbol{X})$ is the tangent space to $\mathscr{S}$ at $\boldsymbol{X}$, and the tensor

$$P(\boldsymbol{X}) = \mathbf{1} - \boldsymbol{n}(\boldsymbol{X}) \otimes \boldsymbol{n}(\boldsymbol{X}) \tag{A1}$$

projects vectors onto this tangent space.

In continuum mechanics tensors are generally linear transformations from $\mathbb{R}^3$ into itself, but of interest here are tensor fields $\mathbf{T}$ on $\mathscr{S}$ with the property that, at each $\boldsymbol{X}$ in $\mathscr{S}$, $\mathbf{T}(\boldsymbol{X})$ is a linear transformation from the tangent space at $\boldsymbol{X}$ into $\mathbb{R}^3$. These two notions of a tensor field may be reconciled by extending $\mathbf{T}(\boldsymbol{X})$ to vectors normal to $\mathscr{S}$ with the requirement that $\mathbf{T}(\boldsymbol{X})$ annihilate such vectors. Precisely, a *superficial tensor field* $\mathbf{T}$ on $\mathscr{S}$ is a function that associates with each $\boldsymbol{X}$ in $\mathscr{S}$ a linear transformation $\mathbf{T}(\boldsymbol{X})$ from $\mathbb{R}^3$ into $\mathbb{R}^3$ such that

$$\mathbf{T}\boldsymbol{n} = \mathbf{0}. \tag{A2}$$

$\mathbf{T}$ then admits a unique decomposition into *tangential* and *normal components* $\mathbf{T}_{\tan}$ and $\mathbf{t}$, respectively:

$$\mathbf{T} = \mathbf{T}_{\tan} + \boldsymbol{n} \otimes \mathbf{t}, \quad \mathbf{T}_{\tan} = \boldsymbol{P}\mathbf{T}, \quad \mathbf{t} = \mathbf{T}^T\boldsymbol{n}; \tag{A3}$$

given any vector field $\boldsymbol{v}$,

$$\mathbf{T}\boldsymbol{v} = \mathbf{T}_{\tan}\boldsymbol{v} + (\mathbf{t} \cdot \boldsymbol{v})\boldsymbol{n} \tag{A4}$$

with $\mathbf{T}_{\tan}\boldsymbol{v}$ a tangential vector field on $\mathscr{S}$. (Note that the *normal* component $\mathbf{t}$ of $\mathbf{T}$ is a *tangential vector field.*)

I define the surface gradient $\nabla_{\mathscr{S}}$ on $\mathscr{S}$ through the chain rule. Let $\varphi(\boldsymbol{X})$ be a smooth scalar field on $\mathscr{S}$ and $\boldsymbol{v}(\boldsymbol{X})$ a smooth vector field on $\mathscr{S}$. Then given any curve $\boldsymbol{z}(t)$ on $\mathscr{S}$,

$$\varphi(\boldsymbol{z})^{\cdot} = \nabla_{\mathscr{S}}\varphi(\boldsymbol{z}) \cdot \boldsymbol{z}^{\cdot}, \quad \boldsymbol{v}(\boldsymbol{z})^{\cdot} = \nabla_{\mathscr{S}}\boldsymbol{v}(\boldsymbol{z})\boldsymbol{z}^{\cdot} \tag{A5}$$

(which defines $\nabla_{\mathscr{S}}\boldsymbol{v}$ only on vectors tangent to $\mathscr{S}$, but, in accord with (A2), $\nabla_{\mathscr{S}}\boldsymbol{v}$ is extended by requiring that $(\nabla_{\mathscr{S}}\boldsymbol{v})\boldsymbol{n} = \mathbf{0}$). Then $\nabla_{\mathscr{S}}\varphi$ is a tangential vector field, while $\nabla_{\mathscr{S}}\boldsymbol{v}$ is a superficial tensor field. The surface divergence of $\boldsymbol{v}$ is defined by

$$\operatorname{div}_{\mathscr{S}}\boldsymbol{v} = \operatorname{tr}(\nabla_{\mathscr{S}}\boldsymbol{v}), \tag{A6}$$

while the surface divergence $\operatorname{div}_{\mathscr{S}}\mathbf{T}$ of a superficial tensor field is defined through the identity

$$\boldsymbol{a} \cdot \operatorname{div}_{\mathscr{S}}\mathbf{T} = \operatorname{div}_{\mathscr{S}}(\mathbf{T}^T\boldsymbol{a}) \tag{A7}$$

for every constant vector $\boldsymbol{a}$.

The *curvature tensor* $\mathbf{L}$ and *total curvature* K (twice the mean curvature) are defined by

$$\mathbf{L} = -\nabla_{\mathscr{S}}\boldsymbol{n}, \quad K = \operatorname{tr}\mathbf{L} = \mathbf{1}\cdot\mathbf{L} = -\operatorname{div}_{\mathscr{S}}\boldsymbol{n}. \tag{A8}$$

As is known, the curvature tensor is symmetric $\mathbf{L} = \mathbf{L}^T$ and (hence) tangential: $\mathbf{L}^T\boldsymbol{n} = \mathbf{0}$.

Let $\mathscr{G}$ denote a smooth subsurface of $\mathscr{S}$, and let $\boldsymbol{\nu}(\boldsymbol{X})$ denote the outward unit normal to the boundary curve $\partial\mathscr{G}$, so that $\mathbf{v}(\boldsymbol{X})$ is *tangent* to $\mathscr{S}$ at each $\boldsymbol{X} \in \partial\mathscr{G}$. The surface divergence theorem then has the form

$$\int_{\partial\mathscr{G}} \boldsymbol{t}\cdot\mathbf{v}\,ds = \int_{\mathscr{G}} \operatorname{div}_{\mathscr{S}}\boldsymbol{t}\,da, \quad \int_{\partial\mathscr{G}} \mathbf{T}\mathbf{v}\,ds = \int_{\mathscr{G}} \operatorname{div}_{\mathscr{S}}\mathbf{T}\,da \tag{A9}$$

for $\boldsymbol{t}$ a tangential vector field and $\mathbf{T}$ a superficial tensor field.

b. Smoothly evolving surfaces

Now let $\mathscr{S}(t)$ depend smoothly on the time t. Let φ° denote the *normal time-derivative*[38] of a scalar, vector, or tensor field φ on $\mathscr{S}$. Then

$$\boldsymbol{n}^\circ = -\nabla_{\mathscr{S}}V, \tag{A10}$$

with V the normal velocity of $\mathscr{S}$.

Let $\mathscr{G}(t)$ denote a smoothly evolving subsurface of $\mathscr{S}(t)$ with $\boldsymbol{\nu}(\boldsymbol{x}, t)$ the outward unit normal to $\partial\mathscr{G}(t)$. The motion of the curve $\partial\mathscr{G}(t)$ may be characterized intrinsically by the velocity field

$$V\boldsymbol{n} + V_{\partial\mathscr{G}}\boldsymbol{\nu}, \tag{A11}$$

where $V_{\partial\mathscr{G}}$, the *tangential edge velocity* of $\mathscr{G}$, is the velocity of $\partial\mathscr{G}$ in the direction of the normal $\boldsymbol{\nu}$.

For φ a superficial scalar field,

$$\frac{d}{dt}\int_{\mathscr{G}} \varphi\,da \quad \text{denotes} \quad \frac{d}{dt}\int_{\mathscr{G}(t)} \varphi(\boldsymbol{X}, t)\,da(\boldsymbol{X}). \tag{A12}$$

Then[39]

$$\frac{d}{dt}\int_{\mathscr{G}} \varphi\,da = \int_{\mathscr{G}} (\varphi^\circ - \varphi K V)\,da + \int_{\partial\mathscr{G}} \varphi V_{\partial\mathscr{G}}\,ds. \tag{A13}$$

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[38] The derivative following the normal trajectories of the surface. Cf. GURTIN [1986, eq. (4.4)].

[39] Cf. PETRYK and MROZ [1986], GURTIN, STRUTHERS and WILLIAMS [1989], ESTRADA and KANWAL [1991], JARIC [1991].

c. *Functions of orientation*

Constitutive equations appropriate to a phase interface generally involve scalar functions $\varphi(\boldsymbol{n})$ and vector functions $\mathbf{f}(\boldsymbol{n})$ of the interface normal $\boldsymbol{n}$. The derivatives $\partial_n\varphi(\boldsymbol{n})$ and $\partial_n\mathbf{f}(\boldsymbol{n})$ are defined by the chain rule. Given any curve $\boldsymbol{n}(t)$ on the unit sphere,

$$\varphi(\boldsymbol{n})^{\cdot} = \{\partial_n\varphi(\boldsymbol{n})\}\cdot\boldsymbol{n}^{\cdot}, \quad \mathbf{f}(\boldsymbol{n})^{\cdot} = \{\partial_n\mathbf{f}(\boldsymbol{n})\}\boldsymbol{n}^{\cdot}; \tag{A14}$$

$\partial_n\varphi(\boldsymbol{n})$ is tangent to the unit sphere, while $\partial_n\mathbf{f}(\boldsymbol{n})$ is defined by (A14) only on vectors perpendicular to $\boldsymbol{n}$, but is extended by requiring that $\{\partial_n\mathbf{f}(\boldsymbol{n})\}\boldsymbol{n} = \mathbf{0}$. Then for $\boldsymbol{n}$ the unit normal field on $\mathscr{S}$, a calculation using the chain rule and (A8) yields the identities

$$\nabla_{\mathscr{S}}\varphi(\boldsymbol{n}) = -\mathbf{L}\partial_n\varphi(\boldsymbol{n}), \quad \nabla_{\mathscr{S}}\mathbf{f}(\boldsymbol{n}) = -\{\partial_n\mathbf{f}(\boldsymbol{n})\}\mathbf{L}, \quad \operatorname{div}_{\mathscr{S}}\mathbf{f}(\boldsymbol{n}) = -\{\partial_n\mathbf{f}(\boldsymbol{n})\}\cdot\mathbf{L}. \tag{A15}$$

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