MULTIPHASE THERMOMECHANICS WITH INTERFACIAL STRUCTURE.

3. EVOLVING PHASE BOUNDARIES IN THE PRESENCE OF BULK DEFORMATION

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1. Introduction.

Previous studies[1] began an investigation whose goal is a *nonequilibrium* thermomechanics of two-phase continua based on Gibbs's notion of a sharp phase-interface endowed with energy, entropy and superficial force. In these studies the underlying continuum is *rigid,* an assumption that forms the basis for a large class of problems discussed by material scientists,[2] but there are situations in which deformation is the paramount concern, examples being shock-induced transformations and mechanical twinning.

In this paper[3] we consider *deformable* two-phase continua in which one of the phases is solid, the other[4] either solid or liquid. The extension to deformable media is not as straightforward as it might appear. One of the chief differences between theories involving phase transitions and the more classical theories of continuum mechanics is the presence of *accretion,* the creation and deletion of material points as the phase interface moves relative to the underlying material, and the interplay between accretion and deformation leads to conceptual difficulties. A major complication is that — because there are two *distinct* kinematical processes — it seems necessary to

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[1] Gurtin [1986,1988a,1988b], in which the underlying physical process is heat conduction: *dynamical* processes generally out of eqilibrium are considered, and restrictions on constitutive equations as well as free-boundary conditions at the interface are derived from balances for force and energy in conjunction with a law of entropy growth. (Cf. Angenent and Gurtin [1989], who discuss the isothermal evolution of the interface.)

[2] Cf., e.g., Mullins and Sekerka [1963,1964].

[3] Our study was motivated by papers of Cahn [1980], Mullins [1981,1984], Cahn and Larche [1982], Alexander and Johnson [1985,1986], and (especially) Leo and Sekerka [1988], all of whom consider deformable media and derive *equilibrium* balance laws for the interface as Euler-Lagrange equations for a global Gibbs function to be stationary. In these references, as in this paper, the individual phases have *different* constitutive equations. A different point of view is taken by Ericksen [1975,1977,1987], Knowles [1979], Gurtin [1983], James [1986ab,1987], Ball and James [1987], Fonseca [1987,1988a], Kinderlehrer [1987], Parry [1987], Chipot and Kinderlehrer [1988], and Abeyaratne and Knowles [1988abc], who consider elastic materials specified by a *single* constitutive relation with phase transitions defined by jumps in deformation gradient induced by constitutive instabilities.

[4] For the solid-solid interaction the interface is assumed coherent; for the solid-liquid interaction the liquid is assumed inviscid.

introduce *two distinct force systems:*[5]

(i) a system of *accretive forces* which acts within the crystal lattice to drive the crystallization process; this system consists of accretive surface stresses within the interface and accretive tractions and moments exerted by the lattice at the interface; these forces are presumed to be purely accretional, they are forces that would be present were there no deformation;

(ii) a system of *deformational forces* to be identified with the more or less standard forces that act in response to the local motion of material points; this system consists of deformational surface stresses within the interface and tractions exerted by the bulk material of the two phases at the interface.

Because of the nonclassical nature of accretive forces, it is not at all clear whether or not there should be an accompanying balance law, let alone what it should be and how it should relate to the more classical momentum balance laws. For that reason *we base most of our considerations on invariance.* Here we find it necessary to introduce a new idea, that of lattice observers: in addition to the standard *spatial observers* who measure the gross velocities of the continuum, *we allow for lattice observers,*[6] *who study the crystal lattice and measure the velocity of the accreting crystal surface.*

We characterize the accretive and deformational forces by the manner in which they expend power: we assume that the accretive and deformational surface stresses expend power over velocities associated with the motion of the interface, that the deformational tractions expend power over corresponding material velocities, and that the accretive traction and moment expend no power. Both the accretive

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[5] That more than one force system is needed is clear from a physical discussion of Cahn [1980], who writes: "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 the surface keeping the number of surface lattice sites constant while changing the form, physical area and poperties" (cf. Gibbs [1878] pp. 314-331).

[6] The use of more than one observer might be useful in other continuum theories, such as theories of liquid crystals, of structured continua, or of mixtures, in which "force"-balance laws over and above the standard laws arise.

and deformational surface stresses perform work related to the accretive motion of the interface; in fact, this work is performed by a certain linear combination of the two stresses, referred to as the *total accretive stress.*

An outline of the paper is as follows. We begin with a fairly thorough discussion of the kinematics of a deforming, accreting crystal, and the manner in which the kinematical quantities transform under changes in spatial and lattice observers.

Next we discuss the underlying mechanics. As the paper is devoted entirely to the physics of the phase interface,[7] we use infinitesimally thin control volumes; that is, control volumes which contain a portion of the interface plus the immediately adjacent bulk material. A basic ingredient of our theory is the *mechanical production* (the outflow of kinetic energy minus the expended power) associated with a control volume. The first law of thermodynamics requires that this production be balanced by the addition of heat and by changes in the internal energy; since heat and energy are invariant quantities, it seems reasonable to presume that the mechanical production itself be invariant. In fact, we use this invariance to derive several important results: invariance under changes in the kinetic description of the interface reduces the tangential part of the total accretive stress to a *surface tension;* invariance under changes in spatial and lattice observer yields the mechanical balance laws of the theory. This latter use of invariance is highly nontrivial: it not only leads to the expected momentum balance laws for the surface,[8] it leads to *additional force and moment balance laws for the accretive system.*

Basic to our theory is the notion of *attachment forces,* which are forces *within the lattice* associated with the attachment and release of atoms as they are exchanged between phases. We analyze

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[7] The basic equations satisfied by the *bulk material* are the standard equations of a one-phase material and can be found, e.g., in Gurtin [1981].

[8] Cf. Gurtin and Podio Guidugli [1989], who use invariance of the mechanical production to deduce balance laws for mass and linear momentum for a "massy" interface separating nondeformable phases.

these forces using bulk control volumes for the individual phases; such control volumes are infinitesimally thin regions which contain bulk material arbitrarily close to the interface, but exclude the interface.

We show that the power expended on an arbitrary control volume (containing the interface) can be decomposed into: *power expended by surface tension in the creation of new surface, power expended in changing the orientation of the surface, power expended in stretching the surface, power expended by the attachment forces in the exchange of atoms between phases, and inertial power expended in the velocity change between phases.*

The conceptual difficulties of the theory concern forces and the manner in which they relate to the underlying kinematics. For that reason we consider next a purely mechanical theory, for which the second law is a dissipation inequality for control volumes: the energy increase plus the energy outflow cannot be greater than the power expended, the relevant energies being the energy of the interface and the bulk energy of the two phases. Again invariance provides an important result: *surface tension equals interfacial energy.*

As constitutive equations we allow the surface energy, the accretive and deformational surface stresses, and the normal attachment force to depend on the bulk deformation gradient F, the normal $\mathbf{n}$ to the interface, the normal speed v of the interface, and a list z of subsidiary variables of lesser importance. We show, as a consequence of the dissipation inequality, that: the surface energy and the accretive and deformational surface stresses are independent of v and z, and depend on F at most through the tangential deformation gradient $\mathbb{F}$; in fact, the energy

$$\psi = \psi^{\wedge}(\mathbb{F},\mathbf{n}) \qquad (1.1)$$

completely determines the surface stresses through relations, the two most important of which are:

$$\mathbb{S} = \partial_{\mathbb{F}}\psi^{\wedge}(\mathbb{F},\mathbf{n}), \qquad \mathbb{C} = -D_{\mathbf{n}}\psi^{\wedge}(\mathbb{F},\mathbf{n}), \qquad (1.2)$$

in which $\mathbb{S}$ is the deformational (Piola-Kirchhoff) surface stress, $\mathbb{C}$ is the normal accretive stress, $\partial_{\mathbb{F}}$ is the partial derivative with respect to $\mathbb{F}$, and D_n is the derivative with respect to n following the interface. A further consequence of the dissipation inequality is an explicit expression for the normal attachment force π:

$$\pi = \mathfrak{k} + \Psi + \beta v, \qquad \beta = \beta\hat{}(F,n,v,z) \geq 0, \tag{1.3}$$

where Ψ is the difference in bulk energies, while $\mathfrak{k}$ is related to changes in momentum and kinetic energy across the interface. Using these results, we are able to show that the the sole source of dissipation is the exchange of atoms between phases, with βv^2 the dissipation per unit interfacial area.

We list the form the resulting equations take when specialized to coherent crystal-crystal interactions and to crystal-melt interactions; in the former case we have the relations[9]

$$\begin{aligned} &\mathrm{div}_{\mathcal{S}}\mathbb{S} + (S_e - S_c)n = \rho v(v_c - v_e), \\ &\Psi_{\mu c} - \Psi_{\mu e} = (S_c n)\cdot(F_c n) - (S_e n)\cdot(F_e n) - \mathfrak{k} - \mathscr{g} - \beta v, \end{aligned} \tag{1.4}$$

with

$$\begin{aligned} &\mathfrak{k} = \tfrac{1}{2}\rho v^2\{|F_c n|^2 - |F_e n|^2\}, \\ &\mathscr{g} = -\psi K - \mathrm{div}_{\mathcal{S}}\mathbb{C} + (F^T\mathbb{S})\cdot\mathbb{L}. \end{aligned} \tag{1.5}$$

The subscripts c and e denote the two phases; $\Psi_{\mu c}$ and $\Psi_{\mu e}$ are the bulk energies per unit reference volume; S_c and S_e are the bulk

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[9] For statical situations: $(1.4)_1$ was derived by Gurtin and Murdoch [1975] as a consequence of balance of forces; $(1.4)_2$ and its counterpart for crystal-melt interactions were derived by Leo and Sekerka [1989] (cf. Johnson and Alexander [1985,1986]) as Euler-Lagrange equations for stable equilibria. In the absence of surface stress and surface energy ($\mathbb{S}=0, \mathbb{C}=0, \psi=0$): $(1.4)_1$ is a standard shock relation; $(1.4)_2$ (with $\beta \neq 0$) was established by Abeyaratne and Knowles [1988c]. Counterparts of (1.4) for a rigid crystal in an inviscid melt were derived by Gurtin [1989]; an analog of $(1.4)_2$ for a rigid system was given by Gurtin [1988b].

Piola-Kirchhoff stresses; F_c and F_e are the bulk deformation gradients; v_c and v_e are the material velocities; ρ is the reference density. The remaining quantities concern the interface: $\mathbb{L}$ is the curvature tensor with κ, its trace, the total curvature, and $\mathrm{div}_{\mathcal{S}}$ is the surface divergence.

Our final step is to enlarge the theory to include thermal influences. We introduce temperature, bulk and superficial internal energies and entropies, and heat flow in conjunction with laws of energy balance and entropy growth. Fortunately, the mechanical results not pertaining to constitutive equations remain valid within this more general context, while the remaining derivations are similar to those of the mechanical theory. In particular, here *surface tension equals interfacial free-energy.*[10]

We generalize the constitutive equations by allowing for a dependence on the temperature θ, and we write an additional constitutive equation for the superficial entropy s. Then, in place of (1.1)-(1.3), we have the relations

$$\begin{aligned} \psi &= \hat{\psi}(\mathbb{F},\theta,\mathbf{n}), & s &= -\partial_\theta \hat{\psi}(\mathbb{F},\theta,\mathbf{n}),\\ \mathbb{S} &= \partial_{\mathbb{F}} \hat{\psi}(\mathbb{F},\theta,\mathbf{n}), & \mathbb{C} &= -D_n \hat{\psi}(\mathbb{F},\theta,\mathbf{n}), \\ \pi &= \Bbbk + \Psi + \beta v, & \beta &= \hat{\beta}(\mathrm{F},\mathbf{n},\theta,v,\mathbf{z}) \geq 0, \end{aligned} \qquad (1.6)$$

with ψ the interfacial free energy.

As before, we list the form the resulting equations take when specialized to coherent crystal-crystal interactions and to crystal-melt interactions; in the former case the basic equations consist of (1.4) and (1.5) in conjunction with the entropy balance[11]

$$s^{\circ} - s\kappa v + [S_{\mu c} - S_{\mu e}]v = \theta^{-1}[\mathbf{h}_c - \mathbf{h}_e]\cdot\mathbf{n} + \theta^{-1}\beta v^2, \qquad (1.7)$$

with $\Psi_{\mu c}$ and $\Psi_{\mu e}$ the bulk free energies per unit reference volume,

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[10] free energy = internal energy - (temperature)(entropy).

[11] Cf. Abeyaratne and Knowles [1988c] for the special case in which surface stress, surface energy, and surface entropy are neglected.

$S_{\mu c}$ and $S_{\mu e}$ the bulk entropies per unit reference volume, and $\mathbf{h}_c$ and $\mathbf{h}_e$ the bulk (Piola-Kirchhoff) heat flux vectors per unit reference area.

I. Kinematics.

2. Preliminary definitions and results.

2.1. Surfaces.[12]

2.1a. Definitions.

The term **vector** will generally signify an element of $\mathbb{R}^3$. Let $\mathbf{n}$ be a *unit vector.* $\mathbb{I}(\mathbf{n})\in\text{lin}(\mathbf{n}^\perp,\mathbb{R}^3)$ is the **inclusion** of $\mathbf{n}^\perp$ into $\mathbb{R}^3$: $\mathbb{I}(\mathbf{n})$ maps $\mathbf{a}\in\mathbf{n}^\perp$ into $\mathbf{a}$ considered as a vector in $\mathbb{R}^3$. $\mathbb{P}(\mathbf{n})$ is the (perpendicular) **projection** from $\mathbb{R}^3$ onto the plane $\mathbf{n}^\perp$: for each $\mathbf{a}\in\mathbb{R}^3$, $\mathbb{P}(\mathbf{n})\mathbf{a}\in\mathbf{n}^\perp$ is defined by

$$\mathbb{P}(\mathbf{n})\mathbf{a} = \mathbf{a} - (\mathbf{a}\cdot\mathbf{n})\mathbf{n}. \tag{2.1}$$

We consider $\mathbb{P}(\mathbf{n})$ as an element of $\text{lin}(\mathbb{R}^3,\mathbf{n}^\perp)$. Thus the codomain of $\mathbb{P}(\mathbf{n})$ is $\mathbf{n}^\perp$ and not $\mathbb{R}^3$; with this agreement,

$$\mathbb{I}(\mathbf{n})^T = \mathbb{P}(\mathbf{n}). \tag{2.2}$$

Let $\mathcal{S}$ denote a smooth,[13] oriented **surface** in $\mathbb{R}^3$ with unit normal field $\mathbf{n}(X)$, the **orientation** of $\mathcal{S}$. Then $\mathbf{n}(X)^\perp$ is the **tangent plane** to $\mathcal{S}$ at $X\in\mathcal{S}$. We use the shorthand

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[12] We use the notation and many of the results of Gurtin and Murdoch [1975], Murdoch [1976,1978], and Gurtin [1986,1988ab]. Given finite-dimensional inner product spaces V and W, $\text{lin}(V,W)$ is the space of linear transformations from V into W; $\text{lin}(V,W)$ is equipped with inner product $A\cdot B=\text{tr}(AB^T)$. Here tr denotes the **trace**, B^T is the **transpose** of B, and we write $u\cdot v$ for the **inner product** of u and v, *regardless of the space in question.* Also, $A\in\text{lin}(V,V)$ is **symmetric** if $A=A^T$, **skew** if $A=-A^T$. The **tensor product** of $v\in V$ and $w\in W$ is the transformation $v\otimes w\in\text{lin}(W,V)$ defined by $(v\otimes w)z=(w\cdot z)v$ for all $z\in W$; for $v,w\in V$, $v\wedge w=v\otimes w-w\otimes v$. The **inverse transpose** B^{-T} of $B\in\text{lin}(V,W)$ is defined by $B^{-T}=(B^{-1})^T=(B^T)^{-1}$. We write "$\times$" for the **cross product** on $\mathbb{R}^3$; for $b\in\mathbb{R}^3$, $(b\times)\in\text{lin}(\mathbb{R}^3,\mathbb{R}^3)$ is the skew transformation defined by $(b\times)z=b\times z$ for all $z\in\mathbb{R}^3$. $Q\in\text{lin}(\mathbb{R}^3,\mathbb{R}^3)$ is a **rotation** if $Q^T=Q^{-1}$ and $\det Q>0$. Here det is the **determinant**.

[13] We omit assumptions of regularity concerning functions, surfaces, regions, etc.

$$\mathbb{I}(X) = \mathbb{I}(n(X)), \qquad \mathbb{P}(X) = \mathbb{P}(n(X)),$$

so that $\mathbb{P}(X)$ is the projection onto the tangent plane at X, while $\mathbb{I}(X)$ is the inclusion of the tangent plane into $\mathbb{R}^3$. The fields $\mathbb{P}$ and $\mathbb{I}$ on $\mathcal{S}$ will be referred to as the **tangential projection** and **tangential inclusion** for $\mathcal{S}$.

We will consistently use the following terminology:

superficial scalar or vector field: a scalar or vector field on $\mathcal{S}$;

tangential vector field: a superficial vector field whose values are tangential to $\mathcal{S}$;

superficial tensor field: a field $\mathbb{C}$ on $\mathcal{S}$ with values $\mathbb{C}(X) \in \mathrm{lin}(n(X)^{\perp}, \mathbb{R}^3)$;

tangential tensor field: a superficial tensor field $\mathbb{C}$ whose values satisfy $\mathbb{C}(X)a \in n(X)^{\perp}$ for each $a \in n(X)^{\perp}$.

Let $\mathbb{T}$ be a tangential tensor field. Although $\mathbb{T}(X)$ maps tangent vectors into tangent vectors, we consider the codomain of $\mathbb{T}(X)$ to be $\mathbb{R}^3$. With this in mind, we refer to a tangential tensor field $\mathbb{T}$ as **symmetric** or **skew** according as $\mathbb{P}(X)\mathbb{T}(X)$ (or equivalently $\mathbb{T}(X)\mathbb{P}(X)$) is symmetric or skew at each $X \in \mathcal{S}$. Similarly, we define the **trace**, $\mathrm{tr}\mathbb{T}$, of a tangential field $\mathbb{T}$ by $\mathrm{tr}\mathbb{T} = \mathrm{tr}(\mathbb{P}\mathbb{T}) = \mathrm{tr}(\mathbb{T}\mathbb{P})$.

Each *tangential* tensor field $\mathbb{T}$ admits the unique decomposition

$$\mathbb{T} = \mathbb{T}_{\mathrm{sym}} + \mathbb{T}_{\mathrm{skw}},$$

where $\mathbb{T}_{\mathrm{sym}}$ and $\mathbb{T}_{\mathrm{skw}}$, respectively, are *symmetric* and *skew* tangential tensor fields called the symmetric and skew parts of $\mathbb{T}$. In fact,

$$\mathbb{T}_{\mathrm{sym}} = \tfrac{1}{2}\mathbb{I}(\mathbb{P}\mathbb{T} + \mathbb{T}^{\mathsf{T}}\mathbb{I}), \qquad \mathbb{T}_{\mathrm{skw}} = \tfrac{1}{2}\mathbb{I}(\mathbb{P}\mathbb{T} - \mathbb{T}^{\mathsf{T}}\mathbb{I}). \tag{2.3}$$

Each superficial tensor $\mathbb{C}$ admits the unique decompositions

$$\mathbb{C} = \mathbb{C}_{\mathrm{tan}} + n \otimes \mathbb{c} = \mathbb{C}_{\mathrm{sym}} + \mathbb{C}_{\mathrm{skw}} + n \otimes \mathbb{c}, \tag{2.4}$$

where $\mathbb{C}_{\mathrm{tan}}$ is a *tangential tensor field,* $\mathbb{C}_{\mathrm{sym}}$ a *symmetric tensor field,* $\mathbb{C}_{\mathrm{skw}}$ a *skew tensor field,* and $\mathbb{c}$ a *tangential vector field;* in fact,

$$\mathbb{c} = \mathbb{C}^{\mathsf{T}}\mathbf{n}; \quad \mathbb{C}_{\mathrm{tan}} = \mathbb{IPC}; \quad \mathbb{C}_{\mathrm{sym}} \textit{ and } \mathbb{C}_{\mathrm{skw}}$$
$$\textit{are the symmetric and skew parts of } \mathbb{C}_{\mathrm{tan}}. \tag{2.5}$$

We will refer to $\mathbb{C}_{\mathrm{tan}}$, $\mathbb{C}_{\mathrm{sym}}$, $\mathbb{C}_{\mathrm{skw}}$, and $\mathbb{c}$, respectively, as the **tangential, symmetric, skew,** and **normal components** of $\mathbb{C}$. If for some scalar field σ,

$$\mathbb{C} = \mathbb{C}_{\mathrm{sym}} = \sigma\mathbb{I},$$

then $\mathbb{C}$ is a **surface tension** σ.

If $\mathbb{C}$ is a superficial tensor field and $\mathbf{Q}$ a rotation, then $\mathbb{C}(X)\mathbf{Q}$ is not defined, since the codomain of $\mathbf{Q}$ is $\mathbb{R}^3$, while the domain of $\mathbb{C}(X)$ is $\mathcal{T} = \mathbf{n}(X)^{\perp}$; for our purposes it is convenient to write $\mathbb{C}(X)\mathbf{Q}$ for the linear transformation of $\mathbf{Q}^{\mathsf{T}}\mathcal{T}$ into $\mathbb{R}^3$ given by

$$[\mathbb{C}(X)\mathbf{Q}]\nu = \mathbb{C}(X)(\mathbf{Q}\nu) \quad \textit{for all} \quad \nu \in \mathbf{Q}^{\mathsf{T}}\mathcal{T}. \tag{2.6}$$

We write $\nabla_{\mathcal{S}}$ for the **surface gradient.**[14] For ϕ a superficial scalar field, $\nabla_{\mathcal{S}}\phi$ is a tangential vector field; for $\mathbf{v}$ a superficial vector field, $\nabla_{\mathcal{S}}\mathbf{v}$ is a superficial tensor field. The trace of $\mathbb{P}\nabla_{\mathcal{S}}\mathbf{v}$ is the **surface divergence** of $\mathbf{v}$:

$$\mathrm{div}_{\mathcal{S}}\mathbf{v} = \mathrm{tr}(\mathbb{P}\nabla_{\mathcal{S}}\mathbf{v}).$$

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[14] Cf., e.g., Gurtin and Murdoch [1975], Gurtin [1988ab]. For $\mathbf{z} = \mathbf{z}(t)$ a curve on $\mathcal{S}$ $\phi(\mathbf{z})^{\cdot} = \nabla_{\mathcal{S}}\phi(\mathbf{z})\cdot\mathbf{z}^{\cdot}$, $\mathbf{v}(\mathbf{z})^{\cdot} = [\nabla_{\mathcal{S}}\mathbf{v}(\mathbf{z})]\mathbf{z}^{\cdot}$; for $\mathbf{v}$ tangential, $\mathbb{P}\nabla_{\mathcal{S}}\mathbf{v}$ is the covariant derivative of $\mathbf{v}$.

Further, for Φ a smooth field on a closed region in $\mathbb{R}^3$ containing $\mathcal{S}$,

$$\nabla_{\mathcal{S}}\Phi = (\nabla\Phi)\mathbb{I}, \tag{2.7}$$

with ∇ the gradient[15] in $\mathbb{R}^3$.

The superficial tensor field

$$\mathbb{L} = -\nabla_{\mathcal{S}}\mathbf{n} \tag{2.8}$$

is the **curvature tensor**. A classical result is that

$$\mathbb{L} \textit{ is tangential and symmetric.} \tag{2.9}$$

The superficial scalar field

$$\kappa = \mathrm{tr}\,\mathbb{L} \tag{2.10}$$

is the **total curvature** (twice the mean curvature).

When $\mathcal{S}$ has a smooth boundary curve $\partial\mathcal{S}$, the **outward unit normal** $\boldsymbol{\nu}$ **to** $\partial\mathcal{S}$ is well defined with $\boldsymbol{\nu}(X)$ *tangent* to $\mathcal{S}$ at each $X\in\partial\mathcal{S}$.

2.1b. Differential and integral identities.

Let $\mathbb{C}$ be a superficial tensor field. Then $\mathrm{div}_{\mathcal{S}}\mathbb{C}$ is the unique vector field on $\mathcal{S}$ with the property

$$\mathbf{a}\cdot\mathrm{div}_{\mathcal{S}}\mathbb{C} = \mathrm{div}_{\mathcal{S}}(\mathbb{C}^{\mathrm{T}}\mathbf{a})$$

for all *constant* vectors $\mathbf{a}$.

The surface gradient and surface divergence obey the usual laws

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[15] ∇, div, and curl (without subscripts) will denote the gradient, divergence, and curl in $\mathbb{R}^3$. When discussing deforming bodies, ∇ and Div are the material gradient and divergence, grad and div the spatial gradient and divergence.

for the differentiation of scalar products and inner products.[16] Less standard are the **identities**:[17]

$$\begin{aligned} &\mathrm{div}_{\mathcal{S}}(\mathbb{C}^{\mathsf{T}}\mathbf{v}) = \mathbf{v}\cdot\mathrm{div}_{\mathcal{S}}\mathbb{C} + \mathbb{C}\cdot\nabla_{\mathcal{S}}\mathbf{v}, \\ &\mathrm{div}_{\mathcal{S}}\mathbb{C} = \mathrm{div}_{\mathcal{S}}\mathbb{C}_{\tan} + (\mathrm{div}_{\mathcal{S}}\mathbb{c})\mathbf{n} - \mathbb{L}\mathbb{c}, \\ &\mathbf{n}\cdot\mathrm{div}_{\mathcal{S}}\mathbb{C} = \mathbb{C}_{\tan}\cdot\mathbb{L} + (\mathrm{div}_{\mathcal{S}}\mathbb{c}). \end{aligned} \tag{2.11}$$

Here $\mathbf{v}$ is a superficial vector field, while $\mathbb{C}$ is a superficial tensor field with $\mathbb{C}_{\tan}$ and $\mathbb{c}$ the corresponding tangential and normal components.

Let $\mathcal{R}$ denote a sufficiently regular subsurface of $\mathcal{S}$, and let ν denote the outward unit normal to the boundary curve $\partial\mathcal{R}$. Then the **surface divergence theorem** (for tensor fields) asserts that, for $\mathbb{C}$ a superficial tensor field,

$$\int_{\partial\mathcal{R}}\mathbb{C}\nu\,ds = \int_{\mathcal{R}}\mathrm{div}_{\mathcal{S}}\mathbb{C}\,da. \qquad (2.12)^{18}$$

We write

$$\mathbf{r}(\mathbf{X}) = \mathbf{X} - \mathbf{X}_0 \tag{2.13}$$

for the position vector from a fixed point $\mathbf{X}_0 \in \mathbb{R}^3$. We then have the following identity,[19] valid for $\mathbb{C}$ a sufficiently smooth superficial tensor field:

$$\int_{\partial\mathcal{R}}\mathbf{r}\wedge\mathbb{C}\nu\,ds = \int_{\mathcal{R}}(\mathbf{r}\wedge\mathrm{div}_{\mathcal{S}}\mathbb{C} + \mathbb{I}\mathbb{C}^{\mathsf{T}} - \mathbb{C}\mathbb{P})\,da,$$

or equivalently, by (2.4),

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[16] Cf. Gurtin and Murdoch [1975], eq. (2.17).

[17] Cf. Gurtin [1988b], eq. (A14).

[18] Cf. Gurtin and Murdoch [1975], eq. (2.14). We write da for the area measure on surfaces, ds for the arc-length increment on curves.

[19] Cf. Gurtin and Murdoch [1975], p. 305.

$$\int_{\partial\mathcal{R}} r\wedge\mathbb{C}\nu\,ds = \int_{\mathcal{R}}\{r\wedge\mathrm{div}_{\mathcal{S}}\mathbb{C} + \mathbf{c}\wedge n - 2\mathbb{C}_{\mathrm{skw}}\mathbb{P}\}\,da, \tag{2.14}$$

with the tangential field $\mathbf{c}$ viewed as having values in $\mathbb{R}^3$.

2.1c. Mappings of surfaces.

Let $\mathfrak{D}_1$ and $\mathfrak{D}_2$ be regular regions[20] in $\mathbb{R}^3$, and write $\mathcal{S}_1 = \partial\mathfrak{D}_1$ and $\mathcal{S}_2 = \partial\mathfrak{D}_2$. Then a **deformation of $\mathfrak{D}_1$ onto $\mathfrak{D}_2$** is a smooth bijection $\mathbf{g}:\mathfrak{D}_1\to\mathfrak{D}_2$ whose gradient

$$\mathbf{G} = \nabla\mathbf{g} \tag{2.15}$$

has strictly positive determinant. Let $X_1\in\mathcal{S}_1$ and $X_2\in\mathcal{S}_2$ satisfy $X_2 = \mathbf{g}(X_1)$. Then a standard identity relates the outward unit normals $\mathbf{n}_1$ and $\mathbf{n}_2$ on $\mathcal{S}_1$ and $\mathcal{S}_2$:

$$\begin{aligned} \mathbf{n}_2(X_2) &= \lambda(X_1)\mathbf{G}(X_1)^{-T}\mathbf{n}_1(X_1), \\ \lambda(X_1) &= |\mathbf{G}(X_1)^{-T}\mathbf{n}_1(X_1)|^{-1}. \end{aligned} \tag{2.16}$$

Further,

$$\mathbf{G}(X_1) \textit{ maps tangent vectors at } X_1\in\mathcal{S}_1 \textit{ to tangent vectors at } X_2\in\mathcal{S}_2. \tag{2.17}$$

Let $\mathbb{P}_i$ and $\mathbb{I}_i$ denote the tangential projection and tangential inclusion for $\mathcal{S}_i$, and let

$$\mathbb{G} = \nabla_{\mathcal{S}_1}\mathbf{g} = \mathbf{G}\mathbb{I}_1. \tag{2.18}$$

$\mathbb{G}(X_1)$ is a linear transformation from the tangent plane at $X_1\in\mathcal{S}_1$ into $\mathbb{R}^3$, and hence cannot be invertible. This lack of invertibility is

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[20] Roughly speaking, a **regular region** $\mathfrak{D}$ is a closed, connected, possibly unbounded region in $\mathbb{R}^3$ whose boundary $\partial\mathfrak{D}$ is a smooth, connected, possibly unbounded surface; the exterior of $\mathfrak{D}$ is the regular region $\mathcal{E} = \mathrm{closure}(\mathbb{R}^3\backslash\mathfrak{D})$.

trivial: by (2.17), $\mathbb{G}(X_1)\tau = \mathbb{P}_2(X_2)\mathbb{G}(X_1)\tau$ for τ tangent at $X_1 \in \mathcal{S}_1$, and $\mathbb{P}_2(X_2)\mathbb{G}(X_1) \in \mathrm{lin}(\mathbf{n}_1(X_1)^\perp, \mathbf{n}_2(X_2)^\perp)$ is invertible. We define the tensor field $\mathbb{G}_{\mathrm{surf}}$ on $\mathcal{S}_1$ by

$$\mathbb{G}_{\mathrm{surf}}(X_1) = \mathbb{P}_2(X_2)\mathbb{G}(X_1); \tag{2.19}$$

then, omitting arguments,

$$\begin{aligned} &(\mathbb{G}_{\mathrm{surf}})^{-1} = \mathbb{P}_1\mathbf{G}^{-1}\mathbb{I}_2, \\ &\mathbf{G} = \mathbb{I}_2(\mathbb{G}_{\mathrm{surf}})\mathbb{P}_1 + (\mathbf{G}\mathbf{n}_1)\otimes\mathbf{n}_1. \end{aligned} \tag{2.20}$$

If we apply the transpose of $(2.20)_2$ to $\mathbb{I}_2$ and use (2.2) and the fact that $\mathbb{P}_2\mathbb{I}_2$ is the identity on $\mathbf{n}_2{}^\perp$, we arrive at the useful identity:

$$\mathbf{G}^{T}\mathbb{I}_2 = \mathbb{I}_1(\mathbb{G}_{\mathrm{surf}})^{T} + \mathbf{n}_1\otimes\mathbb{P}_2\mathbf{G}\mathbf{n}_1. \tag{2.21}$$

We define the **superficial Jacobian** $\det\mathbb{G}$ through the relation

$$\det\mathbb{G}(X_1) = \frac{|\mathbb{G}(X_1)\tau \times \mathbb{G}(X_1)\nu|}{|\tau\times\nu|}, \tag{2.22}$$

where τ and ν are arbitrary vectors in $\mathbf{n}_1(X_1)^\perp$ with $\tau\times\nu \neq 0$ (the particular choice being irrelevant). Then

$$\det\mathbf{G} = \lambda\det\mathbb{G}. \tag{2.23}$$

The superficial Jacobian and the **adjugate** $\mathrm{adj}\,\mathbb{G}$ of $\mathbb{G}$ defined by

$$\mathrm{adj}\,\mathbb{G} = (\det\mathbb{G})(\mathbb{G}_{\mathrm{surf}})^{-T} \tag{2.24}$$

may be used to relate integrals over surfaces and curves in $\mathcal{S}_1$ to corresponding integrals for $\mathcal{S}_2$. Let $\mathcal{R}_i$ denote a sufficiently regular subsurface of $\mathcal{S}_i$ with $\mathcal{R}_2 = g(\mathcal{R}_1)$, and let ν_i denote the *outward unit normal* to the boundary curve $\partial\mathcal{R}_i$. Then, for Φ, v, and $\mathbb{B}_2$, respectively, a scalar, vector, and superficial tensor field on $\mathcal{S}_2$,

$$\begin{aligned} \int_{\mathcal{R}_2} \Phi\, da &= \int_{\mathcal{R}_1} (\Phi \circ g)(\det \mathbb{G})\, da, \\ \int_{\partial\mathcal{R}_2} \mathbb{B}_2 \nu_2\, ds &= \int_{\partial\mathcal{R}_1} \mathbb{B}_1 \nu_1\, ds, \\ \int_{\partial\mathcal{R}_2} v \cdot \mathbb{B}_2 \nu_2\, ds &= \int_{\partial\mathcal{R}_1} (v \circ g) \cdot \mathbb{B}_1 \nu_1\, ds, \end{aligned} \tag{2.25}$$

where

$$\mathbb{B}_1 = (\mathbb{B}_2 \circ g)\, \mathrm{adj}\, \mathbb{G}. \tag{2.26}$$

2.2. Smoothly propagating surfaces.

Let $\mathcal{S}(t)$ $(t \in T)$ denote a one-parameter family of surfaces in $\mathbb{R}^3$, with T, the underlying **time interval**, an open interval of $\mathbb{R}$, and let

$$\begin{aligned} \mathcal{S}_T &= \{ (X,t) : X \in \mathcal{S}(t),\ t \in T \}, \\ (\partial\mathcal{S})_T &= \{ (X,t) : X \in \partial\mathcal{S}(t),\ t \in T \}. \end{aligned} \tag{2.27}$$

Fix $t \in T$ and let $Y(\beta) \in \mathbb{R}^3$ be defined and smooth for β in some neighborhood of t. Then:

(i) $Y(\beta)$ is an **$\mathcal{S}$-trajectory** through X at time t provided $Y(t) = X$ and $Y(\beta) \in \mathcal{S}(\beta)$ for all β;

(ii) $Y(\beta)$ is a **$\partial\mathcal{S}$-trajectory** through X at time t provided $Y(t) = X$ and $Y(\beta) \in \partial\mathcal{S}(\beta)$ for all β.

In either case, we write

$$Y^{\cdot}(\beta) = dY(\beta)/d\beta.$$

We will refer to $\mathcal{S}(t)$ $(t\in T)$ as a **smoothly propagating surface** if:[21]

(i) for each $t\in T$, $\mathcal{S}(t)$ is an oriented, nonintersecting, smooth, possibly unbounded[22] surface with a smooth (possibly empty) boundary-curve $\partial\mathcal{S}(t)$;

(ii) the sets $\mathcal{S}_T$ and $(\partial\mathcal{S})_T$ are smooth manifolds in $\mathbb{R}^3\times\mathbb{R}$, and the orientation $\mathbf{n}(X,t)$ for $\mathcal{S}(t)$ is smooth in (X,t) on $\mathcal{S}_T$;

(iii) given any $t\in T$, there is a *smooth* $\mathcal{S}$-trajectory through each point of $\mathcal{S}(t)$ and a *smooth* $\partial\mathcal{S}$-trajectory through each point of $\partial\mathcal{S}(t)$.

We will consistently write

$\mathcal{S}$ *for the one-parameter family* $\mathcal{S}(t)$ $(t\in T)$.

Superficial fields and *tangential fields* for $\mathcal{S}$ are as specified in Section 2.1; they are defined on $\mathcal{S}_T$, but are superficial or tangential with respect to $\mathcal{S}(t)$ at each $t\in T$ (rather than with respect to $\mathcal{S}_T$), and a similar interpretation applies to the *tangential projection* and *tangential inclusion* for $\mathcal{S}$. Similarly, $\nabla_{\mathcal{S}}$ and $\mathrm{div}_{\mathcal{S}}$ denote the surface gradient and surface divergence on $\mathcal{S}(t)$ for fixed t.

Let $\mathcal{S}$ be a smoothly propagating surface, and let $\mathbf{n}(X,t)$ denote the orientation for $\mathcal{S}(t)$ and $\boldsymbol{\nu}(X,t)$ the outward unit normal to the boundary curve $\partial\mathcal{S}(t)$.

(2A) Lemma.

(i) *Choose* $t\in T$. *Then, for each* $X\in\mathcal{S}(t)$, $v_{\mathcal{S}}(X,t)$ *defined by*

$$v_{\mathcal{S}}(X,t) = Y^{\cdot}(t)\cdot\mathbf{n}(X,t) \tag{2.28}$$

is independent of the $\mathcal{S}$-*trajectory* $Y(\beta)$ *through* X *at* t, *and, for each* $X\in\partial\mathcal{S}(t)$, $v_{(\partial\mathcal{S})\tan}(X,t)$ *defined by*

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[21] Cf. Gurtin [1988a].

[22] As a set in $\mathbb{R}^3$.

$$v_{(\partial\mathcal{S})\tan}(X,t) = Y^{\cdot}(t)\cdot\boldsymbol{\nu}(X,t) \tag{2.29}$$

is independent of the $\partial\mathcal{S}$-trajectory $Y(\beta)$ *through* X *at* t.

(ii) *The field* $(\mathbf{n},-v_{\mathcal{S}})$ *is normal to* $\mathcal{S}_T$; *the fields* $(\mathbf{n},-v_{\mathcal{S}})$ *and* $(\boldsymbol{\nu},-v_{(\partial\mathcal{S})\tan})$ *are normal to* $(\partial\mathcal{S})_T$.

Proof. Choose $(X,t)\in\mathcal{S}_T$ and write $\mathbf{n}=\mathbf{n}(X,t)$. There is a unique scalar α such that $(\mathbf{n},\alpha)$ is normal to $\mathcal{S}_T$ at (X,t). Choose an $\mathcal{S}$-trajectory $Y(\beta)$ through X at t. Since $(Y(\beta),\beta)$ is a curve on $\mathcal{S}_T$, its derivative at $t=\beta$ must be orthogonal to $(\mathbf{n},\alpha)$; hence $\alpha=-Y^{\cdot}(t)\cdot\mathbf{n}$. Thus $v_{\mathcal{S}}(X,t)$ is independent of $Y(\beta)$ and $(\mathbf{n},-v_{\mathcal{S}})$ is normal to $\mathcal{S}_T$.

Similarly, choose $(X,t)\in(\partial\mathcal{S})_T$ and write $\mathbf{n}=\mathbf{n}(X,t)$, $\boldsymbol{\nu}=\boldsymbol{\nu}(X,t)$. There is a unique scalar λ such that $(\boldsymbol{\nu},\lambda)$ is tangent to $\mathcal{S}_T$ and normal to $(\partial\mathcal{S})_T$ at (X,t). The remainder of the proof follows as in the preceding paragraph. ■

The following terminology is useful: $v_{\mathcal{S}}$ is the **normal speed**[23] of $\mathcal{S}$; $v_{(\partial\mathcal{S})\tan}$ is the **intrinsic edge speed** of $\mathcal{S}$;

$$\mathbf{v}_{\mathcal{S}} = v_{\mathcal{S}}\,\mathbf{n} \tag{2.30}$$

is the **normal velocity** of $\mathcal{S}$;

$$\mathbf{v}_{(\partial\mathcal{S})\tan} = v_{(\partial\mathcal{S})\tan}\,\boldsymbol{\nu} \tag{2.31}$$

is the **intrinsic tangential edge velocity** of $\mathcal{S}$;

$$\mathbf{v}_{\partial\mathcal{S}} = \mathbf{v}_{\mathcal{S}} + \mathbf{v}_{(\partial\mathcal{S})\tan} \tag{2.32}$$

is the **intrinsic edge velocity** of $\mathcal{S}$ (Figure 2A).

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[23] We use the term speed even though $v_{\mathcal{S}}$ and $v_{(\partial\mathcal{S})\tan}$ may have negative values.

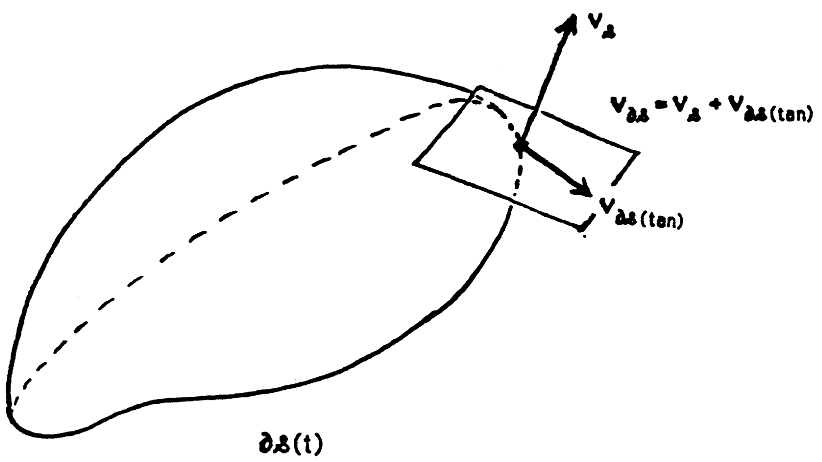

Figure 2A. The intrinsic velocities at the edge of an evolving surface $\mathcal{S}(t)$. $V_{\mathcal{S}}$ is normal to $\mathcal{S}(t)$; $V_{\partial\mathcal{S}(tan)}$ is tangent to $\mathcal{S}(t)$ and normal to $\partial\mathcal{S}(t)$. The plane shown is tangent to $\mathcal{S}(t)$ at the point of $\partial\mathcal{S}(t)$ under consideration.

More generally,[24] a smooth field $\mathbf{v}$ on $\mathcal{S}_T$ is a **velocity field for** $\mathcal{S}$ if

$$\mathbf{v}\cdot\mathbf{n} = V_{\mathcal{S}}\,; \tag{2.33}$$

a smooth field $\mathbf{v}$ on $(\partial\mathcal{S})_T$ is an **edge velocity for** $\mathcal{S}$ if

$$\mathbf{v}\cdot\mathbf{n} = V_{\mathcal{S}}, \qquad \mathbf{v}\cdot\boldsymbol{\nu} = V_{(\partial\mathcal{S})\tan}\,. \tag{2.34}$$

(2B) **Lemma.** *Let* $\mathbf{v}$ *be a smooth vector field on* $\mathcal{S}_T$; *then* $\mathbf{v}$ *is a velocity field for* $\mathcal{S}$ *if and only if, given any* $t\in T$ *and any* $X\in\mathcal{S}(t)$, *there is a locally unique* $\mathcal{S}$*-trajectory* $Y(\beta)$ *through* X *at* t *with*

$$Y^{\cdot}(\beta) = \mathbf{v}(Y(\beta),\beta) \tag{2.35}$$

for all β *near* t. *An analogous statement applies with "*$\mathcal{S}$*" replaced by "*$\partial\mathcal{S}$*" and "velocity field" by "edge velocity".*

Proof. We will prove that portion of the Lemma regarding $\mathcal{S}$. The "if" assertion is a direct consequence of (2.28) and the definition of a smoothly-evolving surface. To establish the "only if" assertion assume that $\mathbf{v}$ is a velocity field. Choose $t\in T$ and $X\in\mathcal{S}(t)$. Then near $\beta=t$ there is is a locally unique solution $Y(\beta)$ of (2.35) that passes through X at t. We have only to show that $Y(\beta)\in\mathcal{S}(\beta)$. But this follows from the fact that, because of (2.33) and (2Aii), the vector $(d/d\beta)(Y(\beta),\beta)$ is, for each β, tangential to $\mathcal{S}_T$ at $(Y(\beta),\beta)$, so that $(Y(\beta),\beta)$ describes a curve on $\mathcal{S}_T$. ∎

The trajectories corresponding to the the normal velocity are

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[24] An evolving surface described in parametric form $\mathbf{x}=\mathbf{x}(p,t)$ (where p ranges in a region in $\mathbb{R}^2$) has an associated velocity field defined by $\partial_t\mathbf{x}(p,t)$. Changes in velocity field then correspond to changes in parametrization; a basic axiom of our theory is that the underlying physics be invariant under reparametrization.

called **normal trajectories**; and the **time derivative** $\Phi^{\circ}(X,t)$ **following** $\mathcal{S}$ of a scalar, vector, or tensor function $\Phi(X,t)$ is defined by

$$\Phi^{\circ}(X,t) = (\partial/\partial\beta)\Phi(\mathcal{Y}(\beta),\beta)\big|_{\beta=t}, \qquad (2.36)$$

with $\mathcal{Y}(\beta)$ the *normal* $\mathcal{S}$-trajectory through X at t. We then have the well known relation

$$n^{\circ} = -\nabla_{\mathcal{S}} v_{\mathcal{S}}. \qquad (2.37)$$

(2C) Transport Theorem.[25] *Let* Φ *be a smooth superficial scalar field on a bounded, smoothly propagating surface* $\mathcal{S}$. *Then*

$$(d/dt)\Big\{\int_{\mathcal{S}(t)}\Phi\, da\Big\} = \int_{\mathcal{S}(t)}(\Phi^{\circ} - \Phi\kappa v_{\mathcal{S}})\,da + \int_{\partial\mathcal{S}(t)}\Phi\, v_{(\partial\mathcal{S})\tan}\,ds. \qquad (2.38)$$

We will refer to $\mathcal{R}(t)$ $(t\in T_0\subset T)$ as a **smoothly propagating subsurface** of $\mathcal{S}$ if $\mathcal{R}$ is a *bounded*, smoothly propagating surface with $\mathcal{R}(t)\subset\mathcal{S}(t)$ at each $t\in T_0$.

2.3. Response functions.

The following notation is convenient:

$$\begin{aligned} \mathrm{Lin}^{+} &= \{\, F\in \mathrm{Lin}(\mathbb{R}^3,\mathbb{R}^3) : \det F > 0 \,\}, \\ \mathrm{Unit} &= \{\, n\in\mathbb{R}^3 : |n| = 1 \,\}. \end{aligned} \qquad (2.39)$$

In discussing phase interfaces we will consider functions

$$\Phi(F,n,v,z) \qquad (2.40)$$

with **domain** $\mathrm{Dom}(\Phi)$ an open set in $\mathrm{Lin}^{+}\times\mathrm{Unit}\times\mathbb{R}\times\mathbb{R}^{p}$ $(p<\infty)$ of the form

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[25] Gurtin, Struthers, and Williams [1989].

$$\mathrm{Dom}(\Phi) = \{ (F,\mathbf{n},v,z) : (F,\mathbf{n},v)\in \mathrm{Lin}^{+}\times \mathrm{Unit}\times \mathbb{R},\ z\in Z(F,\mathbf{n}) \}, \qquad (2.41)$$

where $Z(F,\mathbf{n})$ is an open subset of $\mathbb{R}^{p}$ for each $(F,\mathbf{n})\in \mathrm{Lin}^{+}\times \mathrm{Unit}$. In applications F will be the deformation gradient, $\mathbf{n}$ and v the orientation and normal speed of the interface, and $\mathbf{z}$ a list of variables of lesser importance.[26] Let

$$\mathbf{p} = (F,\mathbf{n},v,z).$$

We write

$$\partial_F\Phi(\mathbf{p})\in \mathrm{Lin}(\mathbb{R}^3,\mathbb{R}^3), \quad \partial_n\Phi(\mathbf{p})\in \mathbf{n}^{\perp}, \quad \partial_v\Phi(\mathbf{p})\in \mathbb{R}, \quad \partial_z\Phi(\mathbf{p})\in \mathbb{R}^{p} \qquad (2.42)$$

for the partial derivatives of $\Phi(\mathbf{p})$ with respect to F, $\mathbf{n}$, v, and z.

For the remainder of this section we suppress the arguments v and z, which are irrelevant to our discussion, and we return to our original notation in which $\mathbb{P}(\mathbf{n})$ and $\mathbb{I}(\mathbf{n})$ are the projection and inclusion as defined in Section 2.1a. Given $\mathbf{n}\in \mathrm{Unit}$, a tensor $F\in \mathrm{Lin}^{+}$ admits the unique decomposition

$$F = \mathbb{F}\mathbb{P}(\mathbf{n}) + \mathbb{f}\otimes \mathbf{n}, \qquad \mathbb{F}\in \mathrm{Lin}(\mathbf{n}^{\perp},\mathbb{R}^3), \qquad \mathbb{f}\in \mathbb{R}^3, \qquad (2.43)$$

with

$$\mathbb{F} = F\,\mathbb{I}(\mathbf{n}), \qquad \mathbb{f} = F\mathbf{n} \qquad (2.44)$$

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[26] When we study coherent crystal-crystal interactions F will be the deformation gradient in one of the phases, $F+\mathbf{u}\otimes\mathbf{n}$ the deformation gradient in the other; here we take $Z(F,\mathbf{n})$ to be the set of all $\mathbf{u}\in\mathbb{R}^3$ with $F+\mathbf{u}\otimes\mathbf{n}\in \mathrm{Lin}^{+}$. More generally, $\mathrm{Dom}(\Phi)$ might be an open subset of a manifold in $\mathrm{Lin}^{+}\times\mathrm{Unit}\times\mathbb{R}\times\mathbb{R}^{p}$ to allow for constraints on z dependent on F, $\mathbf{n}$, and v.

(so that $\mathbb{F}$ is simply the restriction of F to $n^{\perp}$). In applications $\mathbb{F}$ and $\mathbb{f}$ represent the tangential and normal deformation gradients relative to the interface. The decomposition (2.43) allows us to consider $\Phi(F,n)$ as a function

$$\Phi^{\sim}(\mathbb{F},\mathbb{f},n) = \Phi(\mathbb{F}\mathbb{P}(n) + \mathbb{f}\otimes n, n) \tag{2.45}$$

of the "components" $\mathbb{F}$ and $\mathbb{f}$ relative to n. The partial derivatives $\partial_{\mathbb{F}}\Phi(F,n)\in \mathrm{Lin}(n^{\perp},\mathbb{R}^3)$ and $\partial_{\mathbb{f}}\Phi(F,n)\in\mathbb{R}^3$ are then the corresponding partial derivatives of $\Phi^{\sim}(\mathbb{F},\mathbb{f},n)$:

$$\partial_{\mathbb{F}}\Phi(F,n)\cdot\mathbb{A} + \partial_{\mathbb{f}}\Phi(F,n)\cdot\mathbb{a} = (d/d\beta)\Phi(G(\beta),n)\big|_{\beta=0}, \tag{2.46}$$

where

$$G(\beta) = \mathbb{G}(\beta)\mathbb{P}(n) + \mathbb{g}(\beta)\otimes n \tag{2.47}$$

is a curve in Lin^{+} with $\mathbb{G}(0)=\mathbb{F}$, $\mathbb{G}^{\cdot}(0)=\mathbb{A}$, $\mathbb{g}(0)=\mathbb{f}$, $\mathbb{g}^{\cdot}(0)=\mathbb{a}$.

The partial derivative of $\Phi^{\sim}(\mathbb{F},\mathbb{f},n)$ with respect to n is not as easy to define, since both $\mathbb{F}$ and $\mathbb{f}$ depend on the choice of n. Given $n,n'\in\mathrm{Unit}$, $n\neq n'$, let $Q(n',n)$ denote the rotation of n' into n about the axis orthogonal to n' and n, and let $Q(n,n)$ be the identity on $\mathbb{R}^3$. Then the components $\mathbb{F}'=F'\mathbb{I}(n')$ and $\mathbb{f}'=F'n'$ of $F'=FQ(n',n)$ relative to n' are, modulo the rotation $Q(n',n)$, the same as those for F with respect to n. We define the partial derivative $D_n\Phi(F,n)\in n^{\perp}$ (or $D_n\Phi^{\sim}(\mathbb{F},\mathbb{f},n)$) with respect to n **following the surface**[27] as follows:

$$D_n\Phi(F,n)\cdot a = (d/d\beta)\Phi(FQ(k(\beta),n),k(\beta))\big|_{\beta=0} \tag{2.48}$$

for $k(\beta)$ a smooth curve in Unit satisfying $k(0)=n$, $k^{\cdot}(0)=a$.

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[27] In applications n will be the outward unit normal to the crystal surface.

(2D) Lemma.

$$\begin{aligned} \partial_{\mathbb{F}}\Phi(F,n) &= \partial_F\Phi(F,n)\mathbb{I}(n), \\ \partial_{\mathbb{f}}\Phi(F,n) &= \partial_F\Phi(F,n)n, \\ D_n\Phi(F,n) &= \partial_n\Phi(F,n) + \partial_{\mathbb{F}}\Phi(F,n)^T\mathbb{f} - \mathbb{F}^T\partial_{\mathbb{f}}\Phi(F,n). \end{aligned} \tag{2.49}$$

Proof. By (2.46),

$$\partial_{\mathbb{F}}\Phi(F,n)\cdot\mathbb{A} + \partial_{\mathbb{f}}\Phi(F,n)\cdot\mathbb{a} = \partial_F\Phi(F,n)\cdot\{\mathbb{A}\mathbb{P}(n) + \mathbb{a}\otimes n\},$$

which implies $(2.49)_{1,2}$, since $\mathbb{P}(n)^T = \mathbb{I}(n)$. Next, for $k(\beta)$ as in (2.48),

$$(d/d\beta)Q(k(\beta),n)\big|_{\beta=0} = n\otimes a - a\otimes n,$$

and thus, as a consequence of (2.48),

$$D_n\Phi(F,n)\cdot a = \partial_n\Phi(F,n)\cdot a + \partial_F\Phi(F,n)\cdot\{F(n\otimes a - a\otimes n)\};$$

therefore, since a is an arbitrary vector in $n^\perp$,

$$D_n\Phi(F,n) = \partial_n\Phi(F,n) + \mathbb{P}(n)[\partial_F\Phi(F,n)^TFn - F^T\partial_F\Phi(F,n)n],$$

which, with (2.43), (2.44), and $(2.49)_{1,2}$, yields $(2.49)_3$. ■

We say that Φ is **intrinsic to the surface** if

$$\Phi(F_1,n) = \Phi(F_2,n) \quad \textit{whenever} \quad F_1\mathbb{I}(n) = F_2\mathbb{I}(n). \tag{2.50}$$

Roughly speaking, Φ is intrinsic to the surface if Φ depends on F only through $\mathbb{F}\,(= F\mathbb{I}(n))$; in applications, with n the outward normal to the surface and F the deformation gradient, (2.50) implies that Φ depends on F only through the *tangential* gradient. Conditions more useful than (2.50) are furnished by the following

(2E) Lemma. *Let* $\mathfrak{D} = \mathrm{Lin}^{+} \times \mathrm{Unit}$. *The following are equivalent:*

(i) Φ *is intrinsic to the surface;*

(ii) *given any* $(F,n) \in \mathfrak{D}$, $\Phi(F,n) = \Phi(F + u \otimes n, n)$ *for all* u *with* $F + u \otimes n \in \mathrm{Lin}^{+}$;

(iii) $\partial_{\mathbb{f}} \Phi(F,n) = 0$ *for all* $(F,n) \in \mathfrak{D}$, *so that* $\Phi^{\sim}(\mathbb{F},\mathbb{f},n)$ *is independent of* $\mathbb{f}$;

(iv) $\partial_{\mathbb{F}} \Phi(F,n)\mathbb{P}(n) = \partial_{F} \Phi(F,n)$ *for all* $(F,n) \in \mathfrak{D}$.

Proof. Choose $(F,n) \in \mathfrak{D}$, $u \in \mathbb{R}^3$. Since $(u \otimes n)\mathbb{I}(n) = 0$, we may conclude from (2.43) that (i) $\Leftrightarrow$ (ii). Next, by $(2.49)_2$, for $F(\beta) = F + \beta u \otimes n$,

$$(d/d\beta)\Phi(F(\beta),n) = \partial_F \Phi(F(\beta),n) \cdot (u \otimes n) = \partial_{\mathbb{f}} \Phi(F(\beta),n) \cdot u \qquad (2.51)$$

whenever $F(\beta) \in \mathrm{Lin}^{+}$. Since $F(\beta) \in \mathrm{Lin}^{+}$ for sufficiently small β, if (ii) holds, then (2.51) vanishes at $\beta = 0$, and this yields (iii). Conversely, assume that (iii) holds. Let $F + u \otimes n \in \mathrm{Lin}^{+}$. Then $F(\beta) \in \mathrm{Lin}^{+}$ for $0 \leq \beta \leq 1$ and, by (iii), (2.51) vanishes for all such β; this yields (ii). Hence (ii) $\Leftrightarrow$ (iii). Finally, by $(2.49)_2$, (iii) $\Leftrightarrow$ (iv). ■

(2F) Lemma. *Let* Φ *be intrinsic to the surface. Then* $\partial_{\mathbb{F}} \Phi$ *and* $D_n \Phi$ *are intrinsic to the surface, but* $\partial_n \Phi$ *is intrinsic if and only if* $\partial_{\mathbb{F}} \Phi = 0$, *in which case* Φ *is independent of* F *and* $D_n \Phi = \partial_n \Phi$.

Proof. Choose F_1, F_2 with $F_1 \mathbb{I}(n) = F_2 \mathbb{I}(n)$, and let $F_i(\beta) = F_i + \beta \mathbb{A} \mathbb{P}(n)$, with $\mathbb{A} \in \mathrm{Lin}(n^{\perp}, \mathbb{R}^3)$ *arbitrary.* Then $F_1(\beta)\mathbb{I}(n) = F_2(\beta)\mathbb{I}(n)$, and thus differentiating $\Phi(F_i(\beta),n)$ with respect to β at $\beta = 0$ gives $\partial_{\mathbb{F}} \Phi(F_1,n) = \partial_{\mathbb{F}} \Phi(F_2,n)$. Similarly, using the notation of (2.48), $F_1 Q(k(\beta),n)\mathbb{I}(k(\beta)) = F_2 Q(k(\beta),n)\mathbb{I}(k(\beta))$, so that $\Phi(F_1 Q(k(\beta),n),k(\beta)) = \Phi(F_2 Q(k(\beta),n),k(\beta))$ and (2.48) yields

$D_n\Phi(F_1,n) = D_n\Phi(F_2,n)$.

To prove the last assertion of the lemma, suppose that Φ is intrinsic to the surface. Then, by $(2.49)_3$ and Lemma (2Eiii),

$$D_n\Phi(F,n) = \partial_n\Phi(F,n) + \partial_{\mathbb{F}}\Phi(F,n)^T\mathbb{f}, \tag{2.52}$$

and $\partial_n\Phi$ is intrinsic if $\partial_{\mathbb{F}}\Phi = 0$. On the other hand, assume that $\partial_n\Phi$ is intrinsic. Choose $F \in \mathrm{Lin}^+$ and $n \in \mathrm{Unit}$, and let $\mathbf{a}$ be an arbitrary vector. Then $G = F + \varepsilon\mathbf{a}\otimes n$ belongs to Lin^+ for $\varepsilon > 0$ sufficiently small, and $F\mathbb{I}(n) = G\mathbb{I}(n)$; thus (2.52) yields

$$\partial_{\mathbb{F}}\Phi(F,n)^T(Fn - Gn) = \partial_{\mathbb{F}}\Phi(F,n)^T\mathbf{a} = 0$$

and $\partial_{\mathbb{F}}\Phi(F,n) = 0$. ■

3. The kinematics of evolving crystals.

3.1. Crystal lattices. Crystals.

By a **uniform label change** we mean an *affine* transformation g of $\mathbb{R}^3$ onto $\mathbb{R}^3$ whose gradient ∇g has strictly positive determinant.

A **crystal lattice** is a set $\mathcal{L}$ together with a family of bijections of $\mathcal{L}$ onto $\mathbb{R}^3$, called **configurations** (of $\mathcal{L}$), such that:[28]

(i) if μ and λ are configurations, then $\mu \circ \lambda^{-1}$ is a uniform label change;

(ii) if μ is a configuration and g a uniform label change, then $g \circ \mu$ is a configuration.

We assume that a **crystal lattice** $\mathcal{L}$ is prescribed. We use the following notation and terminology: points $X \in \mathcal{L}$ are **material points**; $\mathrm{X} = \mu(X)$ is the material point X **labelled** by its position X in the configuration μ; if μ_1 and μ_2 are configurations, then $g = \mu_2 \circ \mu_1^{-1}$ and $G = \nabla g$ are the **label change** and **label gradient** from μ_1 to μ_2.

We assign to each configuration μ of $\mathcal{L}$ a strictly positive (constant) **mass density** ρ_μ, with densities ρ_1 and ρ_2 for arbitrary configurations μ_1 and μ_2 related by

$$\rho_2 = \rho_1 \det G. \tag{3.1}$$

By a **crystal** (of the lattice $\mathcal{L}$) we mean a subset C of the lattice such that $C_\mu = \mu(C)$ is a regular region in some (and hence every) configuration μ. The set ∂C defined by $\mu(\partial C) = \partial(C_\mu)$ is then independent of μ and represents the **crystal surface**; C_μ and ∂C_μ are the *crystal and crystal surface labelled in* μ.

3.2. Motion of an evolving crystal.

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[28] Our definition is patterned after Noll's [1958] definition of a body. Thus the terms "crystal lattice" and "configuration" might more appropriately be called "uniform crystal lattice" and "uniform configuration".

In contrast to standard continuum mechanics, we allow evolving crystals to gain and lose material points by *accretion* at the crystal surface. The next definition makes this precise.

Let $C(t)$ $(t \in T)$ be a one-parameter family of crystals with *time* t as parameter. Then $C(t)$ $(t \in T)$ is an **evolving crystal** if $\partial C_\mu(t)$ $(t \in T)$ is a smoothly propagating surface for some (and hence every) configuration μ.

Our interest is in describing crystals which *deform* as they evolve. Each such time-dependent deformation, or *motion,* is described by a time-dependent mapping $\varkappa(t)$ that carries $C(t)$ onto a region $c(t)$ in $\mathbb{R}^3$. It is convenient to write

$$\varkappa(t)(X) = \varkappa(X,t),$$

so that $x = \varkappa(X,t)$ is the point of space occupied by the material point X at time t in the motion. The differential properties of motions are best described by labelling material points X by their positions X in a configuration μ. Thus we write

$$\varkappa_\mu(X,t) = \varkappa(\mu^{-1}(X),t)$$

for $X \in C_\mu(t)$, so that

$$c(t) = \varkappa(C(t),t) = \varkappa_\mu(C_\mu(t),t) \tag{3.2}$$

(Figure 3A).

Precisely, a **crystal motion** is a one-parameter family of mappings $\varkappa(t) : C(t) \to c(t)$ $(t \in T)$ with the following properties:

(i) $C(t)$ $(t \in T)$ is an evolving crystal;

(ii) for some (and hence every) configuration μ, the mapping $X \mapsto \varkappa_\mu(X,t)$ is a deformation of $C_\mu(t)$ onto $c(t)$ at each $t \in T$, and the mapping $(X,t) \mapsto \varkappa_\mu(X,t)$ is smooth.

Let μ, the **reference configuration**, be a fixed configuration of the lattice. Assume that a crystal motion $\varkappa(t) : C(t) \to c(t)$ $(t \in T)$ is given. Then $C_\mu(t)$ consists of the points of the lattice (labelled in

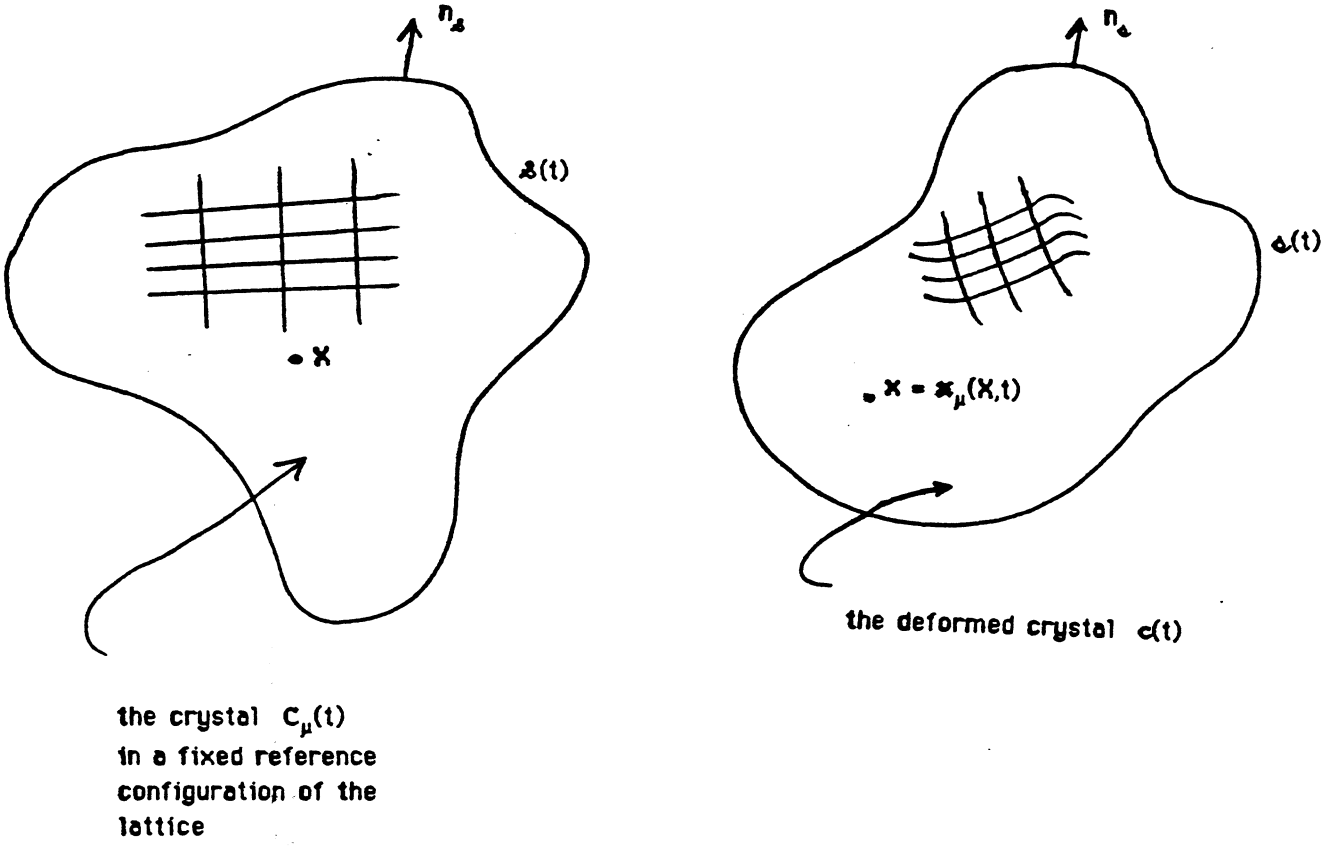

Figure 3A. A crystal motion

μ) which comprise the crystal at time t, while $c(t)$ is the region in space occupied by the *deformed* crystal at time t. The following notation and terminology are useful: $\mathbf{x} = \chi(X,t)$ is the **place** occupied by the material point X at time t; $(\mathbf{X},t) \mapsto \chi_\mu(\mathbf{X},t)$ describes the **motion relative to μ** with material points X **labelled** by their positions $\mathbf{X} = \mu(X)$ in μ;

$$F(\mathbf{X},t) = \nabla \chi_\mu(\mathbf{X},t) \tag{3.3}$$

is the **deformation gradient relative to μ**;

$$\rho_c(\mathbf{x},t) = \rho_\mu \det F(\mathbf{X},t)^{-1}, \qquad (3.4)[29]$$

is the **crystal density** at $\mathbf{x} \in c(t)$ in the motion;

$$\mathcal{S}(t) = \partial C_\mu(t), \qquad \mathcal{D}(t) = \partial c(t) \tag{3.5}$$

are the **reference** and **deformed surfaces**. In addition:

$\nabla_{\mathcal{S}}$, $\nabla_{\mathcal{D}}$	surface gradients on $\mathcal{S}$ and $\mathcal{D}$;
$\mathrm{div}_{\mathcal{S}}$, $\mathrm{div}_{\mathcal{D}}$	surface divergences on $\mathcal{S}$ and $\mathcal{D}$;
$\mathbf{n}_{\mathcal{S}}$, $\mathbf{n}_{\mathcal{D}}$	outward[30] normals for $\mathcal{S}$ and $\mathcal{D}$;
$\mathbb{P}_{\mathcal{S}}$, $\mathbb{P}_{\mathcal{D}}$	tangential projections for $\mathcal{S}$ and $\mathcal{D}$;
$\mathbb{I}_{\mathcal{S}}$, $\mathbb{I}_{\mathcal{D}}$	tangential inclusions for $\mathcal{S}$ and $\mathcal{D}$;
$\mathbb{L}$	curvature tensor for $\mathcal{S}$;
κ	total curvature of $\mathcal{S}$.

Then, by (2.16),

$$\mathbf{n}_{\mathcal{D}}(\mathbf{x},t) = \ell(\mathbf{X},t)F(\mathbf{X},t)^{-\mathrm{T}}\mathbf{n}_{\mathcal{S}}(\mathbf{X},t), \tag{3.6}$$

---

[29] Here and in what follows, in equations relating functions $f(\mathbf{x},t)$ and functions $g(\mathbf{X},t)$, it will always be understood that $\mathbf{x} = \chi_\mu(\mathbf{X},t)$; in fact, we will often omit arguments entirely.

[30] With respect to $\partial C_\mu(t)$ and $\partial c(t)$, respectively.

with

$$\ell = |F^{-T} n_{\mathscr{S}}|^{-1} \tag{3.7}$$

the change in length scale in the direction perpendicular to the crystal surface.

The **tangential deformation gradient**[31] $\mathbb{F}(X,t)$ is defined at each $X \in \mathscr{S}(t)$ by

$$\mathbb{F}(X,t) = \nabla_{\mathscr{s}} \boldsymbol{x}_{\mu}(X,t) = F(X,t)\mathbb{I}_{\mathscr{S}}(X,t). \tag{3.8}$$

$\mathbb{F}(X,t)$ is a linear transformation from the tangent plane at $X \in \mathscr{S}(t)$ into $\mathbb{R}^3$, but $\mathbb{F}(X,t)$ actually *maps tangent vectors at* $X \in \mathscr{S}(t)$ *to tangent vectors at* $x \in \mathscr{s}(t)$. The deformation gradient F is completely determined by $\mathbb{F}$ and the **normal deformation gradient**

$$\mathfrak{f}(X,t) = F(X,t)n_{\mathscr{S}}(X,t) \tag{3.9}$$

through

$$F = \mathbb{F}\mathbb{P}_{\mathscr{S}} + \mathfrak{f} \otimes n_{\mathscr{S}}. \tag{3.10}$$

As in our discussion of (2.19), $\mathbb{F}(X,t)$ is not invertible, but the **superficial deformation gradient**

$$\mathbb{F}_{\mathrm{surf}}(X,t) = \mathbb{P}_{\mathscr{s}}(x,t)\mathbb{F}(X,t) \tag{3.11}$$

is, and

$$\mathbb{F}(X,t) = \mathbb{I}_{\mathscr{s}}(x,t)\mathbb{F}_{\mathrm{surf}}(X,t). \tag{3.12}$$

We define the **superficial Jacobian**

---

[31] Cf. Gurtin and Murdoch [1975].

$$J = \det \mathbb{F} \tag{3.13}$$

through the obvious analog of (2.22), so that, by (2.23),

$$\det F = J\ell . \tag{3.14}$$

Further, guided by (2.24), we define the **adjugate** of $\mathbb{F}$ through

$$\operatorname{adj} \mathbb{F} = J(\mathbb{F}_{surf})^{-T} . \tag{3.15}$$

In view of (3.7) and (3.14), the superficial Jacobian (3.13) may be considered a function $J = J\hat{}(F, \mathbf{n})$, $\mathbf{n} = \mathbf{n}_{\mathcal{S}}$, with

$$J\hat{}(F, \mathbf{n}) = |F^{-T}\mathbf{n}| \det F . \tag{3.16}$$

Then (cf. Section 2.3)

$$\partial_{\ell} J\hat{}(F, \mathbf{n}) = 0. \tag{3.17}$$

Less trivially, the formula

$$\partial_F(\det F) = (\det F)F^{-T} \tag{3.18}$$

and a lengthy calculation yields the identity

$$\partial_{\mathbb{F}} J\hat{}(F, \mathbf{n}) = \mathbb{I}_{\mathcal{S}} \operatorname{adj} \mathbb{F} , \tag{3.19}$$

Further, (3.16) implies that $J\hat{}(F\mathbf{Q}, \mathbf{Q}^T\mathbf{n}) = J\hat{}(F, \mathbf{n})$ for any rotation $\mathbf{Q}$; hence (2.48) has the interesting consequence:

$$D_{\mathbf{n}} J\hat{}(F, \mathbf{n}) = 0. \tag{3.20}$$

We denote by $\mathbf{v}_c(\mathbf{x},t)$ the **velocity of material points**:

$$v_c(x,t) = (\partial/\partial t)\chi_\mu(\mathsf{X},t) = (\partial/\partial t)\chi(X,t) \qquad (3.21)$$

for $x = \chi(X,t) = \chi_\mu(\mathsf{X},t)$.

Let $Y(\beta)$ denote an $\mathcal{S}$-trajectory through X at time t. Then

$$\mathsf{Y}(\beta) = \mu^{-1}(Y(\beta)) \qquad (3.22)$$

defines a "trajectory" in the lattice $\mathcal{L}$ through $\mathsf{X} = \mu^{-1}(X)$ at t; we will refer to $\mathsf{Y}(\beta)$ as the **intrinsic material trajectory** corresponding to $Y(\beta)$.

Let v be an arbitrary velocity field for $\mathcal{S}$. Fix t and $X \in \mathcal{S}(t)$, let $Y(\beta)$ denote an $\mathcal{S}$-trajectory through X at time t, and suppose that $Y(\beta)$ corresponds to v in the sense of Lemma (2B). Further, let $\mathsf{Y}(\beta)$ denote the intrinsic material trajectory corresponding to $Y(\beta)$. Then

$$y(\beta) = \chi_\mu(\mathsf{Y}(\beta),\beta) = \chi(Y(\beta),\beta) \qquad (3.23)$$

is an $\mathscr{s}$-trajectory through $x = \chi_\mu(\mathsf{X},t)$ at t, so that, by Lemma (2B),

$$\mathfrak{v}(x,t) = (d/d\beta)y(\beta)\big|_{\beta=t} \qquad (3.24)$$

defines a velocity field for $\mathscr{s}$. We will refer to $\mathfrak{v}$ as the **velocity field for $\mathscr{s}$ induced by v**. By (3.3) and (3.21),

$$\mathfrak{v}(x,t) = v_c(x,t) + F(X,t)v(X,t). \qquad (3.25)$$

We write $v_{\mathcal{S}}$ for the **normal velocity** of $\mathcal{S}$. It is important to note that the corresponding induced velocity field for $\mathscr{s}$,

$$\mathfrak{v}_{\mathscr{s}}(x,t) = v_c(x,t) + F(X,t)v_{\mathcal{S}}(X,t), \qquad (3.26)$$

is generally *not* normal. In fact, the normal speed of $\mathscr{s}$ is easily obtained from the relation

$$(\boldsymbol{\upsilon}_{\mathcal{D}} - \mathbf{v}_c)\cdot\mathbf{n}_{\mathcal{D}} = \ell v_{\mathcal{S}}, \tag{3.27}$$

which follows from (2.30), (3.6), and (3.26).

It is important to note the difference between the velocities $\mathbf{v}_c$, $\mathbf{v}_{\mathcal{S}}$, and $\boldsymbol{\upsilon}_{\mathcal{D}}$. Fix t and choose $X\in\mathcal{S}(t)$ and $x\in\mathcal{D}(t)$. Then $\mathbf{v}_c(x,t)$ is the velocity of the *material point* which at time t occupies the place x on the *deformed surface* $\mathcal{D}(t)$. $\mathbf{v}_{\mathcal{S}}(X,t)$, the *normal velocity of the undeformed surface* $\mathcal{S}(t)$, gives the rate at which the crystal surface is moving through the lattice $\mathcal{L}$, as measured in the configuration μ. This velocity is governed solely by *accretion* at the crystal surface; it is independent of the manner in which the crystal is deforming. On the other hand, $\boldsymbol{\upsilon}_{\mathcal{D}}(x,t)$ is a *velocity field for the deforming crystal surface* $\mathcal{D}(t)$; as is clear from (3.26), $\boldsymbol{\upsilon}_{\mathcal{D}}(x,t)$ *is effected by both accretion and deformation.* The fields $\mathbf{v}_{\mathcal{S}}(X,t)$, $v_{\mathcal{S}}(X,t)$, and $\boldsymbol{\upsilon}_{\mathcal{D}}(x,t)$ depend on the choice of reference configuration μ; we will refer to these respective fields as the **accretive velocity**, the **accretive speed**, and the **total velocity** of the crystal surface, relative to μ.

It is useful to consider the gradient $(\nabla_{\mathcal{S}}\boldsymbol{\upsilon}_{\mathcal{D}})(X,t)$ of $\boldsymbol{\upsilon}_{\mathcal{D}}$ considered as a function $\boldsymbol{\upsilon}_{\mathcal{D}}(\varkappa_\mu(X,t),t)$ of X on $\mathcal{S}(t)$; by the chain-rule

$$(\nabla_{\mathcal{S}}\boldsymbol{\upsilon}_{\mathcal{D}})(X,t) = \nabla_{\mathcal{D}}\boldsymbol{\upsilon}_{\mathcal{D}}(x,t)\mathbb{F}_{surf}(X,t). \tag{3.28}$$

We then have the following important **identities**:

$$\begin{aligned}
\nabla_{\mathcal{S}}\mathbf{v}_{\mathcal{S}} &= -(\mathbf{n}_{\mathcal{S}}\otimes\mathbf{n}_{\mathcal{S}}{}^\circ)\mathbb{I}_{\mathcal{S}} - v_{\mathcal{S}}\mathbb{L},\\
\nabla_{\mathcal{S}}\boldsymbol{\upsilon}_{\mathcal{D}} &= \{\mathbf{F}^\circ - \mathbf{F}(\mathbf{n}_{\mathcal{S}}\otimes\mathbf{n}_{\mathcal{S}}{}^\circ)\}\mathbb{I}_{\mathcal{S}} - v_{\mathcal{S}}\mathbf{F}\mathbb{L}.
\end{aligned} \tag{3.29}$$

The first of (3.29) follows from (2.8) and (2.36). To verify the second, let $\mathbf{a}$ be an arbitrary tangential vector field for $\mathcal{S}$. Then (2.7), (2.8), (3.9), and the symmetry of $\nabla\mathbf{F} = \nabla\nabla\varkappa_\mu$ yields

$$[\nabla_{\mathcal{S}}\mathfrak{f}]a = [(\nabla_{\mathcal{S}}F)a]n_{\mathcal{S}} - F\mathbb{L}a = [(\nabla F)n_{\mathcal{S}} - F\mathbb{L}]a,$$

so that

$$\nabla_{\mathcal{S}}\mathfrak{f} = [(\nabla F)n_{\mathcal{S}}]\mathbb{1}_{\mathcal{S}} - F\mathbb{L}.$$

Thus, using a superscript dot to denote the material time-derivative (with respect to t holding X fixed), we find, with the aid of (2.7), (3.26), and (2.37), that

$$\begin{aligned}\nabla_{\mathcal{S}}\mathscr{v}_{\mathscr{s}} = \nabla_{\mathcal{S}}[v_c + Fv_{\mathcal{S}}] &= (\nabla\chi_\mu{}^{\cdot})\mathbb{1}_{\mathcal{S}} + \nabla_{\mathcal{S}}(v_{\mathcal{S}}\mathfrak{f}) \\ &= (F^{\cdot})\mathbb{1}_{\mathcal{S}} + v_{\mathcal{S}}(\nabla_{\mathcal{S}}\mathfrak{f}) + [\mathfrak{f}\otimes(\nabla_{\mathcal{S}}v_{\mathcal{S}})]\mathbb{1}_{\mathcal{S}} \\ &= [F^{\cdot} + (\nabla F)v_{\mathcal{S}}]\mathbb{1}_{\mathcal{S}} - (\mathfrak{f}\otimes n_{\mathcal{S}}{}^{\circ})\mathbb{1}_{\mathcal{S}} - v_{\mathcal{S}}F\mathbb{L},\end{aligned}$$

which yields $(3.29)_2$, since $F^{\circ} = F^{\cdot} + (\nabla F)v_{\mathcal{S}}$ (cf. (2.36)).

Let $\mathcal{R}$ be a smoothly propagating subsurface of $\mathcal{S}$. Then

$$\mathscr{r}(t) = \chi_\mu(\mathcal{R}(t),t) \tag{3.30}$$

defines a smoothly propagating subsurface of $\mathscr{s}$. As before, if v is an edge velocity for $\mathcal{R}$, then (3.25) defines an edge velocity $\mathscr{v}$ for $\mathscr{r}$, the **edge velocity for $\mathscr{s}$ induced by v**. We write $v_{\partial\mathcal{R}}$ for the **intrinsic edge velocity** of $\mathcal{R}$,

$$\mathscr{v}_{\partial\mathscr{r}}(x,t) = v_c(x,t) + F(X,t)v_{\partial\mathcal{R}}(X,t) \tag{3.31}$$

for the corresponding induced, but not necessarily intrinsic, edge velocity for $\mathscr{r}$. In view of (2.32), $v_{\partial\mathcal{R}} = v_{\mathcal{S}} + v_{(\partial\mathcal{R})\tan}$; thus (3.26) has the following counterpart:

$$\mathscr{v}_{\partial\mathscr{r}}(x,t) = \mathscr{v}_{\mathscr{s}}(x,t) + F(X,t)v_{(\partial\mathcal{R})\tan}(X,t). \tag{3.32}$$

3.3. Notation to be used in subsequent sections.

For the remainder of the paper - unless stated to the contrary - we will use the notation and terminology of this chapter. In particular, μ is a reference configuration, fixed once and for all; $\boldsymbol{\chi}(t) : C(t) \rightarrow c(t)$ $(t \in T)$ is a crystal motion;

$$\mathscr{S}(t) = \partial C_\mu(t), \qquad \mathscr{s}(t) = \partial c(t) \tag{3.33}$$

are the reference and deformed surfaces; $\mathbb{R}$ is a smoothly evolving subsurface of $\mathscr{S}$ with

$$\mathscr{r}(t) = \boldsymbol{\chi}_\mu(\mathbb{R}(t),t) \tag{3.34}$$

the corresponding deformed subsurface; $\boldsymbol{\nu}(X,t)$ and $\boldsymbol{\tau}(x,t)$ are the outward unit normals to $\partial\mathbb{R}(t)$ and $\partial\mathscr{r}(t)$. We will often omit the argument t when considering integrals over $\mathbb{R}(t)$, $\mathscr{r}(t)$, $\partial\mathbb{R}(t)$, and $\partial\mathscr{r}(t)$.

3.4. The environment.

We assume that the crystal is surrounded by an ancillary phase that supplies atoms during accretion. For now we will not model this phase in detail; our only assumptions concern its behavior at the crystal surface. We therefore associate with the crystal motion two fields defined for $x \in \mathscr{s}(t)$ and $t \in T$:

$v_e(x,t)$ **environmental velocity,**
$\rho_e(x,t)$ **environmental density.**

The vector $v_e(x,t)$ is the velocity of the material exterior to the crystal, while $\rho_e(x,t) > 0$ is its mass density per unit deformed volume.

Much of the theory we will develop for the crystal surface will be independent of the environment. We will, however, demonstrate the particular form of our results for two specific environments. The first consists of an inviscid melt. The second occurs when the crystal exterior is a crystal consisting of another phase of the original material, and the interaction between phases is coherent. We will discuss this second environment in more detail in the next section.

3.5. Coherent crystal-crystal interactions.[32]

Suppose that the environment consists of a second solid phase of the crystal material, with the same crystal lattice $\mathcal{L}$ appropriate to both phases. Here it is convenient to refer to this second phase as the e-phase, and to the original phase as the c-phase. By a **coherent two-phase crystal motion** we mean a pair

$$\chi_c(t):\mathcal{C}(t)\to\mathscr{c}(t), \qquad \chi_e(t):\mathcal{E}(t)\to\mathscr{e}(t), \qquad t\in T, \tag{3.35}$$

of crystal motions, such that, for some (and hence every) configuration μ:

(i) at each $t\in T$, the sets $\mathcal{C}_\mu(t)$ and $\mathcal{E}_\mu(t)$ are exterior to each other, as are the sets $\mathscr{c}(t)$ and $\mathscr{e}(t)$;

(ii) $\chi_{c\mu}$ and $\chi_{e\mu}$, the motions relative to μ, are continuous across the interface $\mathcal{S}=\partial\mathcal{C}_\mu$ in the sense that, for any $t\in T$, $\chi_{c\mu}(X,t)=\chi_{e\mu}(X,t)$ at each $X\in\mathcal{S}(t)$.

For such a motion, we will identify the crystal with $\mathcal{C}$, the environment with $\mathcal{E}$, so that $\mathbf{n}_{\mathcal{S}}(X,t)$ is the outward unit normal to $\mathcal{S}(t)=\partial\mathcal{C}_\mu(t)$, $\mathbf{n}_{\mathscr{s}}(x,t)$ is the outward unit normal to $\mathscr{s}(t)=\partial\mathscr{c}(t)$, and so forth. Then, by (3.26), the corresponding deformation gradients ($F=F_c$ for phase c, F_e for phase e) and velocities satisfy the standard compatibility relations[33]

$$\begin{aligned} \mathscr{v}_{\mathscr{s}} &= v_c + F_c v_{\mathcal{S}} = v_e + F_e v_{\mathcal{S}}, \\ F_c - F_e &= u\otimes\mathbf{n}_{\mathcal{S}}, \end{aligned} \tag{3.36}$$

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[32] Cf. Robin [1974], Larche and Cahn [1978].

[33] Cf., e.g., Truesdell and Toupin [1960], Sect. 185.

so that

$$u = (F_c - F_e)n_{\mathcal{S}} = \mathbb{f}_c - \mathbb{f}_e \tag{3.37}$$

and

$$F_c \mathbb{I}_{\mathcal{S}} = F_e \mathbb{I}_{\mathcal{S}} = \mathbb{F}. \tag{3.38}$$

In addition,

$$\rho_\mu = \rho_c \det F_c = \rho_e \det F_e, \tag{3.39}$$

and the formulas (3.6) and (3.7) hold for both F_c and F_e, but with $\ell = \ell_c, \ell_e$.

4. Changes in observer.

A crucial difference between our theory and the more classical theories of continuum mechanics is that we have *two essentially independent velocities to be measured by observers: the velocity* $\mathbf{v}_c$ *of material points and the accretive velocity* $\mathbf{v}_{\mathscr{S}}$ *of the crystal surface.* Because of this we allow for two *distinct* classes of observers: a class of *spatial observers* that observes the motion of the deforming crystal, and a class of *lattice observers* that observes the evolution of the crystal surface as measured in some configuration of the lattice. As is usual, it is not the observers themselves that are needed, it is the notion of a change in observer.

Precisely, **changes in spatial and lattice observers** are defined by smooth transformations

$$\begin{aligned} \mathbf{x} &\mapsto \mathbf{x}^* = \mathbf{Q}(t)\mathbf{x} + \mathbf{q}(t), \\ \mathbf{X} &\mapsto \mathbf{X}^* = \mathbf{L}(t)\mathbf{X} + \mathbf{l}(t), \end{aligned} \tag{4.1}$$

with $\mathbf{Q}(t)$ and $\mathbf{L}(t)$ *rotations* and $\mathbf{q}(t)$ and $\mathbf{l}(t)$ vectors at each $t \in T$. The corresponding time-derivatives

$$\begin{aligned} \mathbf{w}(\mathbf{x},t) &= \mathbf{Q}^{\cdot}(t)\mathbf{x} + \mathbf{q}^{\cdot}(t), \\ \mathbf{w}_L(\mathbf{X},t) &= \mathbf{L}^{\cdot}(t)\mathbf{X} + \mathbf{l}^{\cdot}(t) \end{aligned} \tag{4.2}$$

represent the velocities of the new observers relative to the old, while $\mathrm{curl}\,\mathbf{w}$ and $\mathrm{curl}\,\mathbf{w}_L$ are the corresponding spins. Since $\mathbf{Q}(t)^T\mathbf{Q}(t)$ and $\mathbf{L}(t)^T\mathbf{L}(t)$ are equal to the identity on $\mathbb{R}^3$, $\mathbf{Q}(t)^T\mathbf{Q}^{\cdot}(t)$ and $\mathbf{L}(t)^T\mathbf{L}^{\cdot}(t)$ are skew; thus there are vectors $\boldsymbol{\omega}(t)$ and $\boldsymbol{\omega}_L(t)$, smooth in t, such that

$$\mathbf{Q}(t)^T\mathbf{Q}^{\cdot}(t) = \boldsymbol{\omega}(t)\times, \qquad \mathbf{L}(t)^T\mathbf{L}^{\cdot}(t) = \boldsymbol{\omega}_L(t)\times. \tag{4.3}$$

It is convenient to let

$$\mathbf{R}(\mathbf{X}) = \mathbf{X} - \mathbf{X}_0, \qquad \mathbf{r}(\mathbf{x}) = \mathbf{x} - \mathbf{x}_0$$

denote the position vectors from *fixed points* $\mathbf{X}_0$ and $\mathbf{x}_0$, and to write

$$\mathbf{u}(t) = \mathbf{Q}(t)^T \mathbf{q}^{\cdot}(t) + \boldsymbol{\omega}(t) \times \mathbf{x}_0, \qquad \mathbf{u}_L(t) = \mathbf{L}(t)^T \mathbf{l}^{\cdot}(t) + \boldsymbol{\omega}_L(t) \times \mathbf{X}_0;$$

then

$$\begin{aligned} \mathbf{v}(\mathbf{x},t) &= \mathbf{Q}(t)\{\boldsymbol{\omega}(t) \times \mathbf{r}(\mathbf{x}) + \mathbf{u}(t)\}, \\ \mathbf{v}_L(\mathbf{X},t) &= \mathbf{L}(t)\{\boldsymbol{\omega}_L(t) \times \mathbf{R}(\mathbf{X}) + \mathbf{u}_L(t)\}, \\ \operatorname{curl} \mathbf{v} &= \mathbf{Q}\boldsymbol{\omega}, \qquad \operatorname{curl} \mathbf{v}_L = \mathbf{L}\boldsymbol{\omega}_L. \end{aligned} \tag{4.4}$$

Under the change in lattice observer (4.1) a "fixed configuration" μ transforms to a "time-dependent configuration" $\mu^*(t)$ $(t \in T)$ with values $\mu^*(t)(X) = \mu^*(X,t)$ given by

$$\mu^*(X,t) = \mathbf{L}(t)\mu(X) + \mathbf{l}(t).$$

Let $C(t)$ $(t \in T)$ be an evolving crystal. Under this change in lattice observer the crystal surface $\mathcal{S}(t) = \partial C_\mu(t)$, as observed in μ, transforms to the surface $\mathcal{S}^*(t) = \partial C_{\mu^*(t)}(t) = \mathbf{L}(t)\mathcal{S}(t) + \mathbf{l}(t)$, and the outward normal $\mathbf{n}_{\mathcal{S}}(X,t)$ to $\mathcal{S}(t)$ transforms to the outward normal

$$(\mathbf{n}_{\mathcal{S}})^*(X^*,t) = \mathbf{L}(t)\mathbf{n}_{\mathcal{S}}(X,t) \tag{4.5}$$

to $\mathcal{S}^*(t)$.

Let V be an *arbitrary* velocity field for $\mathcal{S}$, and let $Y(\beta)$ denote an $\mathcal{S}$-trajectory through X at time t which corresponds to V in the sense of Lemma (2B). To the new observer this trajectory appears as the $\mathcal{S}^*$-trajectory

$$Y^*(\beta) = \mu^*(Y(\beta),\beta) = \mathbf{L}(\beta)Y(\beta) + \mathbf{l}(\beta), \qquad Y^*(t) = X^*, \tag{4.6}$$

with $Y(\beta)$ the intrinsic material trajectory (3.22) corresponding to $Y(\beta)$. The velocity $v(X,t)$ for $\mathscr{S}$ therefore appears to the new observer as the velocity field $v^*(X^*,t)$ for $\mathscr{S}^*$ given by

$$\begin{aligned} v^*(X^*,t) &= (d/d\beta)Y^*(\beta)\big|_{\beta=t}, \\ &= L(t)v(X,t) + L^{\cdot}(t)X + \mathbf{l}^{\cdot}(t), \\ &= L(t)v(X,t) + \mathbf{v}_L(X,t). \end{aligned} \qquad (4.7)$$

Next, smoothly propagating subsurfaces $\mathscr{R}(t)$ of $\mathscr{S}(t)$ transform to smoothly propagating subsurfaces $\mathscr{R}^*(t) = L(t)\mathscr{R}(t) + \mathbf{l}(t)$ of $\mathscr{S}^*(t)$, and edge velocities v for $\mathscr{R}$ transform to edge velocities v^* for $\mathscr{R}^*$ with $v^*(X^*,t)$ also given by (4.7).

Thus far we have considered quantities which are invariant under changes in spatial observer. Consider next a crystal motion $\chi(t):C(t)\rightarrow c(t)$ $(t\in T)$. Under the observer changes (4.1), $\chi(X,t)$ transforms to the crystal motion $\chi^*(t):C(t)\rightarrow c^*(t)$ $(t\in T)$, with

$$\chi^*(X,t) = \mathbf{Q}(t)\chi(X,t) + \mathbf{q}(t) \qquad (4.8)$$

and $c^*(t) = \mathbf{Q}(t)c(t) + \mathbf{q}(t)$, and the surface $\mathscr{s}(t)$ transforms to the surface $\mathscr{s}^*(t) = \partial c^*(t)$ with outward normal

$$(n_{\mathscr{s}})^*(x^*,t) = \mathbf{Q}(t)n_{\mathscr{s}}(x,t). \qquad (4.9)$$

By (4.8), the deformation gradient (3.3) and the material velocity (3.21) transform according to

$$\begin{aligned} F^*(X^*,t) &= \mathbf{Q}(t)F(X,t), \\ v_c^*(x^*,t) &= \mathbf{Q}(t)v_c(x,t) + \mathbf{w}(x,t). \end{aligned} \qquad (4.10)$$

Let v be a velocity field for $\mathscr{S}$, let $\boldsymbol{\upsilon}$ be the corresponding induced velocity field for $\mathcal{S}$, and let v^* and $\mathfrak{v}^*$ be v and $\mathfrak{v}$ as seen by the new observers, so that v^* is given by (4.7). The $\mathcal{S}$-trajectory $y(\beta)$, which is defined in (3.23) and used in (3.24) to compute $\mathfrak{v}(x,t)$, transforms to the $\mathcal{S}^*$-trajectory $y^*(\beta) = \boldsymbol{\chi}^*(y(\beta),\beta)$; hence

$$\begin{aligned} \mathfrak{v}^*(x^*,t) &= (d/d\beta)y^*(\beta)\big|_{\beta=t}, \\ &= Q(t)\mathfrak{v}(x,t) + \mathbf{w}(x,t). \end{aligned} \tag{4.11}$$

Edge velocities for smoothly propagating subsurfaces of $\mathcal{S}$ are also consistent with this transformation law.

We assume that the transformation rule for the environmental velocity is the same as that for the material velocity:

$$v_e^* = Qv_e + \mathbf{w}. \tag{4.12}$$

II. Mechanics.

5. Control volumes. Mass. Kinetic energy.

5.1. Evolving control volumes.

$\mathscr{R}(t)$ and its image $\mathscr{r}(t)$ are *subsurfaces* of the undeformed and deformed surfaces $\mathscr{S}(t)$ and $\mathscr{s}(t)$. When writing balance laws it is useful to visualize $\mathscr{r}(t)$ as an infinitesimally *thin region* consisting of the crystal and environmental bulk material immediately adjacent to $\mathscr{r}(t)$, and to visualize $\mathscr{R}(t)$ as an infinitesimally *thin region* consisting of those atoms of the crystal lattice immediately adjacent to $\mathscr{R}(t)$ together with those atoms of the environment about to be added to - or just removed from - this portion of the lattice (Figure 5A). With this interpretation, we will refer to the pair

$$R(t) = (\mathscr{R}(t),\mathscr{r}(t)) \qquad (t\in T) \tag{5.1}$$

as an **evolving control volume**. The **physical boundary** of $R(t)$ then consists of: the edges $\partial\mathscr{R}(t)$ and $\partial\mathscr{r}(t)$ of $\mathscr{R}(t)$ and $\mathscr{r}(t)$; the *two sides* of $\mathscr{r}(t)$; the *two sides* of $\mathscr{R}(t)$. These definitions are formal and we will use them only as aids when writing balance laws; *in mathematical expressions, such as integrals,* $\mathscr{R}(t)$ *and* $\mathscr{r}(t)$ *should always be interpreted with their precise mathematical meaning as evolving subsurfaces.*

Under the observer change (4.1) the control volume $R(t)$ transforms to the control volume

$$R^*(t) = (\mathscr{R}^*(t),\mathscr{r}^*(t)) \qquad (t\in T), \tag{5.2}$$

where $\mathscr{R}^*$ and $\mathscr{r}^*$ are the images of $\mathscr{R}$ and $\mathscr{r}$ under (4.1).

5.2 Outflows.

Consider an evolving control volume $R(t)$ $(t\in T)$.

Let $\Phi_c(x,t)$ and $\Phi_e(x,t)$, respectively, denote *bulk densities* of a physical quantity for the crystal and for the environment, with both densities measured per unit *deformed volume.* To ease the discussion,

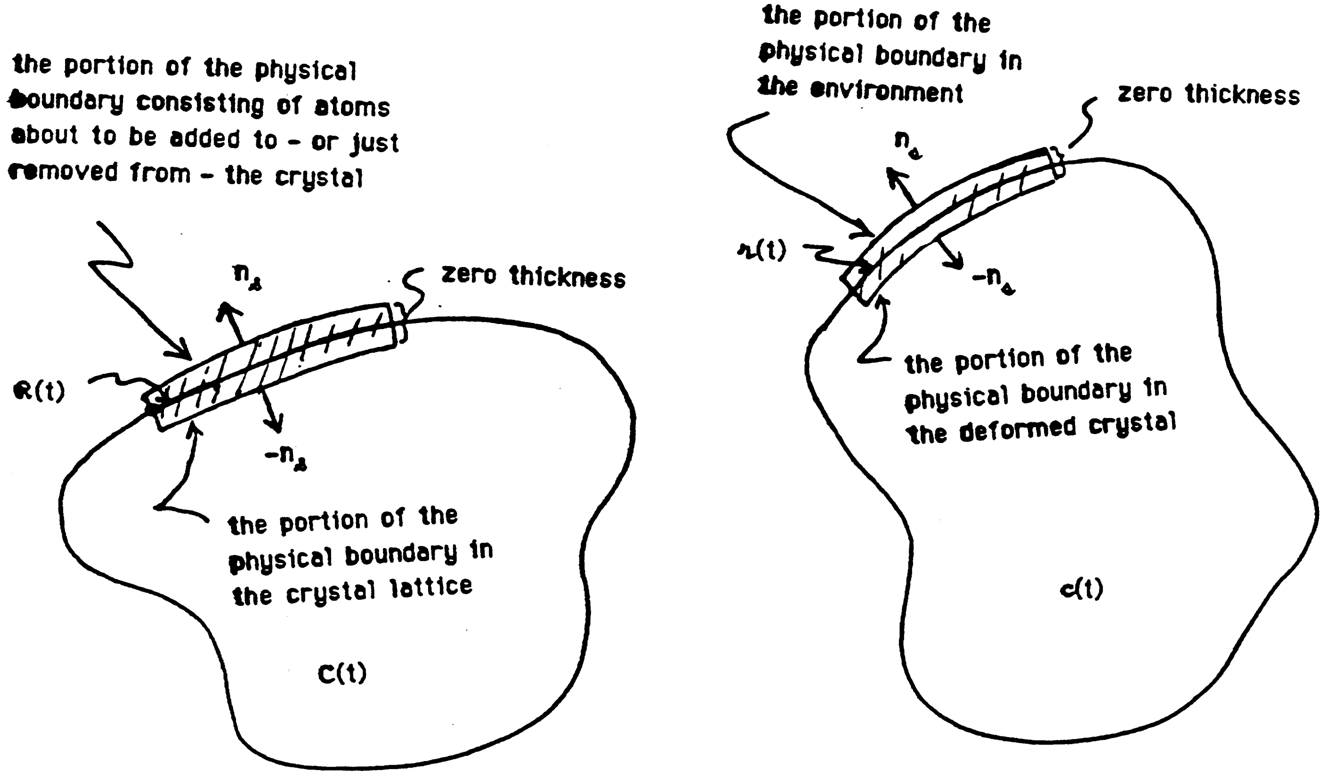

Figure 5A. The control volume R(t) consists of $\mathcal{R}(t)$ and $\mathcal{r}(t)$, considered as infinitesimally thin regions. The physical boundary of R(t) consists of: the two sides of $\mathcal{R}(t)$ and the edge $\partial\mathcal{R}(t)$; the two sides of $\mathcal{r}(t)$ and the edge $\partial\mathcal{r}(t)$.

we will refer to this quantity as *energy,* but it can represent a variety of physical quantities such as mass, kinetic energy, or entropy. The bulk energy of the control volume R(t) is zero, since the volume of R(t) is zero, but, since R(t) is moving relative to the bulk material of the crystal and the environment, R(t) captures and looses bulk energy across its physical boundary. In fact,

$$\int_{\mathscr{r}} \Phi_c(\mathscr{v}_{\mathscr{s}} - v_c) \cdot n_{\mathscr{s}} \, da, \qquad -\int_{\mathscr{r}} \Phi_e(\mathscr{v}_{\mathscr{s}} - v_e) \cdot n_{\mathscr{s}} \, da, \tag{5.3}$$

represent *outflows* of crystal and environmental bulk energy across this boundary. Similarly, if $\Phi_\mu(X,t)$ is the bulk energy of the crystal measured per unit *referential volume,* then

$$\int_{\mathfrak{R}} \Phi_\mu V_{\mathscr{S}} \, da \tag{5.4}$$

represents an *outflow* across the portion of the physical boundary of R(t) that lies in the crystal. This integral actually represents the same physical outflow as $(5.3)_1$; indeed, the energy densities Φ_c and Φ_μ are not independent, but related through

$$\Phi_\mu(X,t) = \det F(X,t)\Phi_c(x,t), \tag{5.5}$$

and, by $(2.25)_1$, (3.14), and (3.27),

$$\int_{\mathfrak{R}} \Phi_\mu V_{\mathscr{S}} \, da = \int_{\mathscr{r}} \Phi_c(\mathscr{v}_{\mathscr{s}} - v_c) \cdot n_{\mathscr{s}} \, da. \tag{5.6}$$

It is clear from this discussion that

$$\begin{aligned} &\int_{\mathscr{r}} \Phi_c(\mathscr{v}_{\mathscr{s}} - v_c) \cdot n_{\mathscr{s}} \, da - \int_{\mathscr{r}} \Phi_e(\mathscr{v}_{\mathscr{s}} - v_e) \cdot n_{\mathscr{s}} \, da = \\ &\int_{\mathfrak{R}} \Phi_\mu V_{\mathscr{S}} \, da - \int_{\mathscr{r}} \Phi_e(\mathscr{v}_{\mathscr{s}} - v_e) \cdot n_{\mathscr{s}} \, da \end{aligned} \tag{5.7}$$

represents the total outflow of "bulk energy" from the control volume R(t) (Figure 5B).

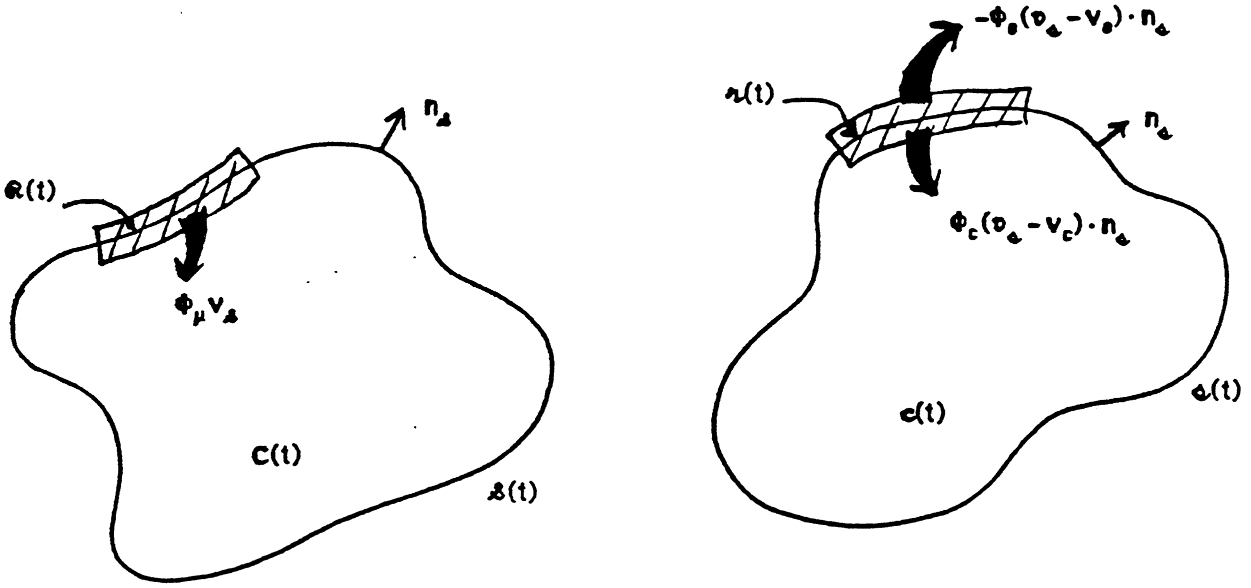

Figure 5B. The dark arrows indicate outflows across the physical boundary of a control volume R(t). The terms involving Φ_c and Φ_μ represent the same outflow measured, respectively, per unit deformed area and per unit referential area.

(5A) Remark. It will be necessary to compute the manner in which outflows of the form (5.3) transform under a change in observer. The term $V_c = (\boldsymbol{\upsilon}_{\mathscr{s}} - \mathbf{v}_c)\cdot\mathbf{n}_{\mathscr{s}}$ represents the normal velocity of $\mathscr{s}$ relative to the deforming crystal. In view of (2.33) with $\mathscr{S}$ replaced by $\mathscr{s}$, we may replace $\boldsymbol{\upsilon}_{\mathscr{s}}$ in the above expression by any velocity field $\boldsymbol{\upsilon}$ for $\mathscr{s}$. Under the change in observer (4.1) the term V_c should be replaced by $V_c{}^* = (\boldsymbol{\upsilon}^* - \mathbf{v}_c{}^*)\cdot(\mathbf{n}_{\mathscr{s}})^*$ with $\boldsymbol{\upsilon}^*$ any velocity field for $\mathscr{s}^*$. In particular, using (4.11) for $\boldsymbol{\upsilon}^*$ in conjunction with (4.9) and (4.10), we see that V_c is invariant under a change in observer: $V_c{}^*(x^*,t) = V_c(x,t)$. An identical argument yields the invariance of the term $V_e = (\boldsymbol{\upsilon}_{\mathscr{s}} - \mathbf{v}_e)\cdot\mathbf{n}_{\mathscr{s}}$.

5.3. Balance of mass. Scaled differences.

We neglect interfacial mass. Balance of mass then requires that there be no net outflow of mass from the evolving control volume R(t). Thus, in view of (5.7) with $\Phi_c = \rho_c$, $\Phi_e = \rho_e$, **balance of mass** is the assertion that

$$\int_{\mathscr{R}} \{\rho_c(\boldsymbol{\upsilon}_{\mathscr{s}} - \mathbf{v}_c)\cdot\mathbf{n}_{\mathscr{s}} - \rho_e(\boldsymbol{\upsilon}_{\mathscr{s}} - \mathbf{v}_e)\cdot\mathbf{n}_{\mathscr{s}}\}da = 0 \qquad (5.8)$$

for every evolving subsurface $\mathscr{R}$; hence

$$\rho_e(\mathbf{v}_e - \boldsymbol{\upsilon}_{\mathscr{s}})\cdot\mathbf{n}_{\mathscr{s}} = \rho_c(\mathbf{v}_c - \boldsymbol{\upsilon}_{\mathscr{s}})\cdot\mathbf{n}_{\mathscr{s}} \equiv \mathscr{m}, \qquad (5.9)$$

with $\mathscr{m}(x,t)$ the **mass flow** across $\mathscr{s}$ in the direction $\mathbf{n}_{\mathscr{s}}$, per unit area. By (3.4), (3.14), and (3.27),

$$\mathscr{m} = -\rho_c \ell v_{\mathscr{S}} = -\rho_\mu J^{-1} v_{\mathscr{S}}, \qquad (5.10)$$

with ρ_μ the crystal density in the reference configuration μ, so that $-\rho_\mu v_{\mathscr{S}}$ represents the mass flow per unit area of $\mathscr{S}$. The relations (3.4), (3.27), (5.9), and (5.10) yield the identities

$$(v_c - v_e) \cdot n_{\mathcal{S}} = \ell(\zeta - 1)v_{\mathscr{S}}, \qquad F^{-1}(v_c - v_e) \cdot n_{\mathscr{S}} = (\zeta - 1)v_{\mathscr{S}},$$
$$\zeta = \rho_c/\rho_e = \rho_\mu/(\rho_e \det F), \tag{5.11}$$

which also express balance of mass.

For the coherent crystal-crystal interaction, the relations (5.11) are consequences of the relations expressed in Section 3.5 and the fact that ρ_μ, the lattice density in the reference configuration μ, is the same for both phases. Therefore,

$$\textit{mass balance is automatically satisfied in a coherent crystal-crystal interaction.} \tag{5.12}$$

The densities are invariant under a change in observer: $\rho_c^*(x^*,t) = \rho_c(x,t)$, $\rho_e^*(x^*,t) = \rho_e(x,t)$. Thus, in view of Remark (5A), the mass flow $\mathfrak{m}$ is invariant:

$$\mathfrak{m}^*(x^*,t) = \mathfrak{m}(x,t). \tag{5.13}$$

The mass balance relations (5.9) and (5.10) allow us to rewrite the outflow relations (5.7) as

$$-\int_{\mathcal{N}} \mathfrak{m}(\rho_c{}^{-1}\Phi_c - \rho_e{}^{-1}\Phi_e)\,da = \int_{\mathcal{R}} \Phi v_{\mathscr{S}}\,da, \tag{5.14}$$

where

$$\Phi = \rho_\mu(\rho_c{}^{-1}\Phi_c - \rho_e{}^{-1}\Phi_e) = \Phi_\mu - (\det F)\zeta\Phi_e. \tag{5.15}$$

The quantity Φ is called a **scaled difference**; we will use this concept often: it will always represent a physical quantity for the crystal minus the same quantity for the environment, with both quantities normalized to the referential volume of the crystal.

For the coherent crystal-crystal interaction (Section 3.5) it is most convenient to use bulk densities measured per unit reference volume for both phases:

$$\Phi_{\mu c}(X,t) = \det F_c(X,t)\Phi_c(x,t), \quad \Phi_{\mu e}(X,t) = \det F_e(X,t)\Phi_e(x,t); \tag{5.16}$$

then, by (3.39), (5.15) becomes

$$\Phi = \Phi_{\mu c} - \Phi_{\mu e}. \tag{5.17}$$

5.4. Kinetic energy.

The bulk **kinetic energy**, per unit deformed volume, of the crystal and environment are given by $\frac{1}{2}\rho_c v_c^2$ and $\frac{1}{2}\rho_e v_e^2$;

$$\mathcal{K}(\mathbb{R}) = \tfrac{1}{2}\int_{\mathfrak{r}}\{\rho_c v_c^2(\boldsymbol{\upsilon}_{\triangle} - v_c)\cdot n_{\triangle} - \rho_e v_e^2(\boldsymbol{\upsilon}_{\triangle} - v_e)\cdot n_{\triangle}\}\,da \tag{5.18}$$

therefore represents the **outflow of kinetic energy** from the evolving control volume R(t). *Since we neglect interfacial mass,* (5.18) represents the only term involving kinetic energy for this control volume. Note that, by (5.9),

$$\mathcal{K}(\mathbb{R}) = \tfrac{1}{2}\int_{\mathfrak{r}}\mathfrak{m}(v_e^2 - v_c^2)\,da. \tag{5.19}$$

Under the observer change (4.1) the control volume R(t) transforms to the control volume $R^*(t)$ given by (5.2), and the kinetic energy $\mathcal{K}(\mathbb{R})$ transforms to a value

$$\mathcal{K}^*(\mathbb{R}^*) = \tfrac{1}{2}\int_{\mathfrak{r}^*}\mathfrak{m}^*\{(v_e^*)^2 - (v_c^*)^2\}\,da, \tag{5.20}$$

which we now compute. By (4.4), (4.10), and (4.12),

$$(v_c^*)^2 = (v_c)^2 + 2v_c\cdot(\omega\times r + u) + (\omega\times r + u)^2,$$
$$(v_e^*)^2 = (v_e)^2 + 2v_e\cdot(\omega\times r + u) + (\omega\times r + u)^2,$$

where we have omitted the arguments (x^*,t) and (x,t) for the starred and unstarred quantities. Changing variable of integration in (5.20) from $\mathbf{x}^*$ to $\mathbf{x}$, and using (5.13), we see that

$$\mathcal{K}^*(\mathcal{R}^*) - \mathcal{K}(\mathcal{R}) = \int_{\mathcal{r}} \mathbf{p}\cdot(\boldsymbol{\omega}\times\mathbf{r} + \mathbf{u})\,da, \tag{5.21}$$

where

$$\mathbf{p} = m(\mathbf{v}_e - \mathbf{v}_c) \tag{5.22}$$

is the **outflow of momentum** from the control volume, per unit deformed area.

6. Accretive, deformational, and environmental forces.

6.1. Force systems.

Basic to our theory are two systems of forces that accompany an accreting, deforming crystal. The first, the *accretive system, consists of forces that arise as a response to the crystallization process* as atoms are added to and removed from the crystal. These forces are presumed to be purely accretional: *they are forces that would be present, were there no deformation.* The second, the *deformational system, consists of forces related to the gross deformation of the crystal.* Since the accretive system accompanies the addition and deletion of *material points,* it is advantageous to consider this system in the reference configuration μ using X as spatial variable. On the other hand, the deformational system is most easily discussed using the variable x in the deformed crystal.

Precisely, the **accretive force system** *relative to* μ consists of three superficial fields for $\mathscr{S}$:

$\mathbb{C}(X,t)$	**accretive surface stress,**
$c(X,t)$	**accretive traction,**
$m(X,t)$	**accretive moment;**

the **deformational force system**[34] consists of three superficial fields for $\mathscr{s}$:

$\mathbb{T}(x,t)$	**deformational surface stress,**
$t_c(x,t)$	**deformational traction,**
$t_e(x,t)$	**environmental traction.**

$\mathbb{C}(X,t)$ is, at each $X \in \mathscr{S}(t)$, a linear transformation that maps tangent vectors $\boldsymbol{\nu}$ to $\mathscr{S}(t)$ at X into (not necessarily tangent) vectors $\mathbb{C}(X,t)\boldsymbol{\nu}$; $\mathbb{T}(x,t)$ is, at each $x \in \mathscr{s}(t)$, a linear transformation

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[34] To parallel the accretive sustem we could allow for a deformational moment exerted on the crystal surface by the crystal bulk. For surfaces whose constitutive equations allow for a dependence on the deformation only through its *first* gradient such a moment is ruled out by thermodynamics. To ease the presentation, we have chosen to omit this moment from the outset. Interestingly, accretive moments are not so precluded, and are, in fact, necessarily present whenever there is anisotropy.

that maps tangent vectors τ to $\mathscr{s}(t)$ at x into (not necessarily tangent) vectors $\mathbb{T}(x,t)\tau$. $\mathbb{C}(X,t)$ represents forces *within the undeformed crystal surface* that perform work during *accretion;* $\mathbb{T}(x,t)$ represents forces *within the deformed crystal surface* that perform work during *deformation.* We write $\mathbb{C}_{tan}$, $\mathbb{C}_{sym}$, $\mathbb{C}_{skw}$, and $\mathbb{c}$, respectively, for the **tangential**, **symmetric**, **skew**, and **normal components** of $\mathbb{C}$ with respect to $\mathscr{S}$; $\mathbb{T}_{sym}$, $\mathbb{T}_{skw}$, and $\mathbb{t}$ for the **symmetric**, **skew**, and **normal components** of $\mathbb{T}$ with respect to $\mathscr{s}$. (cf. (2.5)).

Let $\mathbb{R}(t)$ be a smoothly evolving subsurface of $\mathscr{S}(t)$ with $\mathscr{r}(t)$ the corresponding deformed subsurface, and let $\nu(X,t)$ and $\tau(x,t)$ denote the outward unit normals to the boundary curves $\partial\mathbb{R}(t)$ and $\partial\mathscr{r}(t)$. The forces exerted on the control volume $R(t)=(\mathbb{R}(t),\mathscr{r}(t))$ then consist of (Figure 6A):

$\mathbb{C}\nu$	force per unit length of $\partial\mathbb{R}$,
$\mathbb{T}\tau$	force per unit length of $\partial\mathscr{r}$,
t_c, t_e	forces exerted by the crystal and environment per unit area of $\mathscr{r}$,
c, m	total force and total moment exerted by the crystal and environment, per unit area of $\mathbb{R}$,

where, for convenience, we have omitted arguments. $\mathbb{C}\nu$ is the sum of a tangential force $(\mathbb{C}_{tan})\nu$ and a normal force $(\mathbb{c}\cdot\nu)n_{\mathscr{S}}$, and similarly for $\mathbb{T}\tau$. If $T_c(x,t)$ and $T_e(x,t)$ denote bulk Cauchy stresses for the crystal and the environment, then

$$t_c = -T_c n_{\mathscr{s}}, \qquad t_e = T_e n_{\mathscr{s}}. \tag{6.1}$$

At this point it is not necessary to decompose $\mathbf{c}(X,t)$ and $\mathbf{m}(X,t)$ into crystal and environmental components, but we do stipulate that

$\mathbf{c}$ *and* $\mathbf{m}$ *are indeterminate,*

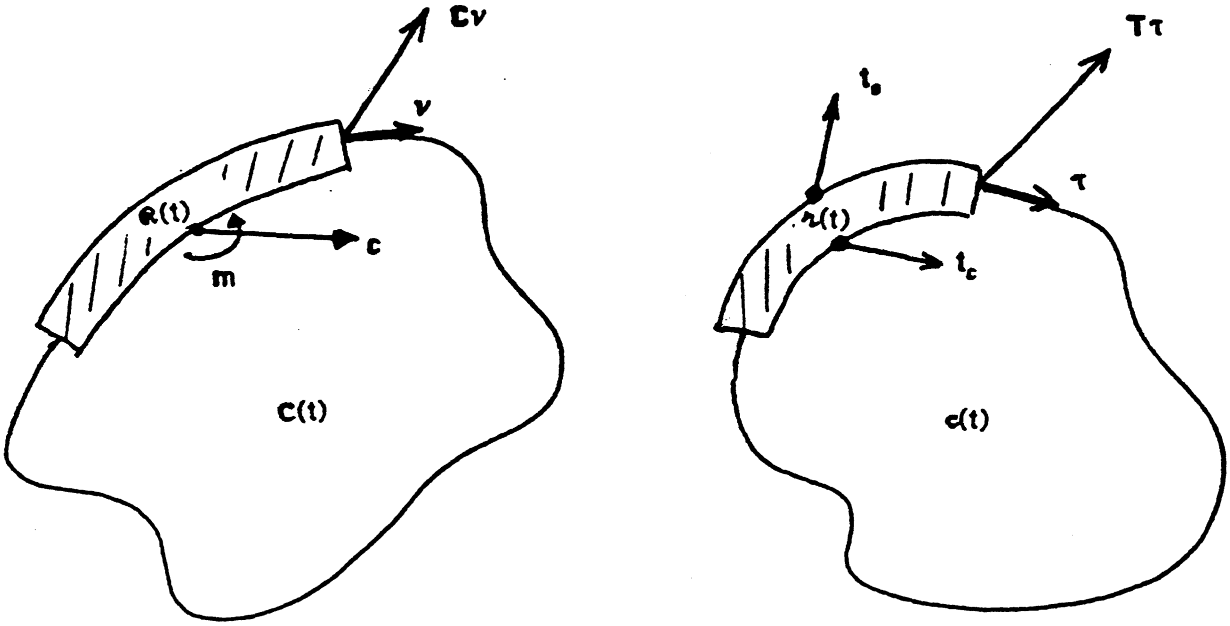

Figure 6A. Forces on a control volume $R(t)=(\mathcal{R}(t),r(t))$. **c** represents the force exerted by the crystal *and* the melt, and similarly for the moment **m**.

since lattice points - as measured in the reference lattice - do not move relative to each other.

Omitting arguments,

$$\int_{\partial \mathscr{r}} \mathbb{T}\tau\,ds + \int_{\mathscr{r}} (t_c + t_e)\,da$$

represents the total deformational force on R(t), while

$$\int_{\partial \mathbb{R}} \mathbb{C}\nu\,ds + \int_{\mathbb{R}} c\,da$$

represents the total accretive force on R(t), and analogous expressions apply to moments.

It is convenient to define the **Piola-Kirchhoff surface stress**[35] $\mathbb{S}(X,t)$ through

$$\mathbb{S}(X,t) = \mathbb{T}(x,t)\,\mathrm{adj}\,\mathbb{F}(X,t), \tag{6.2}$$

with $\mathrm{adj}\,\mathbb{F}$ defined by (3.15), for then, by $(2.25)_2$,

$$\int_{\partial \mathscr{r}} \mathbb{T}\tau\,ds = \int_{\partial \mathbb{R}} \mathbb{S}\nu\,ds \tag{6.3}$$

6.2. Expended power.

We characterize forces by the manner in which they expend power (perform work). Let $R(t) = (\mathbb{R}(t), \mathscr{r}(t))$ be an evolving control volume, and let ν and τ denote the outward unit normals to $\partial\mathbb{R}$ and $\partial\mathscr{r}$. $\mathbb{C}$ and $\mathbb{T}$ represent stresses *within* the undeformed and deformed crystal surfaces; we therefore assume that $\mathbb{C}\nu$ and $\mathbb{T}\tau$ expend power on R over *edge velocities* for $\mathbb{R}$ and $\mathscr{r}$. t_c and t_e are tractions exerted on portions of the control volume that lie in the crystal and in the environment and hence expend power over corresponding *material velocities.* **c** and **m** *do not expend power*

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[35] Cf. Gurtin and Murdoch [1975], eq. (5.24).

since they act within the lattice, and the lattice points are motionless in the configuration μ. Thus the **power expended** on the evolving control volume $R(t)$ is given by

$$\mathcal{P}(\mathbb{R}) = \int_{\partial\mathbb{R}} \mathbb{C}\nu\cdot v\,ds + \int_{\mathbb{R}} (\mathbf{c}\cdot\mathbf{0} + \mathbf{m}\cdot\mathbf{0})\,da + \int_{\partial\mathfrak{r}} \mathbb{T}\tau\cdot\mathfrak{v}\,ds + \int_{\mathfrak{r}} (t_c\cdot v_c + t_e\cdot v_e)\,da, \tag{6.4}$$

where v is an edge velocity for $\mathbb{R}$ with $\mathfrak{v}$ the corresponding induced edge velocity for $\mathfrak{r}$. (Here we have written $\mathbf{c}\cdot\mathbf{0} + \mathbf{m}\cdot\mathbf{0}$ as a reminder that the power expended by the accretive traction and acretive moment vanish only because the velocity and spin of the lattice are zero; these terms will contribute under changes in observer.)

Using the Piola-Kirchhoff stress $\mathbb{S}$ in conjunction with $(2.25)_3$ and (3.25),

$$\int_{\partial\mathfrak{r}} \mathbb{T}\tau\cdot\mathfrak{v}\,ds = \int_{\partial\mathfrak{r}} \mathbb{T}\tau\cdot v_c\,ds + \int_{\partial\mathbb{R}} F^T\mathbb{S}\nu\cdot v\,ds, \tag{6.5}$$

so that the deformational stress expends power in two ways: over the velocity v_c of those material points currently on the crystal surface, and over the "purely accretive" velocity v of the crystal surface. By (6.5),

$$\int_{\partial\mathbb{R}} \mathbb{C}\nu\cdot v\,ds + \int_{\partial\mathfrak{r}} \mathbb{T}\tau\cdot\mathfrak{v}\,ds = \int_{\partial\mathbb{R}} (\mathbb{C} + F^T\mathbb{S})\nu\cdot v\,ds + \int_{\partial\mathfrak{r}} \mathbb{T}\tau\cdot v_c\,ds, \tag{6.6}$$

showing that the power expended on the edges $\partial\mathbb{R}$ and $\partial\mathfrak{r}$ of the control volume can be considered as an accretive part

$$\int_{\partial\mathbb{R}} (\mathbb{C} + F^T\mathbb{S})\nu\cdot v\,ds$$

and a *purely* deformational part

$$\int_{\partial\mathscr{r}} \mathbb{T}\tau \cdot \mathbf{v}_c \, ds.$$

We call

$$\mathbb{A} = \mathbb{C} + \mathbf{F}^{\mathsf{T}}\mathbb{S} \tag{6.7}$$

the **total surface stress**; it represents the stress $\mathbb{C}$ due to accretion alone plus the accretive contribution $\mathbf{F}^{\mathsf{T}}\mathbb{S}$ of the deformational stress $\mathbb{T}$. We write $\mathbb{A}_{\tan}$ and

$$\mathbb{a} = \mathbb{A}^{\mathsf{T}}\mathbf{n}_{\mathscr{s}}, \tag{6.8}$$

for the tangential and normal components of $\mathbb{A}$ with respect to $\mathscr{s}$. Then, by (2.5), (3.8), and (3.9),

$$\mathbb{A}_{\tan} = \mathbb{C}_{\tan} + \mathbb{I}_{\mathscr{s}}\mathbb{F}^{\mathsf{T}}\mathbb{S}, \qquad \mathbb{a} = \mathbb{c} + \mathbb{S}^{\mathsf{T}}\mathbb{f}. \tag{6.9}$$

(6A) **Remark.** It is important to note that $\mathbb{A}_{\tan}$ depends on $\mathbb{C}_{\tan}$, $\mathbb{S}$, and the tangential deformation gradient $\mathbb{F}$, all superficial quantities. On the other hand, the normal component $\mathbb{a}$ of the total stress depends on the *normal* deformation gradient $\mathbb{f}$, *which is not intrinsic to the surface.* In particular, for a coherent crystal-crystal interaction as described in Section 3.5, the definition of $\mathbb{a}$ depends on the crystal phase in which $\mathbf{F}$ is computed.

We assume that the forces transform "naturally" under changes in observer. Precisely, we assume that *under any observer change of the form* (4.1),

$$\begin{aligned} &\mathbb{C}^* = \mathbf{L}\mathbb{C}\mathbf{L}^{\mathsf{T}}, &&\mathbb{T}^* = \mathbf{Q}\mathbb{T}\mathbf{Q}^{\mathsf{T}}, &&\mathbf{c}^* = \mathbf{L}\mathbf{c}, \\ &\mathbf{m}^* = \mathbf{L}\mathbf{m}, &&\mathbf{t}_c^* = \mathbf{Q}\mathbf{t}_c, &&\mathbf{t}_e^* = \mathbf{Q}\mathbf{t}_e, \end{aligned} \tag{6.10}$$

where we have used the convention introduced in the paragraph containing (2.6), and where we have omitted the arguments (X^*,t) and (X,t) for the starred and unstarred accretive fields, and similarly for the deformational fields.

Consider the observer change (4.1). The power expended, as recorded by the new observers, will have terms analogous to those of (6.4). In addition, the new lattice observer does not see the lattice at rest, but sees the lattice moving with the velocity $\mathbf{v}_L(X,t)$ defined in (4.4); hence the power expended, per unit area, by the accretive traction and the accretive moment is $c^*\cdot\mathbf{v}_L + m^*\cdot\mathrm{curl}\,\mathbf{v}_L$. Therefore relative to the new observers the power expended is

$$\begin{aligned}\mathcal{P}^*(\mathbb{R}^*) = {} & \int_{\partial\mathbb{R}^*}\mathbb{C}^*\nu^*\cdot v^*\,ds + \int_{\mathbb{R}^*}(c^*\cdot\mathbf{v}_L + m^*\cdot\mathrm{curl}\,\mathbf{v}_L)\,da \;+ \\ & \int_{\partial\mathfrak{r}^*}\mathbb{T}^*\tau^*\cdot\mathfrak{v}^*\,ds + \int_{\mathfrak{r}^*}(t_c^*\cdot v_c^* + t_e^*\cdot v_e^*)\,da,\end{aligned} \tag{6.11}$$

where $\mathbb{R}^*$ and $\mathfrak{r}^*$ are the images of $\mathbb{R}$ and $\mathfrak{r}$ under (4.1), while $\nu^* = L\nu$ and $\tau^* = Q\tau$ are the outward normals to $\partial\mathbb{R}^*$ and $\partial\mathfrak{r}^*$. By (4.4), (4.7), (4.10), (4.11), (4.12), and (6.10),

$$\begin{aligned}&\mathbb{C}^*\nu^*\cdot v^* = \mathbb{C}\nu\cdot(v + \omega_L\times R + u_L),\\ &c^*\cdot\mathbf{v}_L = c\cdot(\omega_L\times R + u_L), \qquad m^*\cdot\mathrm{curl}\,\mathbf{v}_L = m\cdot\omega_L,\\ &\mathbb{T}^*\tau^*\cdot\mathfrak{v}^* = \mathbb{T}\tau\cdot(\mathfrak{v} + \omega\times r + u),\\ &t_c^*\cdot v_c^* = t_c\cdot(v_c + \omega\times r + u), \qquad t_e^*\cdot v_e^* = t_e\cdot(v_e + \omega\times r + u).\end{aligned}$$

Therefore, changing variables of integration in (6.11) from X^* to X and from x^* to x, and subtracting (6.4) from the resulting relation, we see that

$$\begin{aligned}\mathcal{P}^*(\mathbb{R}^*) - \mathcal{P}(\mathbb{R}) = {} & \int_{\partial\mathfrak{r}}\mathbb{T}\tau\cdot(\omega\times r + u)\,ds + \int_{\mathfrak{r}}(t_c + t_e)\cdot(\omega\times r + u)\,da \;+ \\ & \int_{\partial\mathbb{R}}\mathbb{C}\nu\cdot(\omega_L\times r + u_L)\,ds + \int_{\mathbb{R}}\{c\cdot(\omega_L\times r + u_L) + m\cdot\omega_L\}\,da.\end{aligned} \tag{6.12}$$

7. Invariance of the mechanical production. Momentum balances. Force and moment balances for accretion.

7.1. Mechanical production.

Let $R(t) = (\mathcal{R}(t), r(t))$ be an evolving control volume. The difference

$$\mathcal{E}(\mathcal{R}) = \mathcal{K}(\mathcal{R}) - \mathcal{P}(\mathcal{R}) \tag{7.1}$$

between the outflow of kinetic energy (5.18) and the expended power (6.4) represents the mechanical production of energy, and will be referred to as the **mechanical production** for $R(t)$. The first law of thermodynamics requires that this quantity be balanced by the addition of heat and by changes in the internal energy; since heat and energy are invariant quantities, it seems reasonable to presume that the mechanical production itself be invariant. In fact, we will use invariance of the mechanical production to derive several important results: invariance under changes in the kinetic description of the interface yields the notion of surface tension; invariance under changes in observer yields the mechanical balance laws of the theory. This latter use of invariance is highly nontrivial: it not only leads to the expected momentum balance laws for the surface, it leads to *additional force and moment balance laws for the accretive system.*

Our discussion of invariance is facilitated by the following definitions. Let $\mathfrak{f}(\mathcal{R}, v, \mathbf{w})$ be defined for every evolving subsurface $\mathcal{R}$ of $\mathcal{S}$, and for all velocity fields v and edge velocities $\mathbf{w}$ for $\mathcal{R}$, and suppose that a rule is prescribed giving the value $\mathfrak{f}^*(\mathcal{R}^*, v^*, \mathbf{w}^*)$ of $\mathfrak{f}(\mathcal{R}, v, \mathbf{w})$ under any change in observer (4.1). We then say that:

(i) $\mathfrak{f}$ **is invariant under changes in observer** if, for all $\mathcal{R}$, v, and $\mathbf{w}$, $\mathfrak{f}^*(\mathcal{R}^*, v^*, \mathbf{w}^*) = \mathfrak{f}(\mathcal{R}, v, \mathbf{w})$ for every change in observer (4.1);

(ii) $\mathfrak{f}$ **is invariant under reparametrization**[36] if, for every $\mathcal{R}$, $\mathfrak{f}(\mathcal{R}, v, \mathbf{w})$ *is independent of the choice of velocities* v *and* $\mathbf{w}$ *used to describe the evolution of* $\partial\mathcal{R}$.

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[36] Cf. Footnote 24

A basic **axiom** of our theory is that the

mechanical production be invariant under changes in observer and under reparametrization.

Here it is tacit that, under the change in observer (4.1), the mechanical production $\mathcal{E}(\mathbb{R})$ transform to

$$\mathcal{E}^*(\mathbb{R}^*) = \mathcal{K}^*(\mathbb{R}^*) - \mathcal{P}^*(\mathbb{R}^*), \qquad (7.2)$$

with $\mathcal{K}^*(\mathbb{R}^*)$ and $\mathcal{P}^*(\mathbb{R}^*)$ given by (5.20) and (6.11).

The requirement of invariance under changes in observer is nonstandard: in classical continuum mechanics the mechanical production is the rate of change of kinetic energy minus the expended power and is invariant under Galilean changes of observer, *but not more generally* due to the presence of accelerations in the observer change. Here the use of *arbitrarily thin* control volumes and our neglect of interfacial mass renders the control volumes massless, and because of this accelerations in the observer change do not destroy the invariance.[37]

7.2. Invariance under reparametrization. Surface tension.

By (6.6) and (6.7), the hypothesis that $\mathcal{E}$ be invariant under reparametrization is equivalent to the requirement that

$$\int_{\partial\mathbb{R}} \mathbb{A}\nu\cdot\mathbf{v}\,ds \qquad (7.3)$$

be independent of the edge velocity $\mathbf{v}$. Thus (iii) of the Invariance Lemma (Appendix C) yields the

(7A) Surface-Tension Theorem. *The tangential part of the total surface stress* $\mathbb{A}$ *is a surface tension:*

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[37] The requirement of invariance under observer changes could be replace invariance under Galilean changes in observer. This would yield balance of linear momentum $(7.11)_1$ and balance of accretional forces $(7.10)_1$. Using this as motivation, the moment laws $(7.10)_2$ and $(7.11)_2$ could then be adopted as separate axioms.

$$\mathbb{A}_{\tan} = \sigma \mathbb{I}_{\mathcal{S}}, \tag{7.4}$$

with σ *a scalar field called the* **surface tension**.

Note that, by (6.9) and (7.4), the total surface stress has the representation

$$\mathbb{A} = \sigma \mathbb{I}_{\mathcal{S}} + n_{\mathcal{S}} \otimes \mathbb{a}. \tag{7.5}$$

7.3. Invariance under observer changes. Momentum balances. Force and moment balances for accretion.

Let

$$t = t_c + t_e - p, \qquad p = \mathscr{m}(v_e - v_c) \tag{7.6}$$

denote the **total deformational traction** (including the outflow p of momentum). In view of (5.21) and (6.12), invariance of $\mathcal{E}$ under changes in observer is equivalent to the requirement that

$$\begin{aligned}&\int_{\partial\mathscr{r}} \mathbb{T}\tau\cdot(\omega\times r + u)\,ds + \int_{\mathscr{r}} t\cdot(\omega\times r + u)\,da \, + \\ &\int_{\partial\mathbb{R}} \mathbb{C}\nu\cdot(\omega_L\times r + u_L)\,ds + \int_{\mathbb{R}} \{c\cdot(\omega_L\times r + u_L) + m\cdot\omega_L\}\,da = 0,\end{aligned} \tag{7.7}$$

or alternatively, that

$$\begin{aligned}&u\cdot\Big\{\int_{\partial\mathscr{r}} \mathbb{T}\tau\,ds + \int_{\mathscr{r}} t\,da\Big\} = 0,\\ &\omega\cdot\Big\{\int_{\partial\mathscr{r}} r\times\mathbb{T}\tau\,ds + \int_{\mathscr{r}} r\times t\,da\Big\} = 0,\\ &u_L\cdot\Big\{\int_{\partial\mathbb{R}} \mathbb{C}\nu\,ds + \int_{\mathbb{R}} c\,da\Big\} = 0,\\ &\omega_L\cdot\Big\{\int_{\partial\mathbb{R}} R\times\mathbb{C}\nu\,ds + \int_{\mathbb{R}} R\times c\,da + \int_{\mathbb{R}} m\,da\Big\} = 0\end{aligned}$$

for all vectors $\mathbf{u}$, $\boldsymbol{\omega}$, $\mathbf{u}_L$, and $\boldsymbol{\omega}_L$. This yields the **momentum balances**

$$\begin{aligned}&\int_{\partial\mathscr{r}} \mathbb{T}\tau\,ds + \int_{\mathscr{r}} (\mathbf{t}_c + \mathbf{t}_e)\,da = \int_{\mathscr{r}} \mathscr{m}(\mathbf{v}_e - \mathbf{v}_c)\,da,\\ &\int_{\partial\mathscr{r}} \mathbf{r}\times\mathbb{T}\tau\,ds + \int_{\mathscr{r}} \mathbf{r}\times(\mathbf{t}_c + \mathbf{t}_e)\,da = \int_{\mathscr{r}} \mathbf{r}\times\{\mathscr{m}(\mathbf{v}_e - \mathbf{v}_c)\}\,da,\end{aligned} \tag{7.8}$$

as well as the **force and moment balances for accretion**

$$\begin{aligned}&\int_{\partial\mathbb{R}} \mathbb{C}\nu\,ds + \int_{\mathbb{R}} \mathbf{c}\,da = \mathbf{0},\\ &\int_{\partial\mathbb{R}} \mathbf{R}\times\mathbb{C}\nu\,ds + \int_{\mathbb{R}} \mathbf{R}\times\mathbf{c}\,da + \int_{\mathbb{R}} \mathbf{m}\,da = \mathbf{0},\end{aligned} \tag{7.9}$$

which must hold for all smoothly propagating subsurfaces $\mathbb{R}$ and $\mathscr{r}$ of $\mathscr{S}$ and $\mathscr{s}$.

(7B) Remark. Here we see a major difference between the theory presented here and the more standard theories of continuum mechanics. In classical continuum mechanics, where there are only deformational forces, the stress can be expressed per unit deformed area (Cauchy stress) or per unit undeformed area (Piola-Kirchhoff stress), but both of these quantities represent the same force. Here $\mathbb{T}$ and $\mathbf{t}_c$ represent a force system within the *deformed crystal,* while $\mathbb{C}$ and $\mathbf{c}$ represent a *completely different* force system within the *crystal lattice;* and these two force systems are generally unequal even when the former is "pulled back" to the undeformed crystal. This difference is characterized by the manner in which the two systems perform work, and is exemplified by the fact that there are two sets of mechanical balance laws, one for each system. This underlines the importance of using an invariant basis to derive these balance laws.

(7C) Local Balance Laws.

(i) *The force and moment balances for accretion are equivalent to*

$$\begin{aligned} &\mathrm{div}_{\mathcal{S}}\mathbb{C} + \mathbf{c} = 0, \\ &\mathbf{m}\times = 2\mathbb{C}_{\mathrm{skw}}\mathbb{P}_{\mathcal{S}} - \mathbb{c}\wedge\mathbf{n}_{\mathcal{S}}. \end{aligned} \tag{7.10}$$

(ii) *The momentum balances are equivalent to*

$$\begin{aligned} &\mathrm{div}_{\mathcal{S}}\mathbb{T} + \mathbf{t}_c + \mathbf{t}_e = \mathcal{m}(\mathbf{v}_e - \mathbf{v}_c), \\ &\mathbb{T}_{\mathrm{skw}} = 0, \qquad \mathbb{t} = 0, \end{aligned} \tag{7.11}$$

so that the deformational surface stress is tangential and symmetric.

Proof. We will prove only (i). It is clear from the divergence theorem (2.12) that $(7.9)_1$ and $(7.10)_1$ are equivalent. To complete the proof of (i) it suffices to show that, granted $(7.10)_1$, $(7.10)_2$ is equivalent to $(7.9)_2$. Since $(\mathbf{a}\wedge\mathbf{b})\mathbf{c} = (\mathbf{a}\times\mathbf{b})\times\mathbf{c}$, $(7.9)_2$ is equivalent to

$$\int_{\partial\mathcal{R}} \mathbf{R}\wedge\mathbb{C}\boldsymbol{\nu}\,ds + \int_{\mathcal{R}} \mathbf{R}\wedge\mathbf{c}\,da + \int_{\mathcal{R}} (\mathbf{m}\times)\,da = 0,$$

or alternatively, by (2.14) and (7.10), to

$$\int_{\mathcal{R}} \{\mathbb{c}\wedge\mathbf{n}_{\mathcal{S}} - 2\mathbb{C}_{\mathrm{skw}}\mathbb{P}_{\mathcal{S}} + (\mathbf{m}\times)\}\,da = 0;$$

this relation can hold for all sufficiently regular surfaces $\mathcal{R}$ if and only if $(7.10)_2$ is satisfied. ■

Note that $(7.10)_2$ is equivalent to the two relations

$$\mathbb{c} = \mathbf{n}_{\mathcal{S}}\times\mathbf{m}, \qquad 2\mathbb{C}_{\mathrm{skw}} = \mathbb{I}_{\mathcal{S}}\mathbb{P}_{\mathcal{S}}(\mathbf{m}\times)\mathbb{I}_{\mathcal{S}}. \tag{7.12}$$

7.4. Referential balance laws.

The balance laws expressed in (7C) are difficult to use, chiefly because the independent variable is $\mathbf{X}$ in (7.10) and $\mathbf{x}$ in (7.11). The next result remedies these difficulties. There we discuss only the normal component of the accretive force balance, since that is what arises in applications.

(7D) Referential Balance Laws.

(i) *The momentum balances are equivalent to*[38]

$$\begin{aligned} &\mathrm{div}_{\mathcal{S}}\mathbb{S} + J(t_c + t_e) = \rho_\mu(v_c - v_e)v_{\mathcal{S}}, \\ &\mathbb{S}\mathbb{F}^T = \mathbb{F}\mathbb{S}^T. \end{aligned} \tag{7.13}$$

(ii) *The normal component of the accretive force balance* (7.10)$_1$ *is equivalent to*

$$\sigma K + \mathrm{div}_{\mathcal{S}}\mathbb{c} - (F^T\mathbb{S})\cdot\mathbb{L} + c\cdot n_{\mathcal{S}} = 0. \tag{7.14}$$

Proof. Using (2.25), (6.2), and (7.6), we can write the balance law (7.8)$_1$ in the form

$$\int_{\partial\mathbb{R}}\mathbb{S}\nu\,ds + \int_{\mathbb{R}}Jt\,da = 0. \tag{7.15}$$

Since the smoothly propagating subsurface $\mathbb{R}$ of $\mathcal{S}$ is arbitrary, this, (7.6), and (5.10) yield (7.13)$_1$. Further, (7.11)$_2$, (2.3), (2.5), (3.15), and (6.2) yield

$$\mathbb{P}_{\mathcal{A}}\mathbb{S}(\mathbb{F}_{surf})^T = \mathbb{F}_{surf}\mathbb{S}^T\mathbb{I}_{\mathcal{A}}, \qquad \mathbb{S}^T n_{\mathcal{A}} = 0, \tag{7.16}$$

which, by virtue of (3.11), imply (7.13)$_2$. The converse assertions are established similarly.

Next, by (2.9), $\mathbb{C}\cdot\mathbb{L} = \mathbb{C}_{tan}\cdot\mathbb{L}$; thus (2.11)$_3$, (6.7), (7.4), and the identity $K = \mathbb{I}_{\mathcal{S}}\cdot\mathbb{L}$ yield

$$n_{\mathcal{S}}\cdot\mathrm{div}_{\mathcal{S}}\mathbb{C} = \sigma K - F^T\mathbb{S}\cdot\mathbb{L} + \mathrm{div}_{\mathcal{S}}\mathbb{c}. \tag{7.17}$$

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[38] Cf. Gurtin and Murdoch [1975], p. 307, for the statical version of (7.13).

Substituting (7.17) into $(7.10)_1$ yields (7.14). That (7.14) implies the normal component of $(7.10)_1$ follows upon reversing this argument. ■

(7E) **Remark.** By (2.9), the term $F^T\mathbb{S}\cdot\mathbb{L}$ in (7.14) can be written as $(\mathbb{F}^T\mathbb{S})\cdot(\mathbb{P}_{\mathscr{S}}\mathbb{L})$ and hence involves only superficial quantities.

Suppose that the environment is a melt, modelled as an inviscid fluid. Then

$$t_e = -p_e n_{\mathscr{D}}, \tag{7.18}$$

with $p_e(x,t)$ the **melt pressure** at the crystal surface. By (3.6) and (3.14), $Jn_{\mathscr{D}} = (\det F)F^{-T}n_{\mathscr{S}}$, and therefore

$$Jt_e = -p_e(\det F)F^{-T}n_{\mathscr{S}}. \tag{7.19}$$

The crystal traction is given by $(6.1)_1$ with $T_c(x,t)$ the bulk Cauchy stress; introducing the **bulk Piola-Kirchhoff stress** $S_c(X,t)$ defined by

$$S_c = (\det F)T_cF^{-T}, \tag{7.20}$$

we can express this traction as

$$Jt_c = -S_cn_{\mathscr{S}}. \tag{7.21}$$

Balance of linear momentum $(7.13)_1$ *for a crystal in an inviscid melt therefore has the form*

$$\mathrm{div}_{\mathscr{S}}\mathbb{S} - \{S_c + p_e(\det F)F^{-T}\}n_{\mathscr{S}} = \rho_\mu(v_c - v_e)v_{\mathscr{S}}. \tag{7.22}$$

On the other hand, for the coherent crystal-crystal interaction described in Section 3.5, $\mathbf{S}_c(X,t)$ defined by (7.20) with $\mathbf{F}=\mathbf{F}_c$ and $\mathbf{S}_e(X,t)$ defined by

$$\mathbf{S}_e = (\det\mathbf{F}_e)\mathbf{T}_e\mathbf{F}_e^{-\mathrm{T}} \tag{7.23}$$

are the **bulk Piola-Kirchhoff stresses** for phases c and e. By (3.6), (3.14), and the remark following (3.39), $J\mathbf{n}_{\mathscr{s}} = (\det\mathbf{F}_e)\mathbf{F}_e^{-\mathrm{T}}\mathbf{n}_{\mathcal{S}}$, so that $(6.1)_2$ becomes

$$J\mathbf{t}_e = \mathbf{S}_e\mathbf{n}_{\mathcal{S}}. \tag{7.24}$$

Balance of linear momentum, $(7.13)_1$*, for a coherent crystal-crystal interaction therefore has the form*

$$\mathrm{div}_{\mathcal{S}}\mathbb{S} + (\mathbf{S}_e - \mathbf{S}_c)\mathbf{n}_{\mathcal{S}} = \rho_\mu(\mathbf{v}_c - \mathbf{v}_e)V_{\mathcal{S}}. \tag{7.25}$$

7.5. Invariant form for the expended power.

We now take $\mathbf{v}$ and $\mathfrak{v}$ in (6.4) equal to the intrinsic edge velocity $\mathbf{v}_{\partial\mathbb{R}}$ of $\mathbb{R}$ and the corresponding induced edge velocity $\mathfrak{v}_{\partial\mathscr{r}}$ of $\partial\mathscr{r}$; in view of (7.5), this leads to an *invariant form* for the power expended:

$$\mathcal{P}(\mathbb{R}) = \int_{\partial\mathbb{R}}\mathbb{C}\nu\cdot\mathbf{v}_{\partial\mathbb{R}}\,ds + \int_{\partial\mathscr{r}}\mathbb{T}\tau\cdot\mathfrak{v}_{\partial\mathscr{r}}\,ds + \int_{\mathscr{r}}(\mathbf{t}_c\cdot\mathbf{v}_c + \mathbf{t}_e\cdot\mathbf{v}_e)\,da. \tag{7.26}$$

8. Bulk interaction between phases. Attachment forces.

8.1. Forces describing bulk interactions.

One of the chief differences between theories involving phase transitions and the more classical theories of continuum mechanics is the creation and deletion of material points as the phase interface moves relative to the underlying material. This phenomenon involves only bulk material and the relevant forces may be isolated using (evolving) bulk control volumes $R(t)=(\mathscr{R}(t),\mathscr{r}(t))$ that exclude the interface. Each such $R(t)$ is generated by an evolving subsurface $\mathscr{R}(t)$ and its image $\mathscr{r}(t)$; what makes these control volumes different from those that *include* the interface is the interpretation of their physical boundary. Formally, the **physical boundary of a bulk control volume** $R(t)$ **for the crystal** consists of: the two sides of $\mathscr{r}(t)$ representing the portions of $R(t)$ in the *deformed crystal* that interact with the interface and with the remainder of the deformed crystal; the two sides of $\mathscr{R}(t)$ representing the portions of $R(t)$ in the *crystal lattice* that interact with the interface and with the remainder of the lattice (Figure 8A). The **physical boundary** of a **bulk control volume for the environment** is defined analogously. Note that, for any such control volume,

the net outflow of kinetic energy vanishes, (8.1)

since the energy entering one side of $\mathscr{r}(t)$ leaves the other side.

Force balance for bulk control volumes requires further structure (Figure 8B). We decompose the accretive traction $\mathbf{c}(\mathbf{X},t)$ into crystal and environmental components

$$\mathbf{c}(\mathbf{X},t) = \mathbf{c}_c(\mathbf{X},t) + \mathbf{c}_e(\mathbf{X},t) \tag{8.2}$$

and introduce **attachment forces**

$$\boldsymbol{\pi}_c(\mathbf{X},t), \qquad \boldsymbol{\pi}_e(\mathbf{X},t)$$

and **bulk-interface interactions**

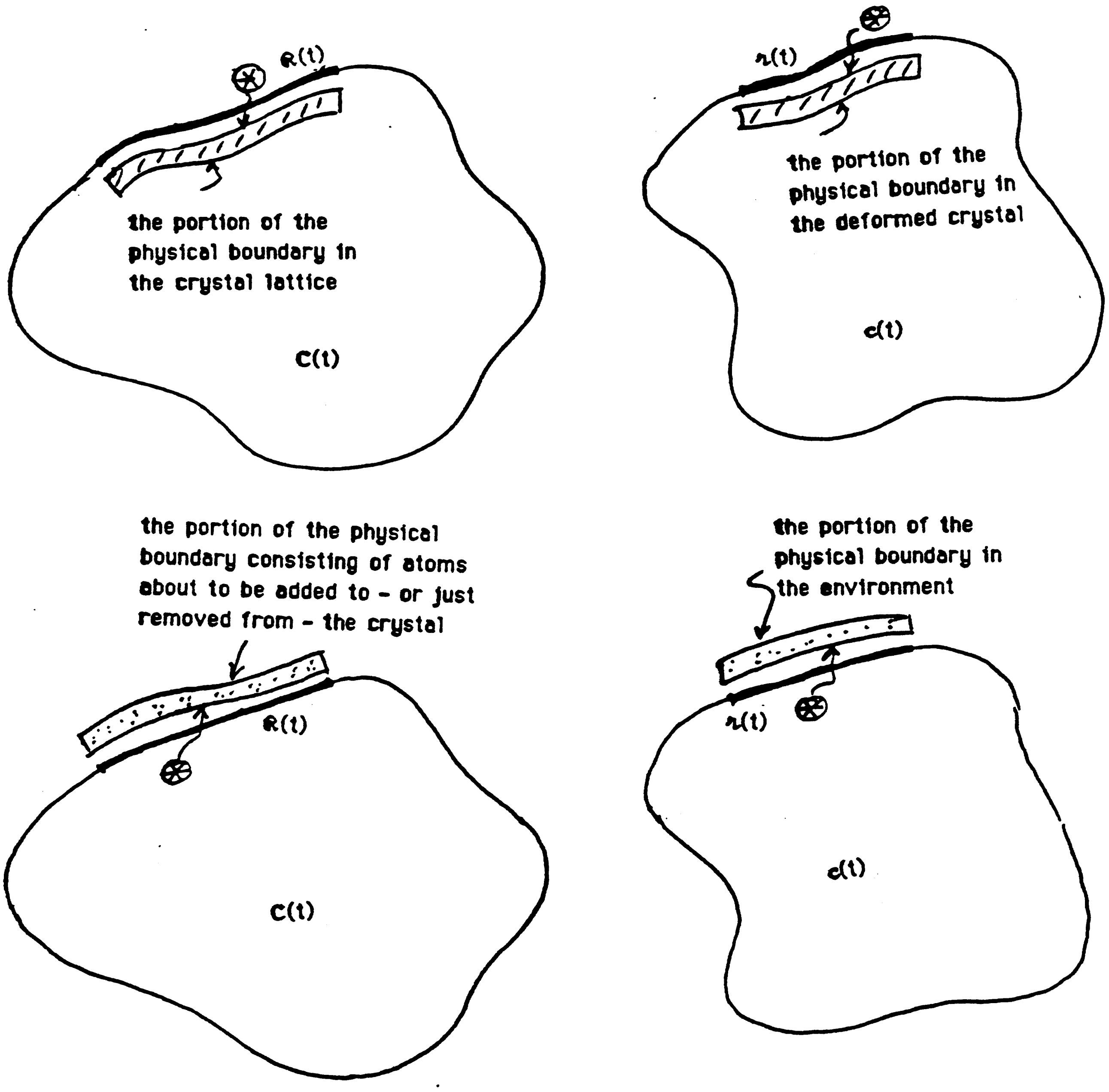

Figure 6A. $R(t)=(\mathcal{R}(t),r(t))$ considered as a bulk control volume for the crystal (shaded) and as a bulk control volume for the environment (dotted). ⊛ designates the portion of the corresponding physical boundaries that interact with the interface.

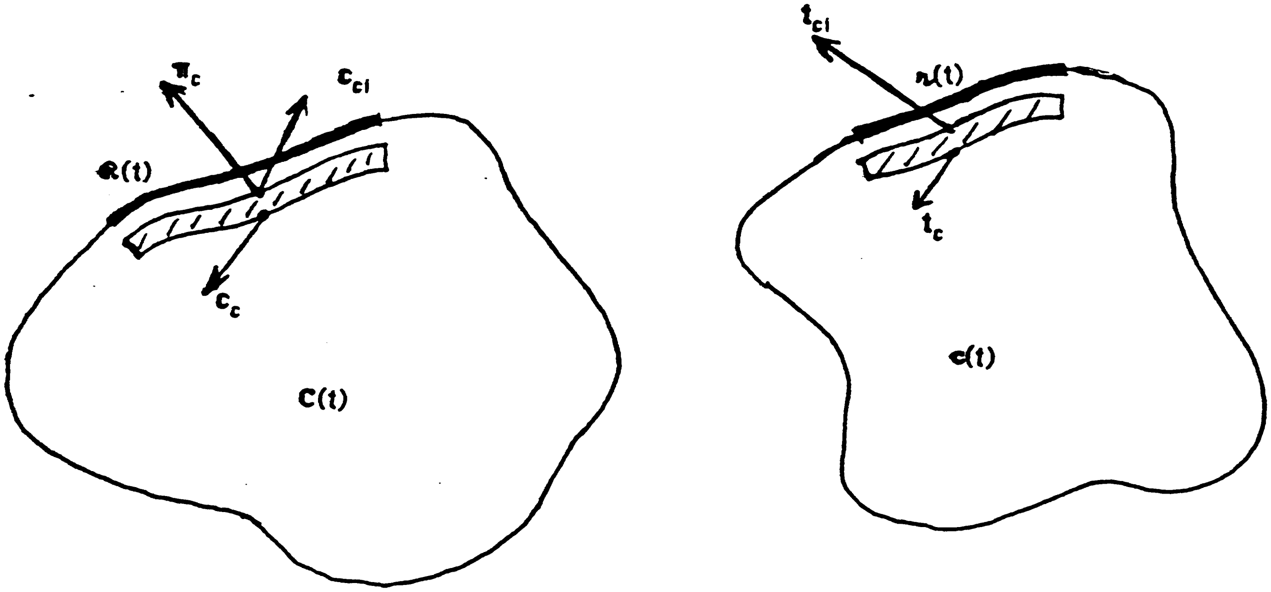

Figure 8B. Forces on a bulk control volume $R(t)=(\mathcal{R}(t),r(t))$ for the crystal.

$$\mathbf{c}_{ci}(X,t), \qquad \mathbf{c}_{ei}(X,t), \qquad \mathbf{t}_{ci}(x,t), \qquad \mathbf{t}_{ei}(x,t)$$

defined for $X \in \mathscr{B}(t)$ and $x \in \mathscr{E}(t)$. $\boldsymbol{\pi}_c(X,t)$ and $\boldsymbol{\pi}_e(X,t)$ are forces *within the lattice* associated with the attachment and release of atoms as they are exchanged between phases, while $\mathbf{c}_{ci}(X,t)$ and $\mathbf{c}_{ei}(X,t)$ are forces *exerted by the interface.* $\boldsymbol{\pi}_c(X,t)$ and $\mathbf{c}_{ci}(X,t)$ act on the atoms of the crystal lattice; $\boldsymbol{\pi}_e(X,t)$ and $\mathbf{c}_{ei}(X,t)$ act on the atoms of the environment which are about to become - or just were - part of the crystal lattice. $\mathbf{t}_{ci}(x,t)$ and $\mathbf{t}_{ei}(x,t)$ are forces exerted by the interface on the deformed crystal and on the environment. The forces associated with the symbols $\mathbf{c}$ and $\boldsymbol{\pi}$ depend on the choice of reference configuration μ.

8.2. Power expended in bulk. Consequences of invariance.

As before we use invariance to derive associated balance laws. By (8.1) we may restrict our attention to power; in particular, to

$$\mathcal{P}_c(\mathbb{R}) = \int_{\mathbb{R}} (\mathbf{c}_c \cdot \mathbf{0} + \boldsymbol{\pi}_c \cdot \mathbf{0} + \mathbf{c}_{ci} \cdot \mathbf{v})\,da + \int_{r} (\mathbf{t}_c \cdot \mathbf{v}_c + \mathbf{t}_{ci} \cdot \mathfrak{v})\,da, \qquad (8.3)$$

the *power expended on bulk control volumes for the crystal,* and to

$$\mathcal{P}_e(\mathbb{R}) = \int_{\mathbb{R}} (\mathbf{c}_e \cdot \mathbf{0} + \boldsymbol{\pi}_e \cdot \mathbf{0} + \mathbf{c}_{ei} \cdot \mathbf{v})\,da + \int_{r} (\mathbf{t}_e \cdot \mathbf{v}_e + \mathbf{t}_{ei} \cdot \mathfrak{v})\,da, \qquad (8.4)$$

the *power expended on bulk control volumes for the environment.* Here $\mathbf{v}$ is a velocity field for $\mathscr{B}$ and $\mathfrak{v}$ the corresponding induced velocity for $\mathscr{E}$. In these relations $\mathbf{c}_{ci}$, $\mathbf{c}_{ei}$, $\mathbf{t}_{ci}$, and $\mathbf{t}_{ei}$ are forces exerted by the interface and hence expend power over appropriate surface velocities; $\boldsymbol{\pi}_c$ and $\boldsymbol{\pi}_e$ are forces within the lattice and hence expend power over the velocity of the lattice (which is zero in the configuration μ).

We assume that the forces and power transform as follows under an observer change (4.1): for $q = c,e$,

$$\mathbf{c}_q{}^* = \mathbf{L}\mathbf{c}_q, \quad \mathbf{c}_{qi}{}^* = \mathbf{L}\mathbf{c}_{qi}, \quad \boldsymbol{\pi}_q{}^* = \mathbf{L}\boldsymbol{\pi}_q, \quad \mathbf{t}_{qi}{}^* = \mathbf{Q}\mathbf{t}_{qi},$$

$$\mathcal{P}_q{}^*(\mathscr{R}^*) = \int_{\mathscr{R}^*}(\mathbf{c}_q{}^* \cdot \mathbf{w}_L + \boldsymbol{\pi}_q{}^* \cdot \mathbf{w}_L + \mathbf{c}_{qi}{}^* \cdot \mathbf{v}^*)da + \int_{\mathscr{r}^*}(\mathbf{t}_q{}^* \cdot \mathbf{v}_q{}^* + \mathbf{t}_{qi}{}^* \cdot \mathfrak{v}^*)da.$$

A basic **axiom** of our theory is that the

> *power expended in bulk on the crystal and on*
> *the environment be invariant under changes*
> *in observer and under reparametrization.*

As before, the presumption of invariance has important consequences.

(8A) Interactive Force Balance. *For* $q = c, e$,

$$\boldsymbol{\pi}_q + \mathbf{c}_{qi} = -\mathbf{c}_q, \qquad \mathbf{t}_{qi} = -\mathbf{t}_q, \qquad \mathbb{P}_{\mathscr{S}}(\mathbf{c}_{qi} + J\mathbf{F}^{\mathsf{T}}\mathbf{t}_{qi}) = 0. \quad (8.5)$$

Proof. An argument strictly analogous to that used to derive (7.10) and (7.11) shows that the invariance of $\mathcal{P}_q$ under changes in observer is equivalent to the first two relations in (8.5). Next, isolating the terms in (8.3) and (8.4) that depend on $\mathbf{v}$ (and $\mathfrak{v}$), we find, using $(2.25)_1$ and (3.25), that invariance of $\mathcal{P}_q$ under reparametrization is equivalent to the requirement that

$$\int_{\mathscr{R}}(\mathbf{c}_{qi} + J\mathbf{F}^{\mathsf{T}}\mathbf{t}_{qi}) \cdot \mathbf{v}\, da$$

be independent of the choice of velocity field $\mathbf{v}$, and the third of (8.5) follows from (i) of the Invariance Lemma (Appendix C). ■

The balance relations (8.5) allow us to express the power expended in bulk *invariantly* as

$$\mathcal{P}_q(\mathscr{R}) = \int_{\mathscr{r}}\mathbf{t}_q \cdot (\mathbf{v}_q - \mathfrak{v}_{\mathscr{A}})da - \int_{\mathscr{R}}(\mathbf{c}_q + \boldsymbol{\pi}_q) \cdot \mathbf{v}_{\mathscr{S}}\, da \qquad (8.6)$$

for $q = c, e$.

III. Mechanical theory.

9. Energies. Global laws for energy. Reduced dissipation inequality.

9.1. Global laws for energy.

We endow the crystal, the environment, and the crystal surface with energies:[39]

$\psi(X,t)$ superficial energy,
$\Psi_c(x,t)$ crystal bulk energy,
$\Psi_e(x,t)$ environmental bulk energy.

$\psi(X,t)$, $X \in \mathscr{S}(t)$, represents the energy of the crystal surface, per unit *referential* area; $\Psi_c(x,t)$ and $\Psi_e(x,t)$, $x \in \mathscr{c}(t)$, are the the bulk energies of the crystal and the environment, per unit *deformed* volume. Although the bulk energies are measured per unit volume, they enter this portion of the theory only through their values (limits) *at the crystal surface.*

Consider an evolving control volume $R(t) = (\mathscr{R}(t), \mathscr{r}(t))$ which *includes* both the interface and the adjacent bulk material (cf. Section 5.1 and Figure 5A). Then

$$\int_{\mathscr{R}} \psi \, da$$

represents the superficial energy of $R(t)$, while

$$\int_{\mathscr{r}} \Psi_c (v_\partial - v_c) \cdot n_\partial \, da - \int_{\mathscr{r}} \Psi_e (v_\partial - v_e) \cdot n_\partial \, da = \int_{\mathscr{R}} \Psi v_{\mathscr{S}} \, da$$

represents the outflow of bulk energy from $R(t)$ (cf. (5.7) and (5.15)). Here

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[39] We use the term energy in a generic sense. The thermodynamic potential (free energy, internal energy, etc.) actually represented depends on which thermodynamic theory this *purely mechanical theory* is meant to "approximate". The current theory is independent of such considerations.

$$\Psi = \rho_\mu(\rho_c^{-1}\Psi_c - \rho_e^{-1}\Psi_e) = \Psi_\mu - (\det F)\zeta\Psi_e \qquad (9.1)$$

is the **scaled difference in bulk energies**, while Ψ_μ is the bulk energy per unit referential volume.

For a purely mechanical theory the **second law** is the assertion that *the rate of energy increase plus the energy outflow (including kinetic energy) cannot be greater than the power expended.* A precise statement of this **global dissipation inequality** for the evolving control volume $R(t)$ is

$$(d/dt)\{\int_{\mathbb{R}}\psi\, da\} + \int_{\mathbb{R}}\Psi v_{\mathcal{S}}\, da + \mathcal{K}(\mathbb{R}) \leq \mathcal{P}(\mathbb{R}) \qquad (9.2)$$

for every evolving subsurface $\mathbb{R}$ of $\mathcal{S}$, where $\mathcal{K}(\mathbb{R})$ is the outflow of kinetic energy (5.18), while $\mathcal{P}(\mathbb{R})$ is the expended power (7.26).

We will also postulate energy *balances* for the bulk material (near the interface). Since *bulk* control volumes exhibit neither outflows of bulk energy nor outflows of kinetic energy, the **bulk energy balances** take the simple form

$$\mathcal{P}_c(\mathbb{R}) = \mathcal{P}_e(\mathbb{R}) = 0 \qquad (9.3)$$

for every evolving subsurface $\mathbb{R}$ of $\mathcal{S}$, where $\mathcal{P}_c(\mathbb{R})$ and $\mathcal{P}_e(\mathbb{R})$, given by (8.6), are the power expenditures in bulk.

9.2. The accretive balance law.

By (8.6) and (9.3), we have the **local balances**

$$Jt_q\cdot(v_q - \mathfrak{v}_{\diamond}) = (c_q + \pi_q)\cdot v_{\mathcal{S}} \qquad (q = c,e), \qquad (9.4)$$

which, by (8.2), combine to give

$$(c\cdot n_{\mathcal{S}} + \pi)v_{\mathcal{S}} = Jt_c\cdot(v_c - \mathfrak{v}_{\diamond}) + Jt_e\cdot(v_e - \mathfrak{v}_{\diamond}), \qquad (9.5)$$

with

$$\pi = (\pi_c + \pi_e)\cdot n_{\mathcal{S}} \tag{9.6}$$

the (normal) **net attachment force**. Using (3.26) and (7.14), we may rewrite (9.5) in the form

$$\{\pi + \mathscr{g} + JF^T(t_c + t_e)]\cdot n_{\mathcal{S}}\}v_{\mathcal{S}} + Jt_e\cdot(v_c - v_e) = 0, \tag{9.7}$$

where $\mathscr{g}$ represents the *superficial terms*

$$\mathscr{g} = -\sigma K - \mathrm{div}_{\mathcal{S}}\mathbb{C} + (F^T\mathbb{S})\cdot\mathbb{L}. \tag{9.8}$$

We will refer to (9.7) as the **accretive balance law**; it represents a combination of the bulk energy balances and the normal accretive force balance.

Suppose that the environment is a melt, modelled as an inviscid fluid. Then, using (7.18), (7.21), (3.6), (3.14), and $(5.11)_1$,

$$\begin{aligned}&\{JF^T t_e\cdot n_{\mathcal{S}}\}v_{\mathcal{S}} + Jt_e\cdot(v_c - v_e) = -(\det F)\zeta p_e v_{\mathcal{S}}, \qquad \zeta = \rho_c/\rho_e,\\ &JF^T t_c\cdot n_{\mathcal{S}} = -(S_c n_{\mathcal{S}})\cdot(Fn_{\mathcal{S}}),\end{aligned} \tag{9.9}$$

with p_e the melt pressure and S_c the bulk Piola-Kirchhoff stress in the crystal. Thus *the accretive balance law for a crystal in an inviscid melt has the form*

$$(S_c n_{\mathcal{S}})\cdot(Fn_{\mathcal{S}}) + (\det F)\zeta p_e - \mathscr{g} - \pi = 0, \tag{9.10}$$

provided $v_{\mathcal{S}} \neq 0$.

On the other hand, for the coherent crystal-crystal interaction described in Section 3.5 and the paragraph containing (7.23), the relations (3.36) and (7.24) yield

$$\{JF_c{}^T t_e\cdot n_{\mathcal{S}}\}v_{\mathcal{S}} + Jt_e\cdot(v_c - v_e) = (S_e n_{\mathcal{S}})\cdot(F_e n_{\mathcal{S}})v_{\mathcal{S}}.$$

Thus, by $(9.9)_3$ with $F = F_c$, *the accretive balance law for a coherent crystal-crystal interaction becomes*

$$(S_c n_{\mathcal{S}}) \cdot (F_c n_{\mathcal{S}}) - (S_e n_{\mathcal{S}}) \cdot (F_e n_{\mathcal{S}}) - \mathscr{g} - \pi = 0 \qquad (9.11)$$

provided $v_{\mathcal{S}} \neq 0$.

9.3. The power identity.

The next theorem, one of our main results, is central to the thermodynamics of crystal motions.

(9A) Power Identity.

$$\mathcal{P}(\mathbb{R}) =$$

$$\int_{\mathbb{R}} \{-\sigma \kappa v_{\mathcal{S}} - \mathbb{a} \cdot n_{\mathcal{S}}{}^{\circ} + (\mathbb{S}\mathbb{P}_{\mathcal{S}}) \cdot F^{\circ} + \pi v_{\mathcal{S}} + Jp \cdot \mathfrak{v}_{\diamond}\} da + \int_{\partial\mathbb{R}} \sigma v_{(\partial\mathbb{R})\tan} ds. \qquad (9.12)$$

The left side of (9.12) is the total power expended on an evolving control volume, while the right side catalogs the manner in which this power is used: $-\sigma \kappa v_{\mathcal{S}}$ represents power expended in the *creation of new surface,* $-\mathbb{a} \cdot n_{\mathcal{S}}{}^{\circ}$ power expended in *changing the orientation of the surface,* $(\mathbb{S}\mathbb{P}_{\mathcal{S}}) \cdot F^{\circ}$ power expended in *stretching the surface,* $\pi v_{\mathcal{S}}$ power expended in the *exchange of atoms between phases,* $Jp \cdot \mathfrak{v}_{\diamond}$ (inertial) power expended in the *velocity change between phases* (cf. (7.6)). The final term $\sigma v_{(\partial\mathbb{R})\tan}$ compensates for the tangential motion of the edge $\partial\mathbb{R}$.

Proof of the power identity. By (3.32) in conjunction with $(2.25)_3$, (6.2), (6.7), and (7.4),

$$\int_{\partial\mathcal{R}}\mathbb{C}\nu\cdot v_{\partial\mathcal{R}}\,ds + \int_{\partial\mathscr{r}}\mathbb{T}\tau\cdot\mathfrak{v}_{\partial\mathscr{r}}\,ds =$$
$$\int_{\partial\mathcal{R}}\mathbb{C}\nu\cdot v_{\mathscr{s}}\,ds + \int_{\partial\mathscr{r}}\mathbb{T}\tau\cdot\mathfrak{v}_{\mathscr{d}}\,ds + \int_{\partial\mathcal{R}}\sigma v_{(\partial\mathcal{R})\tan}\,ds;$$

therefore, using (7.6), (7.26), and (9.5), we find that

$$\begin{aligned}\mathcal{P}(\mathcal{R}) = {}&\int_{\partial\mathcal{R}}\mathbb{C}\nu\cdot v_{\mathscr{s}}\,ds + \int_{\mathcal{R}}c\cdot v_{\mathscr{s}}\,da + \int_{\partial\mathscr{r}}\mathbb{T}\tau\cdot\mathfrak{v}_{\mathscr{d}}\,ds + \int_{\mathscr{r}}(t+p)\cdot\mathfrak{v}_{\mathscr{d}}\,da\\ &+ \int_{\mathcal{R}}\pi v_{\mathscr{s}}\,da + \int_{\partial\mathcal{R}}\sigma v_{(\partial\mathcal{R})\tan}\,ds.\end{aligned} \tag{9.13}$$

Next, as a direct consequence of the balance laws (7C),

$$\begin{aligned}&\int_{\partial\mathcal{R}}\mathbb{C}\nu\cdot v_{\mathscr{s}}\,ds + \int_{\mathcal{R}}c\cdot v_{\mathscr{s}}\,da = \int_{\mathcal{R}}\mathbb{C}\cdot\nabla_{\mathscr{s}}v_{\mathscr{s}}\,da,\\ &\int_{\partial\mathscr{r}}\mathbb{T}\tau\cdot\mathfrak{v}_{\mathscr{d}}\,ds + \int_{\mathscr{r}}t\cdot\mathfrak{v}_{\mathscr{d}}\,da = \int_{\mathscr{r}}\mathbb{T}\cdot\nabla_{\mathscr{d}}\mathfrak{v}_{\mathscr{d}}\,da = \int_{\mathcal{R}}\mathbb{S}\cdot\nabla_{\mathscr{s}}\mathfrak{v}_{\mathscr{d}}\,da,\end{aligned} \tag{9.14}$$

where the final identity follows from $(2.25)_1$, (3.28), and (6.2). The integrands of the right sides of (9.14) represent the stress power, per unit area, of the accretional and deformational stresses. By (3.29),

$$\mathbb{C}\cdot\nabla_{\mathscr{s}}v_{\mathscr{s}} + \mathbb{S}\cdot\nabla_{\mathscr{s}}\mathfrak{v}_{\mathscr{d}} = (\mathbb{C} + F^{T}\mathbb{S})\cdot\nabla_{\mathscr{s}}v_{\mathscr{s}} + (\mathbb{S}\mathbb{P}_{\mathscr{s}})\cdot F^{\circ},$$

and this relation, (3.29), (6.7), and (7.5) yield the **stress-power identity:**

$$\mathbb{C}\cdot\nabla_{\mathscr{s}}v_{\mathscr{s}} + \mathbb{S}\cdot\nabla_{\mathscr{s}}\mathfrak{v}_{\mathscr{d}} = \ = -\sigma\kappa v_{\mathscr{s}} - \mathbb{a}\cdot n_{\mathscr{s}}{}^{\circ} + (\mathbb{S}\mathbb{P}_{\mathscr{s}})\cdot F^{\circ}. \tag{9.15}$$

The results (9.13)-(9.15) imply (9.12). ∎

9.4. The reduced dissipation inequality.

By (5.10), (5.19), and (7.6),

$$\mathcal{K}(\mathcal{R}) - \int_{\mathscr{r}} \mathrm{p}\cdot\mathfrak{v}_{\mathfrak{s}}\,da = \int_{\mathcal{R}} \mathscr{k}\,v_{\mathscr{S}}\,da, \tag{9.16}$$

with

$$\mathscr{k} = \tfrac{1}{2}\rho_{\mu}[(\mathrm{v}_c - \mathfrak{v}_{\mathfrak{s}})^2 - (\mathrm{v}_e - \mathfrak{v}_{\mathfrak{s}})^2]; \tag{9.17}$$

therefore, using (2.38) and (9.12), we can write (9.2) in the form

$$\int_{\mathcal{R}} \{\psi^{\circ} + (\sigma - \psi)K v_{\mathscr{S}} + \mathbb{a}\cdot n_{\mathscr{S}}{}^{\circ} - (\mathbb{S}\mathbb{P}_{\mathscr{S}})\cdot F^{\circ} + (\Psi + \mathscr{k} - \pi)v_{\mathscr{S}}\}\,da \;+ \\ \int_{\partial\mathcal{R}} (\psi - \sigma)v_{(\partial\mathcal{R})\tan}\,ds \;\le\; 0. \tag{9.18}$$

This inequality must hold for every smoothly evolving subsurface $\mathcal{R}$ of $\mathscr{S}$; thus, by (ii) of the Invariance Lemma (Appendix C), we have the

(9B) Tension-Energy Theorem. *The surface tension and superficial energy coincide:*

$$\sigma = \psi. \tag{9.19}$$

If we substitute (9.19) into (9.18) and use the fact that $\mathcal{R}$ is arbitrary, we are led to the **reduced dissipation inequality**

$$\psi^{\circ} + \mathbb{a}\cdot n_{\mathscr{S}}{}^{\circ} - (\mathbb{S}\mathbb{P}_{\mathscr{S}})\cdot F^{\circ} + (\Psi + \mathscr{k} - \pi)v_{\mathscr{S}} \le 0, \tag{9.20}$$

an inequality central to our theory.

10. Constitutive equations. Thermodynamic compatibility.

As constitutive equations for the crystal surface we allow the surface energy and the accretive and deformational surface stress at any point of the surface to depend on the deformation gradient F, the orientation $\mathbf{n} = \mathbf{n}_{\mathcal{S}}$, the normal speed $v = v_{\mathcal{S}}$, and a list z of variables of lesser importance, all evaluated at the same point:

$$\psi = \hat{\psi}(F,\mathbf{n},v,z), \quad \mathbb{T} = \hat{\mathbb{T}}(F,\mathbf{n},v,z), \quad \mathbb{C} = \hat{\mathbb{C}}(F,\mathbf{n},v,z). \tag{10.1}$$

We describe the interaction between phases by a constitutive equation, also of this form, for the normal attachment force:

$$\pi = \hat{\pi}(F,\mathbf{n},v,z). \tag{10.2}$$

We refer to z as the **subsidiary variable**; we require that z contain, as entries, the velocities $\mathbf{v}_c$ and $\mathbf{v}_e$ as well as variables (other than F) which determine the bulk energies Ψ_c and Ψ_e through bulk constitutive equations. With this stipulation, $\mathbb{k}$ and Ψ may be regarded as functions of $(F,\mathbf{n},v,z)$:

$$\mathbb{k} = \hat{\mathbb{k}}(F,\mathbf{n},v,z), \quad \Psi = \hat{\Psi}(F,\mathbf{n},v,z) \tag{10.3}$$

(cf. (9.17) and (9.1)). We assume that the common domain of the *response functions* $\hat{\psi}$, $\hat{\mathbb{T}}$, $\hat{\mathbb{C}}$, and $\hat{\pi}$ is an open set of the form (2.41).

The constitutive equations (10.1) imply corresponding constitutive equations for the Piola-Kirchhoff stress and the *normal* component of the total surface stress,

$$\mathbb{S} = \hat{\mathbb{S}}(F,\mathbf{n},v,z), \quad \mathbb{a} = \hat{\mathbb{a}}(F,\mathbf{n},v,z) \tag{10.4}$$

(cf. (6.2), (6.7)). By (7.4) and (9.19), the *tangential* component of the total surface stress is the surface tension $\sigma = \psi$.

Let $\boldsymbol{\chi}(t): C(t) \to c(t)$ $(t \in T)$ be a crystal motion and $z: \mathcal{S}_T \to Z$

(cf. (2.27)) a smooth function with $\mathbf{z}(\mathbf{X},t)$ interpreted as the subsidiary variable at $\mathbf{X} \in \mathcal{S}(t)$ in this motion. Then the corresponding list $\mathbf{p} = (\mathbf{F}, \mathbf{n}, v, \mathbf{z})$, with $\mathbf{n} = \mathbf{n}_{\mathcal{S}}$ and $v = v_{\mathcal{S}}$, will be referred to as an **admissible process**, and $\mathbf{p}$ together with corresponding fields ψ, $\mathbb{T}$, $\mathbb{C}$, and π generated through the constitutive equations (10.1) and (10.2) will be termed a **constitutive process**.

The presence, in the constitutive equations, of the deformation gradient $\mathbf{F}$ rather than the tangential deformation gradient $\mathbb{F}$ implies a possible dependence on the behavior of the crystal away from - although arbitrarily close to - the crystal surface. We will show, as a consequence of the reduced dissipation inequality, that certain of the constitutive quantities are **intrinsic to the surface** in the sense that they depend depend on $\mathbf{F}$ only through $\mathbb{F} (= \mathbf{F}\mathbb{I}(\mathbf{n}))$ (cf. the sentence containing (2.50) for a precise definition).

The basic thermodynamic **axiom** of the mechanical theory is that *the reduced dissipation inequality* (9.20) *be satisfied in all constitutive processes.*[40] This hypothesis places severe restrictions on the constitutive equations.

(10A) Compatibility Theorem.

(i) *The response functions for the superficial energy (surface tension), the Piola-Kirchhoff surface stress, and the accretive surface stress are intrinsic to the surface, independent of the normal speed and the subsidiary variable, and related through*

---

[40] It is tacit that there are forces available to ensure satisfaction of the underlying balance laws in arbitrarily chosen constitutive processes (cf. Gurtin [1988b], Footnote 13). We chose not to introduce such forces since their introduction tends to complicate the discussion and since it is only here that they are needed. Precisely, we need accretive and deformational body forces $\mathbf{c}_{ext}$ and $\mathbf{b}$. Then $(7.10)_1$ and $(7.11)_1$ become $\mathrm{div}_{\mathcal{S}}\mathbb{C} + \mathbf{c} + \mathbf{c}_{ext} = 0$ (1) and $\mathrm{div}_{\mathcal{S}}\mathbb{T} + \mathbf{t}_c + \mathbf{t}_e + \mathbf{b} = m(\mathbf{v}_e - \mathbf{v}_c)$ (2). Invariance under reparametrization requires that $\mathbf{c}_{ext} + J\mathbf{F}^T\mathbf{b}$ be normal to $\mathcal{S}$. Write $\mathbf{n} = \mathbf{n}_{\mathcal{S}}$ and recall that $\mathbf{c}$ and $\mathbf{m}$ are indeterminate. Given any process we choose: (i) $\mathbf{b}$ to balance (2); (ii) $\mathbf{c}_{ext} \cdot \mathbf{n}$ and $\mathbf{c}_{tan}$ to balance (1); (iii) $\mathbf{m}$ to balance $(7.10)_2$ (accretive moments); (iv) $\mathbf{c} \cdot \mathbf{n}$, $\pi_c - \pi_e$, $(\pi_c + \pi_e)_{tan}$, $\mathbf{c}_{ei}$, $\mathbf{c}_{ci}$, $\mathbf{t}_{ei}$, and $\mathbf{t}_{ci}$ to balance (8.5) (interactive forces) and (9.4) (bulk energy balances).

$$\begin{aligned}&\mathbb{S}^{\wedge}(F,\mathbf{n}) = \partial_{\mathbb{F}}\psi^{\wedge}(F,\mathbf{n}),\\ &\mathbb{C}_{tan}{}^{\wedge}(F,\mathbf{n}) = \psi^{\wedge}(F,\mathbf{n})\mathbb{I}(\mathbf{n}) - \mathbf{I}(\mathbf{n})\mathbb{F}^{T}\partial_{\mathbb{F}}\psi^{\wedge}(F,\mathbf{n}),\\ &\mathbb{c}^{\wedge}(F,\mathbf{n}) = -D_{\mathbf{n}}\psi^{\wedge}(F,\mathbf{n}).\end{aligned} \tag{10.5}$$

(ii) *There is a response function* $\beta^{\wedge}$ *such that the normal attachment force has the form*

$$\pi^{\wedge}(F,\mathbf{n},v,\mathbf{z}) = \Bbbk + \Psi + \beta v, \qquad \beta = \beta^{\wedge}(F,\mathbf{n},v,\mathbf{z}) \geq 0, \tag{10.6}$$

with $\Bbbk$ *and* Ψ *given by* (10.3).

Proof. The requirement that the reduced dissipation inequality hold in every constitutive process is equivalent to the requirement that

$$\begin{aligned}&\partial_{v}\psi^{\wedge}(\mathbf{p})v^{\circ} + \partial_{z}\psi^{\wedge}(\mathbf{p})\cdot\mathbf{z}^{\circ} + [\partial_{\mathbf{n}}\psi^{\wedge}(\mathbf{p}) + \mathbb{a}^{\wedge}(\mathbf{p})]\cdot\mathbf{n}^{\circ} +\\ &[\partial_{F}\psi^{\wedge}(\mathbf{p}) - \mathbb{S}^{\wedge}(\mathbf{p})\mathbb{P}(\mathbf{n})]\cdot F^{\circ} + [\Bbbk^{\wedge}(\mathbf{p}) + \Psi^{\wedge}(\mathbf{p}) - \pi^{\wedge}(\mathbf{p})]v \leq 0\end{aligned} \tag{10.7}$$

in every admissible process $\mathbf{p} = (F,\mathbf{n},v,\mathbf{z})$. In view of the Variation Lemma proved in Appendix C, given any $\mathbf{p}_0 = (F_0,\mathbf{n}_0,v_0,\mathbf{z}_0)$ in the domain of the response functions, there is an admissible process $\mathbf{p}$ such that, at some point and time, $\mathbf{p} = \mathbf{p}_0$ but $(F^{\circ},\mathbf{n}^{\circ},v^{\circ},\mathbf{z}^{\circ})$ is arbitrary. Thus

$$\begin{aligned}&\partial_{v}\psi^{\wedge}(\mathbf{p}) = 0, \quad \partial_{z}\psi^{\wedge}(\mathbf{p}) = \mathbf{0}, \quad \mathbb{a}^{\wedge}(\mathbf{p}) = -\partial_{\mathbf{n}}\psi^{\wedge}(\mathbf{p}),\\ &\mathbb{S}^{\wedge}(\mathbf{p})\mathbb{P}(\mathbf{n}) = \partial_{F}\psi^{\wedge}(\mathbf{p}), \quad [\pi^{\wedge}(\mathbf{p}) - \Bbbk^{\wedge}(\mathbf{p}) - \Psi^{\wedge}(\mathbf{p})]v \geq 0,\end{aligned} \tag{10.8}$$

with $\mathbf{p} = (F,\mathbf{n},v,\mathbf{z})$ an arbitrary element of the domain of the response functions, and $\psi^{\wedge}$ is independent of v and $\mathbf{z}$. Further, $(2.48)_2$ and $(10.8)_4$ imply $\partial_{\mathbb{f}}\psi^{\wedge} = \mathbf{0}$, so that, by Lemma (2Eiii), $\psi^{\wedge}$ is intrinsic to the surface; Lemma (2Eiv) and $(10.8)_4$ then yield $(10.5)_1$. Next, (2.50), (6.9), (7.4), (10.5), and the relation $\sigma = \psi$ imply $(10.5)_{2,3}$, while the remaining assertions of (i) follow from (10.5) and Lemma (2F). Finally, $(10.8)_5$ implies the existence of a function $\beta\hat{}(F,n,v,z) \geq 0$ such that (iii) is satisfied. ■

(10B) Remarks

(1) By (6.2) and $(10.5)_1$, the response function $\mathbb{T}\hat{}$ for the deformational surface stress is intrinsic to the surface and given by

$$\mathbb{T}\hat{}(F,n) = \partial_{\mathbb{F}}\psi\hat{}(F,n)(\mathrm{adj}\,\mathbb{F})^{-1}. \tag{10.9}$$

(2) By (10.8), the normal component of the total surface stress satisfies

$$\mathbb{a}\hat{}(F,n) = -\partial_n\psi\hat{}(F,n), \tag{10.10}$$

and, by Lemma (2F), is *intrinsic to the surface if and only if* $\psi\hat{}$ *is independent of the deformation gradient* (cf. Remark (6A)).

(3) The Compatibility Theorem allows us to write the constitutive equations (10.1) and $(10.4)_1$ in the form (cf. Lemma (2Eiii))

$$\begin{aligned} \psi &= \psi\hat{}(\mathbb{F},n), & \mathbb{T} &= \mathbb{T}\hat{}(\mathbb{F},n), \\ \mathbb{C} &= \mathbb{C}\hat{}(\mathbb{F},n), & \mathbb{S} &= \mathbb{S}\hat{}(\mathbb{F},n). \end{aligned} \tag{10.11}$$

(4) We interpret the symmetry relation expressed in $(7.11)_{2,3}$ or $(7.13)_2$ as a restriction on the response function $\mathbb{S}\hat{}$ or $\mathbb{T}\hat{}$, and hence, by $(10.5)_1$, on $\psi\hat{}$.

(5) The relations (10.5) yield the Gibbs relation

$$\psi^{\circ} + \mathbb{a}\cdot n^{\circ} - (\mathbb{S}\mathbb{P}_{\delta})\cdot F^{\circ} = 0, \tag{10.12}$$

which shows that the surface itself does not dissipate energy. A further confirmation of this is found upon computing the right side of

(9.2) minus the left; the result, the **total dissipation**, is given by

$$\int_{\mathcal{R}} \beta v_{\mathcal{S}}^{2} da \geq 0, \tag{10.13}$$

so that *the only source of dissipation is in the exchange of atoms between phases.*

(6) Consider the coherent crystal-crystal interaction (Section 3.5) described by constitutive equations of the form

$$\begin{aligned} \psi &= \hat{\psi}(F_c, F_e, n, v), & \mathbb{T} &= \hat{\mathbb{T}}(F_c, F_e, n, v), \\ \mathbb{C} &= \hat{\mathbb{C}}(F_c, F_e, n, v), & \pi &= \hat{\pi}(F_c, F_e, n, v), \end{aligned} \tag{10.14}$$

with *domain* subject to the constraint $F_c \mathbb{I}(n) = F_e \mathbb{I}(n) = \mathbb{F}$ (cf. (3.38)). Then for every F_c, F_e, and $\mathbf{n}$ in this domain there is a $u \in \mathbb{R}^3$ such that

$$F_c - F_e = u \otimes n. \tag{10.15}$$

Because of (10.15), the constitutive equations (10.14) fall within our framework: we simply take $F = F_c$ and allow $\mathbf{u}$ to enter the list[41] z. Thus ψ, $\mathbb{T}$, $\mathbb{C}$, and $\mathbb{S}$ can depend on F_c and F_e only through the common tangential gradient $\mathbb{F}$. Here it should be emphasized that the normal component $\mathbb{a}$ of the total surface stress is defined (cf. (6.9)) relative to the *normal deformation gradient* $\mathbb{f} = F_c n$ *for phase* c (cf. (2) above).

---

[41] Cf. Footnote 26

11. Basic equations for the crystal surface.

The basic equations of the mechanical theory, expressed using the referential description and the abbreviations

$$n = n_{\mathscr{S}}, \qquad V = V_{\mathscr{S}}, \qquad \rho = \rho_{\mu},$$

consist of: **balance of mass**

$$\begin{aligned} &F^{-1}(v_c - v_e)\cdot n = (\zeta - 1)V, \\ &\zeta = \rho_c/\rho_e = \rho/(\rho_e \det F), \end{aligned} \qquad (11.1)$$

balance of momentum

$$\mathrm{div}_{\mathscr{S}}\mathbb{S} + J(t_c + t_e) = \rho V(v_c - v_e), \qquad (11.2)$$

and the **accretive balance**

$$\{\Psi + JF^{T}(t_c + t_e)\cdot n + \mathscr{k} + \mathscr{g} + \beta V\}V + Jt_e\cdot(v_c - v_e) = 0, \qquad (11.3)$$

with

$$\begin{aligned} &\mathscr{g} = -\psi K - \mathrm{div}_{\mathscr{S}}\mathbb{C} + (F^{T}\mathbb{S})\cdot\mathbb{L}, \\ &\mathscr{k} = \tfrac{1}{2}\rho[(v_c - \mathfrak{v}_{\mathscr{S}})^2 - (v_e - \mathfrak{v}_{\mathscr{S}})^2], \end{aligned} \qquad (11.4)$$

supplemented by the **thermodynamic relations**

$$\begin{aligned} &\psi = \psi\hat{}(\mathbb{F},n), \quad \mathbb{S} = \partial_{\mathbb{F}}\psi\hat{}(\mathbb{F},n), \quad \mathbb{C} = -D_n\psi\hat{}(\mathbb{F},n), \\ &\beta = \beta\hat{}(F,n,V,z) \geq 0 \end{aligned} \qquad (11.5)$$

(cf. $(5.11)_{2,3}$, (7.13), (9.17), (9.7), (9.8), (10.5), (10.6), (10.11)). Within the full theory, which includes constitutive equations and balance laws for the crystal interior and for the environment, (11.1)-(11.5) constitute free-boundary conditions.

For the environment an **inviscid melt**, as discussed in the paragraph containing (7.18), the basic laws reduce to[42]

$$
\begin{aligned}
&F^{-1}(v_c - v_e)\cdot n = (\zeta - 1)v,\\
&\mathrm{div}_{\mathcal{S}}\mathbb{S} - \{S_c + p_e(\det F)F^{-T}\}n = \rho v(v_c - v_e), \qquad (11.6)\\
&\Psi_\mu - (\det F)\zeta\Psi_e = (S_c n)\cdot(Fn) + (\det F)\zeta p_e - \mathscr{k} - \mathscr{g} - \beta v,
\end{aligned}
$$

supplemented by (11.5) (cf. (7.22), (9.1), (9.10)).

For the **coherent crystal-crystal interaction** described in Section 3.5 and the paragraph containing (7.23), we may use (3.36) to write (9.17) in the form

$$\mathscr{k} = \tfrac{1}{2}\rho v^2\{|F_c n|^2 - |F_e n|^2\},$$

and, using the bulk energies $\Psi_{\mu c}$ and $\Psi_{\mu e}$ measured per unit reference volume (cf. (5.16),(5.17)), the basic laws reduce to

$$
\begin{aligned}
&\mathrm{div}_{\mathcal{S}}\mathbb{S} + (S_e - S_c)n = \rho v(v_c - v_e),\\
& \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad (11.7)\\
&\Psi_{\mu c} - \Psi_{\mu e} = (S_c n)\cdot(F_c n) - (S_e n)\cdot(F_e n) - \mathscr{k} - \mathscr{g} - \beta v,
\end{aligned}
$$

supplemented by (11.5) (cf. (7.25), (9.11)). Because of (5.12), mass balance is not needed. If we let

$$
\begin{aligned}
&s_{av} = \tfrac{1}{2}\{(S_c n) + (S_e n)\},\\
&\mathscr{f}_{av} = \tfrac{1}{2}\{\mathscr{f}_c + \mathscr{f}_e\}, \qquad \mathscr{f}_c = F_c n, \qquad \mathscr{f}_e = F_e n,
\end{aligned}
$$

then we can use (3.36) to write $(11.7)_1$ in the form

---

[42] For statical situations ($v = 0$, $v_c = v_e = 0$): $(11.6)_2$ and $(11.7)_1$ are trivial consequences of eqt. (5.25) of Gurtin and Murdoch [1975]; $(11.6)_3$ and $(11.7)_2$ were derived by Leo and Sekerka [1989] (cf. Johnson and Alexander [1985,1986]) as Euler-Lagrange equations for stable equilibria.

$$\Psi_{\mu c} - \Psi_{\mu e} = \mathbf{s}_{av} \cdot (\mathbb{f}_c - \mathbb{f}_e) + \mathbb{f}_{av} \cdot \mathrm{div}_{\mathscr{s}}\mathbb{S} - \mathscr{g} - \beta v. \qquad (11.8)$$

(11A) Remark. Coherent phase transitions involve jumps in deformation gradient and material velocity, and therefore are kinematically equivalent to shock waves. *When surface stress and surface energy are neglected,* (11.7) reduce to

$$\begin{aligned} &(S_e - S_c)\mathbf{n} = \rho v(v_c - v_e), \\ &\Psi_{\mu c} - \Psi_{\mu e} = (\mathbf{S}_c\mathbf{n}) \cdot (\mathbf{F}_c\mathbf{n}) - (\mathbf{S}_e\mathbf{n}) \cdot (\mathbf{F}_e\mathbf{n}) - \mathscr{k} - \beta v. \end{aligned} \qquad (11.9)$$

The equation $(11.9)_1$ is a standard jump condition for shock waves, but[43] $(11.9)_2$ is not. Indeed, for shock waves $(11.9)_2$ is replaced by the "entropy condition"

$$[\Psi_{\mu c} - \Psi_{\mu e} - (\mathbf{S}_c\mathbf{n}) \cdot (\mathbf{F}_c\mathbf{n}) + (\mathbf{S}_e\mathbf{n}) \cdot (\mathbf{F}_e\mathbf{n}) + \mathscr{k}]v \geq 0,$$

which shows the major difference between shocks in single phase materials and evolving phase boundaries; for shocks the dissipation is specified only to sign, but the dissipation underlying the motion of phase boundaries is specified completely as βv^2, with β a given constitutive modulus.[44] If, in addition, interfacial energy is included, then one would expect severe restrictions on the spontaneous development of phase boundaries,[45] another indication of the major difference between the two phenomena.

---

[43] $(11.9)_2$ was first established by Abeyaratne and Knowles [1988c]. We arrived at $(11.7)_2$ and $(11.9)_2$ independently, motivated by results of Gurtin for nondeformable media ([1988b], eqt. $(5.7)_1$) and for a rigid crystal in an inviscid melt ([1989], eqt. (5.3)). We proposed a one-dimensional version of $(11.9)_2$ during discussions with Slemrod in April 1989.

[44] Cf. the discussion of Abeyaratne and Knowles [1988c].

[45] This possibility was brought to our attention by Slemrod and Rascle (private communication, April, 1989).

IV. Thermodynamic theory.

12. The first two laws.

12.1. Balance of energy. Growth of entropy.

A **thermodynamic system**, relative to μ, consists of accretive and deformational force systems together with seven functions of $X \in \mathcal{S}(t)$ and $t \in T$:

$e(X,t)$	**superficial internal energy,**
$s(X,t)$	**superficial entropy,**
$\theta(X,t)$	**absolute temperature,**
$E(X,t)$	**scaled difference in bulk internal energies,**
$S(X,t)$	**scaled difference in bulk entropies,**
$q(X,t)$	**heat supply,**
$\mathfrak{q}(X,t)$	**apparent heat.**

A basic physical assumption of the theory is that the temperature be continuous across the crystal surface; $\theta(X,t)>0$ then represents the common limit as the surface is approached from the crystal interior and from the environment.

The fields e and s represent the internal energy and entropy of the crystal surface, per unit *referential* area, while E and S are scaled differences as defined in (5.15). It is convenient to define the **superficial free energy** $\psi(X,t)$ and the **scaled difference** $\Psi(X,t)$ **in bulk free energies** through

$$\psi = e - \theta s, \qquad \Psi = E - \theta S. \tag{12.1}$$

Consider an evolving control volume $R(t)=(\mathbb{R}(t),\mathfrak{r}(t))$ that *includes* the interface. Then

$$\int_{\mathbb{R}} e\,da, \qquad \int_{\mathbb{R}} s\,da$$

represent the superficial energy and entropy of $R(t)$, while

$$\int_{\mathcal{R}} E v_{\mathcal{S}}\,da, \qquad \int_{\mathcal{R}} S v_{\mathcal{S}}\,da \tag{12.2}$$

represent outflows of bulk energy and bulk entropy from $R(t)$.

The field q gives the heat supplied to $R(t)$, per unit referential area, from the bulk material of the crystal and from the environment. If $q_c(x,t)$ and $q_e(x,t)$ denote the heat flux vectors for the crystal and the environment, measured per unit deformed area, then

$$q = J(q_c - q_e)\cdot n_{\mathcal{S}}. \tag{12.3}$$

The quantity $\mathfrak{q} v_{(\partial\mathcal{R})\tan}$ gives the heat flow into $R(t)$ across its edge $\partial\mathcal{R}(t)$, per unit referential length, due to the motion of $\partial\mathcal{R}(t)$; thus

$$\int_{\mathcal{R}} q\,da + \int_{\partial\mathcal{R}} \mathfrak{q} v_{(\partial\mathcal{R})\tan}\,ds, \qquad \int_{\mathcal{R}} \theta^{-1} q\,da + \int_{\partial\mathcal{R}} \theta^{-1} \mathfrak{q} v_{(\partial\mathcal{R})\tan}\,ds$$

represent the total heat and entropy flows into $R(t)$. (We neglect heat flow within the interface.)

The accretive and deformational force systems and the kinetic energy enter the thermodynamical laws through the mechanical production $\mathcal{E}(\mathcal{R})$ for $R(t)$, which remains as defined and structured in Section 7, so that the results of that section remain valid.

The *first two laws of thermodynamics* for $R(t)$ are **balance of energy**

$$(d/dt)\Big\{\int_{\mathcal{R}} e\,da\Big\} + \int_{\mathcal{R}} E v_{\mathcal{S}}\,da + \mathcal{E}(\mathcal{R}) = \int_{\mathcal{R}} q\,da + \int_{\partial\mathcal{R}} \mathfrak{q} v_{(\partial\mathcal{R})\tan}\,ds \tag{12.4}$$

and **growth of entropy**

$$(d/dt)\Big\{\int_{\mathcal{R}} s\,da\Big\} + \int_{\mathcal{R}} S v_{\mathcal{S}}\,da \geq \int_{\mathcal{R}} \theta^{-1} q\,da + \int_{\partial\mathcal{R}} \theta^{-1} \mathfrak{q} v_{(\partial\mathcal{R})\tan}\,ds. \tag{12.5}$$

Attachment forces and bulk-interface interactions are as defined in Section 8, and the results of that section remain valid. Further, since bulk control volumes (as defined in Section 8) have no thickness, they have neither bulk internal energy nor bulk entropy, they do not exhibit outflows of bulk internal energy, bulk entropy, or kinetic energy, and they exhibit neither net heat flows nor net entropy flows. Thus energy balance for such control volumes is the requirement that (9.3) hold, while growth of entropy is satisfied automatically. We therefore postulate (9.3), and this renders the results of Sections 9.2 and 9.3 valid.

12.2. Local forms of the thermodynamical laws.

By (2.38), (9.12), (9.17), and (12.1), we may write (12.4) and (12.5) as

$$\int_{\mathcal{R}}\{e^{\circ} + (\sigma - e)\kappa v_{\mathcal{S}} + \mathbb{a}\cdot\mathbf{n}^{\circ} - (\mathbb{S}\mathbb{P}_{\mathcal{S}})\cdot\mathbf{F}^{\circ} + (E + \mathscr{k} - \pi)v_{\mathcal{S}} - q\}\,da$$

$$+ \int_{\partial\mathcal{R}}(e - \sigma - \mathscr{q})v_{(\partial\mathcal{R})\tan}\,ds = 0, \qquad (12.6)$$

$$\int_{\mathcal{R}}\{s^{\circ} - s\kappa v_{\mathcal{S}} + S v_{\mathcal{S}} - \theta^{-1}q\}\,da + \int_{\partial\mathcal{R}}(s - \theta^{-1}\mathscr{q})v_{(\partial\mathcal{R})\tan}\,ds \leq 0,$$

with $\mathscr{k}$ given by (9.17). This relation and inequality must hold for each smoothly evolving subsurface $\mathcal{R}$ of $\mathcal{S}$; thus (ii) of the Invariance Lemma (Appendix C) yields the

(12A) Tension-Energy Theorem. *The surface tension and superficial free energy coincide, while* θs *represents the apparent heat:*

$$\sigma = \psi, \qquad \mathscr{q} = \theta s. \qquad (12.7)$$

If we substitute (12.7) into (12.6), and use (12.1) and the fact that $\mathcal{R}$ is arbitrary, we are led to the

(12B) Local Thermodynamical Laws. *The laws of balance of energy and growth of entropy have the local forms*

$$\begin{aligned} &e^\circ - \theta s K v_{\mathcal{S}} + \mathbb{a}\cdot n^\circ - (\mathbb{S}\mathbb{P}_{\mathcal{S}})\cdot F^\circ + (E + \mathcal{k} - \pi)v_{\mathcal{S}} = q, \\ &s^\circ - s K v_{\mathcal{S}} + S v_{\mathcal{S}} \geq q/\theta, \end{aligned} \tag{12.8}$$

which combine to yield the **reduced free-energy inequality**

$$\psi^\circ + s\theta^\circ + \mathbb{a}\cdot n^\circ - (\mathbb{S}\mathbb{P}_{\mathcal{S}})\cdot F^\circ + (\Psi + \mathcal{k} - \pi)v_{\mathcal{S}} \leq 0. \tag{12.9}$$

The accretive balance remains as in the mechanical theory:

$$\begin{aligned} &\{\pi + \mathcal{g} + JF^T(t_c + t_e)\cdot n_{\mathcal{S}}\}v_{\mathcal{S}} + Jt_e\cdot(v_c - v_e) = 0, \\ &\mathcal{g} = -\sigma K - \operatorname{div}_{\mathcal{S}}\mathbb{C} + (F^T\mathbb{S})\cdot\mathbb{L}. \end{aligned} \tag{12.10}$$

For the environment an *inviscid melt,* it is convenient to express the scaled differences $\Phi = E, S, \Psi$ in terms of bulk densities in the crystal $\Phi_\mu = E_\mu, S_\mu, \Psi_\mu$ per unit referential volume and bulk densities in the melt $\Phi_e = E_e, S_e, \Psi_e$ per unit deformed volume (cf. (9.1):

$$\Phi = \Phi_\mu - (\det F)\zeta\Phi_e. \tag{12.11}$$

On the other hand, for the *coherent crystal-crystal interaction* we will use densities $\Phi_{\mu c} = E_{\mu c}, S_{\mu c}, \Psi_{\mu c}$ and $\Phi_{\mu e} = E_{\mu e}, S_{\mu e}, \Psi_{\mu e}$ per unit reference volume for both phases (cf. (5.16) and (5.17)):

$$\Phi = \Phi_{\mu c} - \Phi_{\mu e} \tag{12.12}$$

It is generally easier to use the bulk Piola-Kirchhoff heat flux vector

$$h_c = (\det F)F^{-1}q_c \tag{12.13}$$

for the crystal; then, by (3.6) and (3.13), we can write (12.3) in the form

$$q = [h_c - (\det F)F^{-1}q_e] \cdot n_{\mathcal{S}}. \qquad (12.14)$$

For the *coherent crystal-crystal interaction* we will use bulk Piola-Kirchhoff heat flux vectors for both phases:

$$h_c = (\det F_c){F_c}^{-1}q_c, \qquad h_e = (\det F_e){F_e}^{-1}q_e; \qquad (12.15)$$

in this case

$$q = (h_c - h_e) \cdot n_{\mathcal{S}}. \qquad (12.16)$$

13. Constitutive equations. Compatibility with thermodynamics.

We consider constitutive equations of the form

$$
\begin{gathered}
e = e\hat{}(F,\theta,\mathbf{n},v,\mathbf{z}), \qquad s = s\hat{}(F,\theta,\mathbf{n},v,\mathbf{z}), \\
\mathbb{T} = \mathbb{T}\hat{}(F,\theta,\mathbf{n},v,z), \qquad \mathbb{C} = \mathbb{C}\hat{}(F,\theta,\mathbf{n},v,z), \\
\pi = \pi\hat{}(F,\theta,\mathbf{n},v,z),
\end{gathered} \tag{13.1}
$$

with $\mathbf{n}=\mathbf{n}_{\mathcal{S}}$, $v=v_{\mathcal{S}}$, and z a subsidiary variable as specified in Section 10, so that

$$
\Bbbk = \Bbbk\hat{}(F,\mathbf{n},v,z), \qquad \Psi = \Psi\hat{}(F,\theta,\mathbf{n},v,z) \tag{13.2}
$$

These constitutive equations imply relations

$$
\psi = \psi\hat{}(F,\theta,\mathbf{n},v,z), \qquad \mathbb{S} = \mathbb{S}\hat{}(F,\theta,\mathbf{n},v,z), \qquad \mathbb{e} = \mathbb{e}\hat{}(F,\theta,\mathbf{n},v,z). \tag{13.3}
$$

A **constitutive process** now consists of: (i) a crystal motion $\boldsymbol{\chi}(t):\mathcal{C}(t)\to c(t)$ $(t\in T)$; (ii) smooth temperature and auxiliary fields $\theta(X,t)$ and $z(X,t)$ defined for $X\in\mathcal{S}(t)$ and $t\in T$; (iii) corresponding fields e, s, $\mathbb{T}$, $\mathbb{C}$, and π generated through the constitutive equations (13.1). The basic thermodynamic **axiom** is now the requirement that *the reduced free-energy inequality* (12.9) *be satisfied in all constitutive processes.* The next theorem is a direct consequence of this axiom; its proof is strictly analogous to that of (10A).

(13A) Thermodynamic Compatibility.

(i) *The response functions for the free and internal superficial energies, the superficial entropy, the Piola-Kirchhoff surface stress, and the accretive surface stress are intrinsic to the surface, independent of the normal speed and the subsidiary variable, and related through*

$$\begin{aligned} &\hat{s}(F,\theta,n) = -\partial_\theta\hat{\psi}(F,\theta,n), \\ &\hat{\mathbb{S}}(F,\theta,n) = \partial_{\mathbb{F}}\hat{\psi}(F,\theta,n), \\ &\hat{\mathbb{C}}_{tan}(F,\theta,n) = \hat{\psi}(F,\theta,n)\mathbb{I}(n) - \mathbb{I}(n)\mathbb{F}^{T}\partial_{\mathbb{F}}\hat{\psi}(F,\theta,n), \\ &\hat{\mathbb{c}}(F,\theta,n) = -D_n\hat{\psi}(F,\theta,n). \end{aligned} \tag{13.4}$$

(ii) *There is a response function* $\hat{\beta}$ *such that the normal attachment force has the form*

$$\hat{\pi}(F,\theta,n,v,z) = \mathscr{k} + \Psi + \beta v, \qquad \beta = \hat{\beta}(F,\theta,n,v,z) \geq 0, \tag{13.5}$$

with $\mathscr{k}$ *and* Ψ *given by* (13.2).

Analogs of the Remarks (10B) hold in the present theory. In particular, we have the *Gibbs relations*

$$\begin{aligned} &\psi^\circ + s\theta^\circ + \mathbb{a}\cdot n^\circ - (\mathbb{S}\mathbb{P}_{\mathscr{S}})\cdot F^\circ = 0, \\ &e^\circ - \theta s^\circ + \mathbb{a}\cdot n^\circ - (\mathbb{S}\mathbb{P}_{\mathscr{S}})\cdot F^\circ = 0. \end{aligned} \tag{13.6}$$

The relation $(13.6)_2$ allows us to simplify the local energy balance $(12.8)_1$; indeed, by (12.1) and (13.5), we have the following result:

(13B) Local Entropy Balance. *Granted the thermodynamic restrictions* (13.4) *and* (13.5), *balance of energy* $(12.8)_1$ *is equivalent to the entropy balance*

$$s^\circ - s\kappa v_{\mathscr{S}} + S v_{\mathscr{S}} = \theta^{-1}(q + \beta v_{\mathscr{S}}{}^2). \tag{13.7}$$

The left side of (12.5) minus the right represents the **total entropy production**, which, by (13.7) (cf. $(12.6)_2$, $(12.7)_2$), is

$$\int_{\mathscr{R}} \theta^{-1}\beta v_{\mathscr{S}}{}^2 da \geq 0, \tag{13.8}$$

so that *the only source of entropy production is in the exchange of atoms between phases.*

14. Basic equations for the crystal surface.

The basic equations of the thermodynamical theory, expressed using the referential description and the abbreviations $\mathbf{n}=\mathbf{n}_{\mathcal{S}}$, $v=v_{\mathcal{S}}$, $\rho=\rho_{\mu}$, consist of: **balance of mass**

$$F^{-1}(\mathbf{v}_c-\mathbf{v}_e)\cdot\mathbf{n} = (\zeta-1)v,$$
$$\zeta = \rho_c/\rho_e = \rho/(\rho_e \det F), \tag{14.1}$$

balance of momentum

$$\mathrm{div}_{\mathcal{S}}\mathbb{S} + J(\mathbf{t}_c+\mathbf{t}_e) = \rho v(\mathbf{v}_c-\mathbf{v}_e), \tag{14.2}$$

the **accretive balance**

$$\{\Psi + JF^T(\mathbf{t}_c+\mathbf{t}_e)\cdot\mathbf{n} + \mathfrak{k} + \mathfrak{g} + \beta v\}v + J\mathbf{t}_e\cdot(\mathbf{v}_c-\mathbf{v}_e) = 0,$$
$$\mathfrak{g} = -\psi K - \mathrm{div}_{\mathcal{S}}\mathbb{C} + (F^T\mathbb{S})\cdot\mathbb{L}, \tag{14.3}$$
$$\mathfrak{k} = \tfrac{1}{2}\rho[(\mathbf{v}_c-\mathfrak{v}_{\mathcal{A}})^2 - (\mathbf{v}_e-\mathfrak{v}_{\mathcal{A}})^2],$$

the **entropy balance** (energy balance)

$$s^{\circ} - sKv + Sv = \theta^{-1}(q + \beta v^2), \tag{14.4}$$

and the **thermodynamic relations**

$$\psi = \psi\hat{}(\mathbb{F},\theta,\mathbf{n}),\quad s = -\partial_\theta\psi\hat{}(\mathbb{F},\theta,\mathbf{n}),\quad \mathbb{S} = \partial_{\mathbb{F}}\psi\hat{}(\mathbb{F},\theta,\mathbf{n}),$$
$$\mathbb{C} = -D_{\mathbf{n}}\psi\hat{}(\mathbb{F},\mathbf{n}),\qquad \beta = \beta\hat{}(F,\theta,\mathbf{n},v,z) \geq 0. \tag{14.5}$$

Within the full theory, which includes constitutive equations and balance laws for the crystal interior and for the environment, (14.1)-(14.5) constitute free-boundary conditions.

For the environment an **inviscid melt**, the basic laws reduce to

$$\begin{aligned}
&\mathbf{F}^{-1}(\mathbf{v}_c - \mathbf{v}_e)\cdot\mathbf{n} = (\zeta - 1)V,\\
&\mathrm{div}_{\mathcal{S}}\mathbb{S} - \{\mathbf{S}_c + p_e(\det\mathbf{F})\mathbf{F}^{-\mathsf{T}}\}\mathbf{n} = \rho V(\mathbf{v}_c - \mathbf{v}_e),\\
&\Psi_\mu - (\det\mathbf{F})\zeta\Psi_e = (\mathbf{S}_c\mathbf{n})\cdot(\mathbf{F}\mathbf{n}) + (\det\mathbf{F})\zeta p_e - \mathscr{k} - \mathscr{g} - \beta V,\\
&s^\circ - s\kappa V + [S_\mu - (\det\mathbf{F})\zeta S_e]V =\\
&\qquad\qquad \theta^{-1}[\mathbf{h}_c - (\det\mathbf{F})\mathbf{F}^{-1}\mathbf{q}_e]\cdot\mathbf{n} + \theta^{-1}\beta V^2,
\end{aligned} \tag{14.6}$$

supplemented by (14.5).

For the **coherent crystal-crystal interaction** the basic laws reduce to[46]

$$\begin{aligned}
&\mathrm{div}_{\mathcal{S}}\mathbb{S} + (\mathbf{S}_e - \mathbf{S}_c)\mathbf{n} = \rho V(\mathbf{v}_c - \mathbf{v}_e),\\
&\Psi_{\mu c} - \Psi_{\mu e} = (\mathbf{S}_c\mathbf{n})\cdot(\mathbf{F}_c\mathbf{n}) - (\mathbf{S}_e\mathbf{n})\cdot(\mathbf{F}_e\mathbf{n}) - \mathscr{k} - \mathscr{g} - \beta V,\\
&s^\circ - s\kappa V + [S_{\mu c} - S_{\mu e}]V = \theta^{-1}[\mathbf{h}_c - \mathbf{h}_e]\cdot\mathbf{n} + \theta^{-1}\beta V^2,
\end{aligned} \tag{14.7}$$

supplemented by (14.5). We could also use $(14.7)_2$ in the form (11.8).

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[46] Abeyaratne and Knowles [1988c] derive $(14.7)_{2,3}$ for the special case in which surface stress, surface energy, and surface entropy are negligible (cf. Remark 11A).

Appendices.

Appendix A. Change in reference configuration.

A1. Kinematics.

Let μ_1 and μ_2 be configurations of the lattice, with g and $G = \nabla g$ the label change and label gradient from μ_1 to μ_2. Further, let $\mathcal{S}_1(t) = \partial C_{\mu_1}(t)$, $n_1 = n_{\mathcal{S}_1}$, $\mathbb{P}_1 = \mathbb{P}_{\mathcal{S}_1}$, $\mathbb{I}_1 = \mathbb{I}_{\mathcal{S}_1}$, $\chi_1 = \chi_{\mu_1}$, $F_1 = F_{\mu_1}$, and so forth; and similarly for the quantities corresponding to μ_2. Let $X_1 \in \mathcal{S}_1(t)$ and $X_2 \in \mathcal{S}_2(t)$ satisfy $X_2 = g(X_1)$. Then

$$\begin{aligned} \chi_2(X_2,t) &= \chi_1(g^{-1}(X_2),t), \\ F_2(X_2,t) &= F_1(X_1,t)G^{-1}, \end{aligned} \tag{A1}$$

so that, by (2.16) (applied to G^{-1}), $(2.20)_1$, and (3.8),

$$\mathbb{F}_2 = F_2\mathbb{I}_2 = F_1G^{-1}\mathbb{I}_2 = F_1\mathbb{I}_1\mathbb{P}_1G^{-1}\mathbb{I}_2 = \mathbb{F}_1(\mathbb{G}_{surf})^{-1}, \tag{A2}$$

and (3.11) yields

$$(\mathbb{F}_{surf})_2 = (\mathbb{F}_{surf})_1(\mathbb{G}_{surf})^{-1}, \tag{A3}$$

where, for convenience, we have omitted arguments. Similarly,

$$J_1 = J_2 \det \mathbb{G}, \tag{A4}$$

so that, by (2.24),

$$\operatorname{adj}\mathbb{F}_1 = (\operatorname{adj}\mathbb{F}_2)(\operatorname{adj}\mathbb{G}), \tag{A5}$$

Each $\mathcal{S}_1$-trajectory $Y_1(\beta)$ through X_1 at t induces an $\mathcal{S}_2$-trajectory $Y_2(\beta) = g(Y_1(\beta))$ through X_2 at t, and $Y_2^{\cdot}(\beta) = GY_1^{\cdot}(\beta)$. We may therefore use Lemma (2B) to conclude that each velocity field[47]

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[47] Here we write v_1 and v_2 for arbitrary velocity fields, $v_{\mathcal{S}_1}$ and $v_{\mathcal{S}_2}$ for normal velocities.

$\mathbf{v}_1$ for $\mathcal{S}_1$ induces a velocity field $\mathbf{v}_2$ for $\mathcal{S}_2$ through

$$\mathbf{v}_2 = \mathbf{G}\mathbf{v}_1. \tag{A6}$$

What is important about this pairing is that, by (3.25), (A1), and the invariance of $\mathbf{v}_c$ under reference changes, the corresponding induced velocities $\boldsymbol{\upsilon}_1$ and $\boldsymbol{\upsilon}_2$ are invariant:

$$\boldsymbol{\upsilon}_1 = \boldsymbol{\upsilon}_2. \tag{A7}$$

This result holds also for edge velocities and corresponding induced edge velocities for smoothly propagating subsurfaces $\mathbb{R}_1$ and $\mathbb{R}_2$ of $\mathcal{S}_1$ and $\mathcal{S}_2$ provided $\mathbb{R}_2(t) = \mathbf{g}(\mathbb{R}_1(t))$.

The transformation (A6) does not generally preserve the normality of velocity fields. If in (A6) we take $\mathbf{v}_1$ to be the normal velocity $\mathbf{v}_{\mathcal{S}_1}$ and use (2.16) and the fact that $(\mathbf{v}_2 \cdot \mathbf{n}_2)\mathbf{n}_2 = \mathbf{v}_{\mathcal{S}_2}$, we arrive at the transformation rules

$$V_{\mathcal{S}_2} = \lambda V_{\mathcal{S}_1}, \qquad \mathbf{v}_{\mathcal{S}_2} = \lambda^2 \mathbf{G}^{-\mathrm{T}} \mathbf{v}_{\mathcal{S}_1}, \qquad \lambda = |\mathbf{G}^{-\mathrm{T}} \mathbf{n}_1|^{-1}. \tag{A8}$$

A2. Invariance under change in reference configuration.

The accretive force system is defined relative to a given reference configuration μ, and this renders the expended power possibly dependent on the choice of μ. We now deduce transformation laws for accretive forces under changes in reference which ensure the invariance of the expended power (and hence of the mechanical production, since the outflow of kinetic energy is independent of the choice of reference).

Let μ_1 and μ_2 be configurations of the lattice, let $\mathbb{C}_1$ and $\mathbf{c}_1$ denote the accretive stress and accretive traction for μ_1, and let $\mathbb{C}_2$ and $\mathbf{c}_2$ denote the analogous quantities for μ_2. Further, (using the notation of Section 3.3) let $\mathbf{g}$ and $\mathbf{G} = \nabla\mathbf{g}$ designate the label change and label gradient from μ_1 to μ_2; let $\mathbb{R}_1$ and $\mathbb{R}_2$ denote smoothly propagating subsurfaces of $\mathcal{S}_1$ and $\mathcal{S}_2$, with $\mathbb{R}_2(t) = \mathbf{g}(\mathbb{R}_1(t))$ so that

$r(t) = \boldsymbol{\chi}_1(\mathbb{R}_1(t),t) = \boldsymbol{\chi}_2(\mathbb{R}_2(t),t)$; let ν_1 and ν_2 denote the outward unit normals to $\partial\mathbb{R}_1$ and $\partial\mathbb{R}_2$. Then relative to the configuration μ_i $(i=1,2)$ the expended power (6.4) is given by

$$\mathcal{P}_i = \int_{\partial\mathbb{R}_i} \mathbb{C}_i\nu_i \cdot \mathbf{v}_i\,ds + \int_{\partial r} \mathbb{T}\tau \cdot \boldsymbol{\upsilon}_i\,ds + \int_{r} (\mathbf{t}_c \cdot \mathbf{v}_c + \mathbf{t}_e \cdot \mathbf{v}_e)\,da, \tag{A9}$$

with $\mathbf{v}_i$ an edge velocity for $\partial\mathbb{R}_i$ and $\boldsymbol{\upsilon}_i$ the corresponding induced edge velocity for r. (Here it is tacit that the deformational and environmental systems are independent of the choice of reference.) Since $\mathcal{P}_i$ is independent of the choice of $\mathbf{v}_i$, we may choose $\mathbf{v}_1$ arbitrarily and $\mathbf{v}_2 = \mathbf{G}\mathbf{v}_1$ (cf. (A6)), so that $\boldsymbol{\upsilon}_1 = \boldsymbol{\upsilon}_2$ (cf. (A7)), to verify that $\mathcal{P}_1 = \mathcal{P}_2$ if and only if

$$\int_{\partial\mathbb{R}_1} \mathbb{C}_1\nu_1 \cdot \mathbf{v}_1\,ds = \int_{\partial\mathbb{R}_2} \mathbb{C}_2\nu_2 \cdot \mathbf{G}\mathbf{v}_1\,ds,$$

or equivalently, using $(2.25)_3$ and the fact that $\mathbf{v}_1$ and $\mathbb{R}_1$ are arbitrary,

$$\mathbb{C}_1 = \mathbf{G}^{\mathsf{T}}\mathbb{C}_2\,\mathrm{adj}\,\mathbb{G}, \tag{A10}$$

which is the *transformation law for the accretive stress.*

Next, $(2.25)_2$, the fact that $\mathbf{G}$ is constant, and the requirement that the accretive force systems relative to the two configurations be consistent with the balance laws $(7.9)_1$ yield

$$\begin{aligned}
0 &= \int_{\partial\mathbb{R}_2} \mathbf{G}^{\mathsf{T}}\mathbb{C}_2\nu_2\,ds + \int_{\mathbb{R}_2} \mathbf{G}^{\mathsf{T}}\mathbf{c}_2\,da \\
&= \int_{\partial\mathbb{R}_1} \mathbf{G}^{\mathsf{T}}\mathbb{C}_2(\mathrm{adj}\,\mathbb{G})\nu_1\,ds + \int_{\mathbb{R}_1} (\det\mathbb{G})\mathbf{G}^{\mathsf{T}}\mathbf{c}_2\,da \\
&= \int_{\partial\mathbb{R}_1} \mathbb{C}_1\nu_1\,ds + \int_{\mathbb{R}_1} (\det\mathbb{G})\mathbf{G}^{\mathsf{T}}\mathbf{c}_2\,da,
\end{aligned}$$

so that

$$\int\limits_{\mathbb{R}_1} \mathbf{c}_1 da = \int\limits_{\mathbb{R}_1} (\det\mathbb{G})\mathbf{G}^T\mathbf{c}_2 da.$$

Since $\mathbb{R}_1$ is arbitrary, this implies the *transformation law for the accretive traction:*

$$\mathbf{c}_1 = (\det\mathbb{G})\mathbf{G}^T\mathbf{c}_2. \tag{A11}$$

Next, (A5) and (6.2) yield the *transformation law for the Piola-Kirchhoff stress:*

$$\mathbb{S}_1 = \mathbb{S}_2 \operatorname{adj}\mathbb{G}, \tag{A12}$$

and this, (A1) and (6.7) yield the *transformation law for the total surface stress:*

$$\mathbb{A}_1 = \mathbf{G}^T\mathbb{A}_2 \operatorname{adj}\mathbb{G}. \tag{A13}$$

The law (A13) implies corresponding transformation rules for the surface tensions σ_1 and σ_2 and the normal parts $\mathbb{a}_1$ and $\mathbb{a}_2$ of the total surface stress, where, by (7.5),

$$\mathbb{A}_i = \sigma_i \mathbb{I}_i + \mathbf{n}_i \otimes \mathbb{a}_i. \tag{A14}$$

Indeed, if substitute $\mathbb{A}_2$ in the form (A14) into (A13), and use (2.16) and (2.21), we find that

$$(\det\mathbb{G})^{-1}\mathbb{A}_1 = \sigma_2\mathbb{I}_1 + \mathbf{n}_1 \otimes (\mathbb{G}_{\mathrm{surf}})^{-1}[\lambda\mathbb{a}_2 + \sigma_2\mathbb{P}_2\mathbf{G}\mathbf{n}_1], \tag{A15}$$

and therefore, taking $\mathbb{A}_1$ as given by (A14) and using (2.17), we find that

$$\sigma_1 = (\det\mathbb{G})\sigma_2, \qquad \mathbb{a}_1 = (\operatorname{adj}\mathbb{G})^T[\lambda\mathbb{a}_2 + \sigma_2\mathbb{P}_2\mathbf{G}\mathbf{n}_1]. \tag{A16}$$

Finally, if ψ_i and Ψ_i denote the superficial and (crystal) bulk energies relative to μ_i $(i=1,2)$. Then, by (2.23), $(2.25)_1$, and $(A8)_1$, under the transformations

$$\psi_1 = (\det \mathbb{G})\psi_2, \qquad \Psi_1 = (\det G)\Psi_2 \tag{A17}$$

the corresponding terms in (9.2) are independent of the choice of reference configuration; these transformations coupled with those given in (A10)-(A12) (which ensure the invariance of the expended power) render the global dissipation inequality independent of the choice of reference.

Similar considerations apply in the thermodynamical theory.

Appendix B. Material symmetry.

We now deduce the manner in which the response functions $\psi\hat{}$, $\mathbb{C}\hat{}$, and $\mathbb{T}\hat{}$ in (10.1) transform under a change in reference.[48] Thus let μ_1 and μ_2 be configurations, and let $\psi_i\hat{}$, $\mathbb{C}_i\hat{}$, and $\mathbb{T}_i\hat{}$ denote these response functions relative to μ_i $(i=1,2)$. Then, since the deformational surface stress is invariant under a change in reference, we may use (2.16), (A1), (A10), and (A17) to conclude that

$$\begin{aligned} \psi_2\hat{}(F,n) &= (\det\mathbb{G})^{-1}\psi_1\hat{}(FG,|G^T n|^{-1}G^T n), \\ \mathbb{C}_2\hat{}(F,n) &= G^{-T}\,\mathbb{C}_1\hat{}(FG,|G^T n|^{-1}G^T n)(\operatorname{adj}\mathbb{G})^{-1}, \\ \mathbb{T}_2\hat{}(F,n) &= \mathbb{T}_1\hat{}(FG,|G^T n|^{-1}G^T n), \end{aligned} \tag{B1}$$

with G the label gradient from μ_1 to μ_2.

We use the term **unimodular tensor** for a tensor $G \in \mathrm{lin}(\mathbb{R}^3,\mathbb{R}^3)$ with $\det G = 1$. The symmetry group for the material relative to a configuration μ consists of those changes in reference which leave the material response and density unaltered. Modulo an inconsequential translation, each such change in reference can be identified with a unimodular label-gradient G. Thus, guided by (B1), we define the **symmetry group**[49] $\mathcal{G}_\mu$, relative to a configuration μ, to be the group of all unimodular tensors G such that the response functions relative to μ satisfy

$$\begin{aligned} \psi\hat{}(F,n) &= (\det\mathbb{G})^{-1}\psi\hat{}(FG,|G^T n|^{-1}G^T n), \\ G^T\,\mathbb{C}\hat{}(F,n)(\operatorname{adj}\mathbb{G}) &= \mathbb{C}\hat{}(FG,|G^T n|^{-1}G^T n), \\ \mathbb{T}\hat{}(F,n) &= \mathbb{T}\hat{}(FG,|G^T n|^{-1}G^T n) \end{aligned} \tag{B2}$$

for all $F \in \mathrm{Lin}^+$ and $n \in \mathrm{Unit}$.

A **solid** is, by definition, a material whose symmetry group $\mathcal{G}_\mu$,

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[48] The response function $\pi\hat{}$ could also be included provided we specify the manner in which the subsidiary variable z transforms under a change in reference.

[49] For a single-phase bulk material this definition as well as those of "solid" and "fluid" are due to Noll [1958]. Cf. also Truesdell and Noll [1965], Sect. 31, Gurtin [1981], Sect. 25.

relative to some configuration μ, is a subgroup of the group of all rotations. The particular configurations μ with this property are then referred to as **undistorted**. In contrast, **fluids** are defined by the requirement that, relative to some (and hence every) configuration μ, $\mathfrak{D}_\mu$ contains *all* unimodular tensors. As is clear from our choice of terminology (lattice, crystal, etc.), our interest lies chiefly in solids; even so, our ideas seem appropriate also to fluids.

We require that the constitutive equations be invariant under changes in spatial observer. By virtue of $(4.10)_1$ and (6.10), this is equivalent to the requirement that, for all rotations $\mathbf{Q}$,

$$\begin{aligned} \hat{\psi}(\mathbf{F},\mathbf{n}) &= \hat{\psi}(\mathbf{QF},\mathbf{n}), \\ \hat{\mathbb{C}}(\mathbf{F},\mathbf{n}) &= \hat{\mathbb{C}}(\mathbf{QF},\mathbf{n}), \\ \mathbf{Q}\hat{\mathbb{T}}(\mathbf{F},\mathbf{n})\mathbf{Q}^T &= \hat{\mathbb{T}}(\mathbf{QF},\mathbf{n})), \end{aligned} \tag{B3}$$

The restrictions (B3) may be used, in the usual manner,[50] to deduce reduced constitutive equations in terms of superficial strain tensors.

For a solid the conditions (B2) and (B3) may be combined to give the more standard symmetry relations:

$$\begin{aligned} \hat{\psi}(\mathbf{F},\mathbf{n}) &= \hat{\psi}(\mathbf{QFQ}^T,\mathbf{Qn}), \\ \mathbf{Q}\hat{\mathbb{C}}(\mathbf{F},\mathbf{n})\mathbf{Q}^T &= \hat{\mathbb{C}}(\mathbf{QFQ}^T,\mathbf{Qn}), \\ \mathbf{Q}\hat{\mathbb{T}}(\mathbf{F},\mathbf{n})\mathbf{Q}^T &= \hat{\mathbb{T}}(\mathbf{QFQ}^T,\mathbf{Qn})), \end{aligned} \tag{B4}$$

for all (rotations) $\mathbf{Q}\in\mathfrak{D}_\mu$. In deriving (B4), we have used the fact that, by virtue of our convention (2.6), $\hat{\mathbb{C}}(\mathbf{F},\mathbf{n})(\mathrm{adj}\,\mathbb{G}) = \hat{\mathbb{C}}(\mathbf{F},\mathbf{n})\mathbf{G}$ for $\mathbf{G}$ a rotation.

For fluids it is convenient to introduce the energy

$$\psi_0(\mathbf{F},\mathbf{n}) = \hat{J}(\mathbf{F},\mathbf{n})^{-1}\hat{\psi}(\mathbf{F},\mathbf{n}) \tag{B5}$$

per unit deformed area (cf. $(2.25)_1$, (3.16)). Then $(B2)_1$ and $(B3)_1$

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[50] Cf. Gurtin and Murdoch [1975].

combine to give

$$\psi_0(\mathbf{F},\mathbf{n}) = \psi_0(\mathbf{QFG},|\mathbf{G}^T\mathbf{n}|^{-1}\mathbf{G}^T\mathbf{n}) \tag{B6}$$

for all rotations $\mathbf{Q}$ and all unimodular tensors $\mathbf{G}$. In classical treatments of fluid surfaces the surface tension is assumed constant and equal to ψ_0. The next result establishes the consistency of our theory with this classical formulation.

Theorem on Fluid Surfaces. *Let the material be a fluid. Then:*

(i) *the surface energy* ψ_0 *(per unit deformed area) is identically constant;*

(ii) *the deformational surface stress is a surface tension equal to* ψ_0 *and the accretive surface stress vanishes identically:*

$$\mathbb{T} = \psi_0\mathbf{I}_{\mathcal{S}}, \qquad \mathbb{C} = \mathbf{0}. \tag{B7}$$

Proof. Fix $(\mathbf{F},\mathbf{n})$. The choice $\mathbf{G}=(\det\mathbf{F})\mathbf{F}^{-1}\mathbf{Q}^T$ in (B6) yields

$$\psi_0(\mathbf{F},\mathbf{n}) = \psi_0((\det\mathbf{F})\mathbf{1},|\mathbf{F}^{-T}\mathbf{n}|^{-1}\mathbf{Q}\mathbf{F}^{-T}\mathbf{n}),$$

which can hold for all rotations $\mathbf{Q}$ only if $\psi_0(\mathbf{F},\mathbf{n})$ is independent of $\mathbf{n}$. Thus $\psi_0(\mathbf{F},\mathbf{n})=\psi_0(\det\mathbf{F})$ and, by (B5),

$$\hat{\psi}(\mathbf{F},\mathbf{n}) = \hat{J}(\mathbf{F},\mathbf{n})\psi_0(\det\mathbf{F}).$$

Consequently, $(2.49)_2$, (3.17), and (3.18) yield

$$\partial_{\mathbf{n}}\hat{\psi}(\mathbf{F},\mathbf{n}) = \hat{J}(\mathbf{F},\mathbf{n})(\det\mathbf{F})\psi_0'(\det\mathbf{F})\mathbf{F}^{-T}\mathbf{n}. \tag{B8}$$

But $\hat{\psi}$ is intrinsic to the surface, so that, by (9Eiii), (B8) must vanish identically; hence $\psi_0\equiv$constant. Further, this result, (3.19), and $(10.5)_1$ yield

$$\mathbb{S} = \psi_0 \mathbb{I}_{\partial} \,\mathrm{adj}\, \mathbb{F}, \qquad \text{(B9)}$$

and we conclude from (6.2) that $(B7)_1$ is satisfied. Also, by (3.11), $\mathbb{F}^T \mathbb{I}_{\partial} = (\mathbb{F}_{surf})^T$; therefore (3.19) and $(10.5)_2$ with $\partial_{\mathbb{F}}\psi^{\wedge}$ given by (B9) yield $\mathbb{C}_{tan} = 0$, while (3.20) and $(10.5)_2$ imply $\mathbb{C} = 0$; hence $(B7)_2$ is satisfied. ■

Note that $(B7)_2$ and (7.10) imply that the accretive traction also vanishes: $\mathbf{c} = 0$.

Appendix C. Two lemmas.

Invariance Lemma. *Let* $\mathcal{S}$ *be a smoothly propagating surface. Let* f, g, $\mathbf{f}$, *and* $\mathbb{A}$ *be fields on* $\mathcal{S}$, *with* f *and* g *superficial scalar fields,* $\mathbf{f}$ *a superficial vector field, and* $\mathbb{A}$ *a superficial tensor field.*

(i) *If, for all smoothly propagating subsurfaces* $\mathcal{R}$ *of* $\mathcal{S}$,

$$\int_{\mathcal{R}} \mathbf{f}\cdot\mathbf{v}\,da \tag{C1}$$

is independent of the choice of velocity field $\mathbf{v}$ *for* $\mathcal{S}$, *then the tangential component of* $\mathbf{f}$ *vanishes.*

(ii) *If, for all smoothly propagating subsurfaces* $\mathcal{R}$ *of* $\mathcal{S}$,

$$\int_{\mathcal{R}} f\,da + \int_{\partial\mathcal{R}} g\,v_{(\partial\mathcal{R})\tan}\,ds \le 0, \tag{C2}$$

then $g=0$.

(iii) *If, for all smoothly propagating subsurfaces* $\mathcal{R}$ *of* $\mathcal{S}$,

$$\int_{\partial\mathcal{R}} \mathbb{A}\nu\cdot\mathbf{v}\,da \tag{C3}$$

is independent of the choice of edge velocity $\mathbf{v}$ *for* $\mathcal{R}$, *then* $\mathbb{A}_{\tan}$ *is a surface tension. (Here* ν *is the outward unit normal to* $\partial\mathcal{R}$.*)*

Proof. For any (unit) vector $\mathbf{u}$ let $\mathbf{P}(\mathbf{u})\in\mathrm{lin}(\mathbb{R}^3,\mathbb{R}^3)$ be defined by

$$\mathbf{P}(\mathbf{u}) = \mathbf{1} - \mathbf{u}\otimes\mathbf{u}, \tag{C4}$$

with $\mathbf{1}$ the identity on $\mathbb{R}^3$. Let $\mathbf{n}=\mathbf{n}_{\mathcal{S}}$. Throughout the proof $\mathbf{q}(X,t)$ is an arbitrary smooth vector field on $\mathbb{R}^3\times\mathbb{R}$.

The following results will be useful:

(1) If $\mathbb{E}$ is a tangential tensor field, and if, for each $X\in\mathcal{S}$,

$\alpha\cdot\mathbb{E}(X)\beta=0$ whenever α and β are orthogonal vectors orthogonal to $n(X)$, then $\mathbb{E}$ is a surface tension.

(2) The field

$$v = v_{\mathcal{S}} + P(n)q \tag{C5}$$

is a velocity field for $\mathcal{S}$.

(3) Let $\mathcal{R}$ be a smoothly propagating subsurface of $\mathcal{S}$, with ν the outward unit normal to $\partial\mathcal{R}$. Then

$$v = v_{\partial\mathcal{R}} + P(n)P(\nu)q \tag{C6}$$

is an edge velocity for $\mathcal{R}$.

The results (2) and (3) follow from (2.33) and (2.34) (with $\mathcal{S}$ replaced by $\mathcal{R}$). Consider (1). Since $\mathbb{E}$ is tangential, it suffices to show that if $E\in\mathrm{Lin}(\mathbb{R}^2,\mathbb{R}^2)$ satisfies $\alpha\cdot E\beta=0$ whenever $\alpha,\beta\in\mathbb{R}^2$ are orthogonal, then $E=\sigma 1_2$ with 1_2 the identity on $\mathbb{R}^2$. This latter assertion follows using the choices $\alpha=e_1$, $\beta=e_2$ and $\alpha=e_1-e_2$, $\beta=e_1+e_2$, with $e_1=(1,0)$, $e_2=(0,1)$.

Consider now (i)-(iii).

(i) Choose v in (C1) equal to (C5). (C1) is then independent of q only if

$$\int_{\mathcal{R}} P(n)f\cdot q\,da = 0$$

for all q; thus and since $\mathcal{R}$ is arbitrary, $P(n)f=0$, which is the desired conclusion.

(ii) Again let v be defined by (C5). Fix t_0, let $\mathcal{R}_0$ be a sufficiently regular subsurface of $\mathcal{S}(t_0)$, and, for t sufficiently close to t_0, let $\mathcal{R}(t)$ with $\mathcal{R}(t_0)=\mathcal{R}_0$ be the image of $\mathcal{R}_0$ under the trajectories generated by the velocity field v. Then, at $t=t_0$, $V_{(\partial\mathcal{R})\tan}=q\cdot\nu$, with ν the outward unit normal to $\partial\mathcal{R}_0$, and, since q is arbitrary, (C2) yields the conclusion that, at $t=t_0$, $g\nu=0$ on $\partial\mathcal{R}_0$; since t_0 and $\mathcal{R}_0$ are arbitrary, this yields $g=0$.

(iii) Choose a smoothly propagating subsurface $\mathcal{R}$ of $\mathcal{S}$, and take v in (C3) equal to the edge velocity for $\mathcal{R}$ defined by (C6). Then, since the resulting expression must be independent of the choice of q, we may use $(2.5)_1$ to conclude that

$$\int_{\partial\mathcal{R}} (\mathbb{A}_{\tan}\nu)\cdot P(\nu) q\,da = 0.$$

Thus, since q and $\mathcal{R}$ are arbitrary, $P(\nu)\mathbb{A}_{\tan}\nu = \mathbf{0}$ for any tangential vector field ν, and the desired conclusion is a consequence of (1). ■

Let $\mathfrak{D}\subset \mathrm{Lin}^{+}\times\mathrm{Unit}\times\mathbb{R}\times\mathbb{R}^{p}$ denote the common domain of the constitutive equations (10.1), so that $\mathfrak{D}$ is an open set in $\mathrm{Lin}^{+}\times\mathrm{Unit}\times\mathbb{R}\times\mathbb{R}^{p}$ (cf. 2.41). In the next lemma it is convenient to identify the crystal $C(t)$ with the region $C_\mu(t)$ it occupies in the reference configuration μ.

Variation Lemma. *Given*

$$\mathbf{p}_0 = (F_0, n_0, V_0, z_0)\in\mathfrak{D},$$

$$F_1\in \mathrm{Lin}(\mathbb{R}^3,\mathbb{R}^3), \quad n_1\in n_0{}^{\perp}, \quad V_1\in\mathbb{R}, \quad z_1\in\mathbb{R}^p,$$

there is a crystal motion $\boldsymbol{x}(t): C(t)\to c(t)$ $(t\in T)$, *with* $0\in T$, $0\in\partial C(0)$, *such that the corresponding admissible process* $\mathbf{p} = (F, n, V, z)$ *satisfies:*

$$\mathbf{p}(0,0) = \mathbf{p}_0, \qquad \mathbf{p}^{\circ}(0,0) = (F_1, n_1, V_1, z_1). \tag{C7}$$

Proof. Let

$$\begin{aligned}
F(t) &= F_0 + tF_1, \\
\mathbf{n}(t) &= (\mathbf{n}_0 + t\mathbf{n}_1)/(\mathbf{n}_0 + t^2\mathbf{n}_1{}^2)^{\frac{1}{2}}, \\
r(t) &= tv_0 + \tfrac{1}{2}t^2 v_1, \\
z(t) &= z_0 + tz_1.
\end{aligned}$$

Further, let

$$C(t) = \{\, X : X \cdot \mathbf{n}(t) \le r(t) \,\},$$

so that

$$\partial C(t) = \{\, X : X \cdot \mathbf{n}(t) = r(t) \,\}$$

is a plane with normal $\mathbf{n}(t)$ and distance $r(t)$ from the origin, and $C(t)$ is an evolving crystal (on any time interval) with $\mathbf{n}(t)$ as outward normal. The normal velocity v is found by choosing a $\partial C(t)$-trajectory $y(t)$ and differentiating the relation $y(t) \cdot \mathbf{n}(t) = r(t)$; the result is

$$v(y(t),t) = y^{\cdot}(t) \cdot \mathbf{n}(t) = v_0 + tv_1 - y(t) \cdot \mathbf{n}^{\cdot}(t),$$

so that

$$v(X,t) = v_0 + tv_1 - X \cdot \mathbf{n}^{\cdot}(t)$$

for all $X \in \partial C(t)$.

We choose the time interval T $(0 \in T)$ sufficiently small that $(F(t),\mathbf{n}(t),v(X,t),z(t)) \in \mathfrak{D}$ for all $t \in T$ (cf. (2.41)). Then $F(t)$ is the deformation gradient of a crystal motion $\varkappa(t) : C(t) \to c(t)$ $(t \in T)$. Moreover, using (2.36) to compute the normal time derivatives of $F(t)$, $\mathbf{n}(t)$, $v(X,t)$, and $z(t)$, we see that the corresponding admissible process is consistent with (C7). ∎

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