NAMT 92-041

The Dynamics of Solid-Solid Phase Transitions 1. Coherent Interfaces

Morton E. Gurtin Carnegie Mellon University

Research Report No. 92-NA-041

November 1992

Sponsors

U.S. Army Research Office Research Triangle Park NC 27709

National Science Foundation 1800 G Street, N.W. Washington, DC 20550 University Libraries Carnegie Mellon University Pittsburgh, PA 15213-3890

3

7

THE DYNAMICS OF SOLID-SOLID PHASE TRANSITIONS 1. COHERENT INTERFACES

Morton E. Gurtin Department of Mathematics Carnegie Mellon University Pittsburgh, PA 15213

CONTENTS

1. Introduction

2. General notation.

- A. Simple theory without interfacial structure
 - 3. Kinematics. Mass.
 - 3.1. Kinematics.
 - 3.2. Mass. Momentum. Kinetic energy
 - 4. The accretive and deformational force systems
 - 5. Power
 - 6. Energetics. Dissipation inequalities
 - 7. Constitutive equations
 - 8. Evolution equations in the absence of external forces
- B. Theory with interfacial structure
 - 9. Kinematics

10. Force systems

- 11. Power
- 12. Energetics. Dissipation inequalities
- 13. Constitutive equations
- 14. Evolution equations in the absence of external forces
- 15. Theory with bulk diffusion, but without inertia

Appendices

University Libraries Samegie Mellon University Pittsburgh, PA 15213-3890 A. Surfaces

A1. Surfaces

A2. Smoothly evolving surfaces

A3. Interface response functions

B. Localization and variation lemmas

References

1. INTRODUCTION.

This paper begins a two-part series on phase transitions in deformable solids,¹ with and without mass transport,² with the interface between phases sharp and capable of supporting energy and stress. The present study, Part 1, discusses coherent phase transitions;³ Part 2 will discuss incoherent transitions.

In a recent paper $[GS]^4$, Allan Struthers and I developed a continuum thermodynamics of coherent interfaces. Many of the results presented here were derived in [GS], but the development here is different and, I believe, simpler. In particular, I do not use the notions of "bulk interactions between phases" and "attachment forces" as described in Section 8 of [GS]; in fact, I now believe that section to be conceptually flawed.

The development precedes in four steps:

(1) Kinematics. A chief difficulty in the study of dynamical phase transitions is the presence of accretion, the motion of the phase interface relative to the underlying material. The interplay between accretion and deformation requires a kinematical development more complicated than that standard in continuum mechanics.

(2) Mechanics. The standard forces associated with continua arise as a response to the motion of material points. The mechanical description of accretion requires additional forces with their own balance. Following [GS], I refer to the former as *deformational forces*, to the latter as *accretive*

¹Other papers relevant to solid-solid phase transitions are: Brooks [1952], Robin [1974], Cahn [1980], Cahn & Larché [1978,1982,1985], Mullins [1981,1984], Alexander & Johnson [1985,1986], Parry [1987], Pitteri [1987], Fonseca [1989], and Leo & Sekerka [1989], all of whom derive equilibrium balance laws for the interface as Euler-Lagrange conditions for a global Gibbs function to be stationary; Abeyaratne & Knowles [1990,1991] and Truskinovsky [1991], who discuss kinetic relations for the interface neglecting interfacial structure; and Pfenning & Williams [1992], who use measure-theoretic arguments to derive interface conditions starting from general laws for force, energy, and entropy.

²Heat flow and interfacial mass are neglected; their inclusion adds no new difficulties. (Cf. Gurtin & Struthers [1990], who allow for bulk heat flow.)

³For which the reference lattices (homogeneous reference configurations) of the individual phases are coincident (modulo a homogeneous deformation) and the underlying deformations are continuous across the interface. ⁴I write [GS] for the reference "Gurtin & Struthers [1990]".

1

forces.⁵ That more than standard forces may be required is at least intimated by Gibbs,⁶ whose discussion is paraphrased by Cahn [1980] as follows: "solid surfaces can have their physical area changed in two ways, either by creating or destroying surface without changing surface structure and properties per unit area, or by an elastic strain along the surface keeping the number of surface lattice sites constant " Analogous ideas appear in the work of Eshelby,⁷ who introduced the notion of forces on lattice defects. A basic difference between the presentation here and the work of Gibbs, Cahn, and Eshelby is that for them such forces as well as their balances derive from variational principles,⁸ whereas for me "accretive forces" are primitive concepts entering the theory through their own force balance.

(3) Thermomechanics. For a mechanical theory of the type considered here the second law is the requirement that the energy of a body B increase at a rate not greater than the power expended on B plus the energy flow into $B.^9$ Basic to a precise statement of this law is a prescription of the manner in which interfacial forces expend power; I assume that such forces expend power over velocities associated with the motion of the interface through the lattice.¹⁰

(4) Constitutive theory. My development of a suitable constitutive theory is based on an extension of the Coleman-Noll procedure to multiphase continua.¹¹ Basic to this extension is the requirement that the second law be satisfied in any conceivable motion of the material points and phase interface, irrespective of the difficulties involved in producing such motions in the laboratory. The rational application of this procedure

⁵In place of the modifier "accretive", one might use lattice, configurational, structural, or reticular.

⁶[1878] (pp. 314-331).

⁷Cf., e.g., [1975].

⁸In such a derivation the standard force balance would be the Euler-Lagrange equation resulting from arbitrary variations of the deformation; but there is also a relation resulting from arbitrary variations of the interface; this corresponds to the accretive force balance.

⁹This version of the second law follows from appropriate versions of balance of energy and growth of entropy under the assumption of constant temperature (cf. Gurtin [1991]); in this instance what I term "energy" should more appropriately be termed "free energy".

¹⁰Gurtin [1988,1991], [GS].

¹¹Gurtin [1988].

requires the introduction of external fields that ensure balance of force and mass in all such motions. This may seem artificial, but it is no more artificial than a constitutive theory based on a principle of virtual work using arbitrary virtual displacements; in fact, both procedures are introduced with the same goal in mind: to ensure a properly invariant theory consistent with basic physical laws under the widest possible set of circumstances.

I begin with a development of equations appropriate to situations in which mass transport may be neglected. In this case the bulk relations are standard and consist of the momentum balance

$$Div S = \rho y^{**} \tag{1.1}$$

and the constitutive equations

$$\Psi = \hat{\Psi}_{i}(\mathbf{F}), \qquad \mathbf{S} = \partial_{\mathbf{F}} \hat{\Psi}_{i}(\mathbf{F})$$
(1.2)

in each phase i=1,2. Here $\mathbf{y}(\mathbf{X},t)$ describes the motion, $\mathbf{F}=\nabla \mathbf{y}$ is the deformation gradient, ρ is the mass density, Ψ is the bulk energy, and \mathbf{S} is the bulk stress. Here and in what follows:

bulk fields are measured per unit volume and area in the reference lattice,

so that, in particular, S is the Piola-Kirchhoff stress.

The interface — represented by a smoothly evolving surface S = S(t)in the reference lattice — is endowed with interfacial energy ψ , deformational stress **S**, and accretive stress **C**. Among the constitutive equations considered for the interface are relations allowing ψ , **S**, and the normal component **C** of **C** to depend on the normal **n** and the normal velocity V of S, and the interfacial limits F_1 and F_2 of F. A consequence of the second law is that ψ , **S**, and **C** are independent of V and depend on F_1 and F_2 through the tangential deformation gradient **F**. In fact, the energy $\psi = \tilde{\psi}(\mathbf{F}, \mathbf{n})$ determines **S** and **C** through the relations

$$\mathbf{S} = \partial_{\mathbf{F}} \widetilde{\psi}(\mathbf{F}, \mathbf{n}), \qquad \mathbf{C} = -D_{\mathbf{n}} \widetilde{\psi}(\mathbf{F}, \mathbf{n}), \qquad (1.3)$$

in which $\partial_{\mathbf{F}}$ is the partial derivative with respect to \mathbf{F} , while D_n is the derivative with respect to \mathbf{n} following the interface.

Fields that strongly influence the motion of the interface are the bulk and interfacial Eshelby $tensors^{12}$

$$\mathbf{P} = \Psi \mathbf{1} - \mathbf{F}^{\mathsf{T}} \mathbf{S}, \qquad \mathbf{P} = \psi \mathbf{1}_{n} - \mathbf{F}^{\mathsf{T}} \mathbf{S}, \qquad (1.4)$$

respectively, where 1 is the unit tensor, while 1_n is (essentially) the identity on the tangent space n^{\perp} . An important consequence of the thermodynamic development is a relation $\mathbf{P} = \mathbf{C}_{tan}$, identifying the tangential part of the accretive stress \mathbf{C} as the Eshelby tensor for the interface.

The final interface conditions¹³ consist of the compatibility conditions

$$[y^{*}] = -V[F]n,$$
 $[F](1 - n \otimes n) = 0,$ (1.5)

the deformational momentum balance

$$[\mathbf{S}]\mathbf{n} = -\rho[\mathbf{y}] \vee - \mathrm{Div}_{\mathbf{S}} \mathbf{S}, \qquad (1.6)$$

and the normal accretive balance

$$\mathbf{n} \cdot [\mathbf{P}]\mathbf{n} + \frac{1}{2}\rho[|\mathbf{F}\mathbf{n}|^2]\mathbf{V}^2 = -\mathbf{P} \cdot \mathbf{L} - \mathrm{Div}_{\mathbf{S}}\mathbf{C} + \beta \mathbf{V}.$$
(1.7)

Here $\beta = \tilde{\beta}(F_1, F_2, n, V) \ge 0$ is a kinetic modulus, $[\Phi]$ denotes the jump of a ¹²The insight afforded by the use of bulk and surface Eshelby tensors was pointed out to me by P. Podio-Guidugli (private communication).

¹³These interface conditions were derived in [GS], but the development here is different. For statical situations (1.7) was derived by Leo & Sekerka [1989] (cf. Alexander & Johnson [1985,1986]) as an Euler-Lagrange equation for stable equilibria, while (1.6) was derived by Gurtin & Murdoch [1974]. A counterpart of (1.7) for a rigid system was derived by Gurtin [1988]. For dynamical situations without surface energy or stress, (1.7) was proposed by Abeyaratne & Knowles [1990,1991] and Truskinovsky [1991]. bulk field Φ across the interface, \mathbf{L} is the curvature tensor of S, and Div_S is the surface divergence on S.

Next, using a study of Gurtin & Voorhees $[1993]^{14}$ as a guide, I modify the theory to include the bulk diffusion of \mathfrak{A} (unconstrained) species of mobile atoms, neglecting inertia. Each species $\mathfrak{a} = 1, 2, ..., \mathfrak{A}$ is described by a molar density $\rho^{\mathfrak{a}}$, a bulk molar flux $h^{\mathfrak{a}}$, and a chemical potential $\mu^{\mathfrak{a}}$, assumed continuous across the interface. Letting

$$\rho = (\rho^1, \dots, \rho^{\mathfrak{A}}), \quad \mu = (\mu^1, \dots, \mu^{\mathfrak{A}}), \quad H = (h^1, \dots, h^{\mathfrak{A}}), \quad (1.8)$$

I consider bulk constitutive equations

$$\Psi = \hat{\Psi}_{i}(F,\rho), \quad S = \partial_{F}\hat{\Psi}_{i}(F,\rho), \quad \mu = \partial_{\rho}\hat{\Psi}_{i}(F,\rho), \quad H = -D_{i}(F,\rho)\nabla\mu, \quad (1.9)$$

for each phase i, with diffusivity $D_i(\mathbf{F}, \boldsymbol{\rho})$ compatible with the inequality $\Sigma_{\alpha} \mathbf{h}^{\alpha} \cdot \nabla \mu^{\alpha} \leq 0$, where Σ_{α} designates the sum over α from 1 to \mathfrak{A} .

The resulting interface conditions consist of (1.5) and

$$[S]n = -Div_{S}S,$$

$$[\rho^{\alpha}]V = [h^{\alpha}] \cdot n,$$

$$n \cdot [P]n = -P \cdot L - Div_{S}C + \beta V,$$
(1.10)

with the bulk Eshelby tensor P now based on a Gibbs function ω ,

$$\mathbf{P} = \boldsymbol{\omega} \mathbf{1} - \mathbf{F}^{\mathsf{T}} \mathbf{S}, \qquad \boldsymbol{\omega} = \boldsymbol{\Psi} - \boldsymbol{\Sigma}_{\boldsymbol{\alpha}} \, \boldsymbol{\rho}^{\boldsymbol{\alpha}} \, \boldsymbol{\mu}^{\boldsymbol{\alpha}}, \qquad (1.11)$$

but with the interfacial Eshelby tensor \mathbb{P} unchanged (since interfacial mass is neglected). The corresponding bulk relations are (1.8), (1.9), and

$$\operatorname{Div} \mathbf{S} = \mathbf{0},$$
 $(\rho^{\alpha})^* = -\operatorname{Div} \mathbf{h}^{\alpha}.$ (1.12)

¹⁴Who assume linear elastic behavior in bulk and no interfacial elasticity.

2. GENERAL NOTATION.

The notation presented here is sufficiently general to be applicable also to incoherent phase transitions.

6

We will generally omit regularity assumptions.

T designates the time-interval in question. The term region is used to denote a region in \mathbb{R}^3 with sufficiently regular boundary. Let B be a closed region. A deformation φ of B is a smooth bijection of B onto a closed region, with det $\nabla \varphi > 0$.

By an evolving two-phase region $\{\Omega(t), \Omega_1(t), \Omega_2(t); t \in \mathcal{T}\}$ we mean a (possibly) time-dependent region $\Omega(t) \subset \mathbb{R}^3$, $t \in \mathcal{T}$, together with closed subregions $\Omega_1(t)$ and $\Omega_2(t)$ whose union is $\Omega(t)$ and whose intersection $\Gamma(t)$ is a smoothly evolving surface whose orienting unit normal $\mathbf{n}(\mathbf{x},t)$ is directed outward from $\partial\Omega_1(t)$; $\Gamma(t)$ will be referred to as the interface. We will often refer to $\Omega(t)$ or simply Ω as the evolving two-phase region, and we will usually omit the quantifier $t \in \mathcal{T}$.

Let φ be a mapping that associates with each $\mathbf{x} \in \Omega(t)$ and $t \in \mathcal{T}$ a scalar, vector, or tensor¹⁵ $\varphi(\mathbf{x},t)$. Then φ is a **bulk field** (for Ω) if φ is smooth away from the interface and up to the interface from either side. For such a field φ , we denote by $\varphi_i(\boldsymbol{\xi},t)$ the limit of φ at $\boldsymbol{\xi} \in \Gamma(t)$ from $\Omega_i(t)$, by $[\varphi]$ the jump in φ across the interface, and by $\langle \varphi \rangle$ the average value of φ at the interface:

$$\begin{split} \varphi_{i}(\boldsymbol{\xi},t) &= \lim \quad \varphi(\boldsymbol{x},t), \\ & \boldsymbol{x} \rightarrow \boldsymbol{\xi} \\ & \boldsymbol{x} \in \Omega_{i}(t) \end{split} \\ \begin{bmatrix} \varphi \end{bmatrix} &= \varphi_{2} - \varphi_{1}, \qquad \langle \varphi \rangle = (\varphi_{1} + \varphi_{2})/2; \end{split} \tag{2.1}$$

we then have the identities:

$$\begin{aligned} [\varphi \delta] &= [\varphi] \langle \delta \rangle + \langle \varphi \rangle [\delta], \\ \varphi_i &= \langle \varphi \rangle + \frac{1}{2} \delta_i [\varphi], \end{aligned}$$
 (2.2)

 $15_{\text{The term tensor}}$ (without the adjective superficial or the adjective interfacial) denotes a linear transformation of \mathbb{R}^3 into itself. 1 is the unit tensor; Lin⁺ is the set of all tensors F with det F > 0; and Unit is the set of all unit vectors. We use a dot to denote the inner product, \otimes to denote the tensor product, and the superscript T to denote the transpose, regardless of the space in question.

where here and in what follows

$$\delta_i = (-1)^i.$$
 (2.3)

We will also use the notation (2.1) for arbitrary fields $\varphi_1(\mathbf{x},t)$ and $\varphi_2(\mathbf{x},t)$ on the interface (the subscripts here denoting the phase to which the field is associated).

By a control volume (with respect to Ω) we mean a fixed region R with the property that, for some open time-interval $T \subset T$,

$R \subset \Omega(t)$

for all $t \in T$, and either $\Gamma(t) \cap R$ is empty for all $t \in T$ or $\Gamma(t) \cap R$ is a smoothly evolving surface for all $t \in T$; times t in the union of all such T are then *regular times* for R. When writing balance laws the quantifier "for all control volumes R" will mean "for all control volumes R and all regular times for R". When writing balance laws for a control volume R, we will always write

m for the outward unit normal to ∂R .

We label material points by their positions X in a fixed homogeneous reference configuration. A dot denotes the material time-derivative (with respect to time t holding X fixed); ∇ and Div are the material gradient and divergence (with respect to X).

7

A. SIMPLE THEORY WITHOUT INTERFACIAL STRUCTURE.

3. KINEMATICS. MASS.

3.1. KINEMATICS.

We consider a two-phase material with phases labelled i=1,2. We choose a fixed (uniform) **reference lattice** \mathcal{L} identified with \mathbb{R}^3 ; \mathcal{L} assumes the role played by the reference configuration in classical continuum mechanics and should be viewed as a macroscopic interpretation of a microscopic lattice, so that the points of \mathcal{L} fill \mathbb{R}^3 .

A two-phase body is a pair (B_1, B_2) of closed regions in \mathcal{L} whose intersection S is a smooth surface. We will refer to

$$B = B_1 \cup B_2$$

as the body, to points X of B as material points. The region B_i represents the portion of B composed of material of phase i, while S represents the interface between phases. B_i should be viewed as a collection of lattice points together with atoms¹⁶ structured in the manner peculiar to phase i.

Let B be a two-phase body, and let y be a mapping that associates with each material point X in B a point x=y(X) in \mathbb{R}^3 . Then y is a coherent two-phase deformation of B if:

(i) \mathbf{y} restricted to B_i is a deformation of B_i for each i;

(ii) **y** is continuous across the interface.

The set B=y(B) then represents the deformed body, &=y(S) the deformed interface, $B_i=y(B_i)$ the deformed phase i region.

At each time t, let y(t) be a coherent two-phase deformation of a two-phase body $(B_1(t), B_2(t))$, and write y for the mapping $(X,t) \mapsto y(X,t) = y(t)(X)$. Then y is a coherent two-phase motion of B if: (i) the body

 $B = B_1(t) \cup B_2(t)$

is independent of time, with $\{B, B_1(t), B_2(t)\}$ an evolving two-phase region;

16 Our theory is macroscopic; we use the term "atom" for descriptive purposes.

(ii) y is continuous;

(iii) **y** is smooth away from the *interface*

 $S(t) = B_1(t) \cap B_2(t)$ (3.1)

and up to the interface from each side.

Note that $B_1(t)$ and $B_2(t)$ depend on time at most through accretion; away from the *interface* $B_i(t)$ is *independent of time* in the sense that, given any time τ , each point **X** in $\partial B_i(\tau) - S(\tau)$ has a neighborhood N=N(X) such that, for some $\varepsilon > 0$, $N \cap \{\partial B_i(t) - S(t)\}$ is independent of t for all $t \in (\tau - \varepsilon, \tau + \varepsilon)$.

Let y be a coherent two-phase motion of B (Figure 3a).

We use the term *bulk field* to denote a bulk field with respect to $\{B, B_1(t), B_2(t)\}$, the term *interfacial field* to denote a superficial field (Appendix A) with respect to the interface S. Given a bulk field φ , the *limits* φ_i at the interface from phase i, and the *jump* $[\varphi]$ in φ across the interface are as defined in (2.1).

We will consistently write:

$$n(X,t)$$
 for the unit normal to the interface
S(t) directed outward from $\partial B_1(t)$ (3.2)

and V(X,t) for the normal velocity of S(t) in the direction n(X,t). Given a local parametrization X=r(u,t) for S(t), $v(X,t)=(\partial/\partial t)r(u,t)$ satisfies

 $V = \mathbf{v} \cdot \mathbf{n}; \tag{3.3}$

we will refer to interfacial fields \mathbf{v} consistent with (3.3) as admissible velocity fields for the interface.

We write

$$\mathbf{F}(\mathbf{X},t) = \nabla \mathbf{y}(\mathbf{X},t), \qquad \mathbf{y}^{*}(\mathbf{X},t) = (\partial/\partial t)\mathbf{y}(\mathbf{X},t)$$
(3.4)

for the deformation gradient and material velocity. Computing

9

 $(\partial/\partial t)\mathbf{y}(\mathbf{r}(\mathbf{u},t),t)$ — which represents a velocity field $\mathbf{\bar{v}}$ for &(t) — from either side of the interface yields the relations

$$\bar{\mathbf{v}} = (\mathbf{y}^*)_i + \mathbf{F}_i \mathbf{v} \tag{3.5}$$

and (hence) the compatibility conditions

 $[y^{*}] = -[F]v,$ $[F](1 - n \otimes n) = 0.$ (3.6)

The fields \mathbf{v} and $\mathbf{\bar{v}}$ have intrinsic forms

$$\mathbf{v} = \nabla \mathbf{n}, \quad \overline{\mathbf{v}} = \langle \mathbf{y}^* \rangle + \nabla \langle \mathbf{F} \rangle \mathbf{n}, \quad (3.7)$$

which allows us to rewrite $(3.6)_1$ as

$$[\mathbf{y}^*] = -\mathbf{V}[\mathbf{F}]\mathbf{n}. \tag{3.8}$$

By a **referential control volume** R we mean a control volume with respect to $\{B, B_1(t), B_2(t)\}$. Given a bulk field Φ , we write

 $\begin{cases} \int \Phi \, dv \end{cases}^*(t) = (d/dt) \{ \int \Phi(X,t) \, dv(X) \}. \\ R \qquad R \end{cases}$

3.2. MASS. MOMENTUM. KINETIC ENERGY.

We write ρ for the uniform 17 mass density in the reference lattice. Then balance of mass

$$\begin{cases} \int \rho \, dv \end{cases}^* = 0 \tag{3.9}$$

is trivially satisfied for each referential control volume R.

The integrals

$$\int \rho \mathbf{y}^* d\mathbf{v}, \qquad \int \frac{1}{2} \rho |\mathbf{y}^*|^2 d\mathbf{v} \qquad (3.10)$$

R R

¹⁷This assumption is consistent with coherency and a uniform reference lattice; we will be unable to make this assumption when we treat incoherent interfaces.

10

represent the momentum and kinetic energy. By Lemma B1 the time derivatives of these integrals when localized to the interface have densities

$$\mathbf{p} = -\rho[\mathbf{y}^*] \mathbf{V}, \qquad -\frac{1}{2} \rho[|\mathbf{y}^*|^2] \mathbf{V}, \qquad (3.11)$$

with **p** the momentum flow across the interface. By (3.5) and $(3.7)_1$,

$$[|\mathbf{y}^{*}|^{2}] = [|\mathbf{y}^{*} - \bar{\mathbf{v}}|^{2}] + 2[\mathbf{y}^{*}] \cdot \bar{\mathbf{v}} = [|\mathbf{Fn}|^{2}] \nabla^{2} + 2[\mathbf{y}^{*}] \cdot \bar{\mathbf{v}}, \qquad (3.12)$$

and therefore

$$-\frac{1}{2}\rho[|\mathbf{y}^{*}|^{2}]\mathbf{V} = -\mathbf{k}\mathbf{V} + \mathbf{p}\cdot\mathbf{\bar{v}}$$
(3.13)

with (cf. (3.8))

$$\mathbf{\&} = \frac{1}{2} \rho[|\mathbf{Fn}|^2] \mathbf{V}^2 = \frac{1}{2} \rho[|\mathbf{y} - \bar{\mathbf{v}}|^2] = \mathbf{p} \cdot \mathbf{V} \langle \mathbf{F} \rangle \mathbf{n}$$
(3.14)

the (jump in) relative kinetic energy.

4. THE ACCRETIVE AND DEFORMATIONAL FORCE SYSTEMS.

Here forces such as surface tension that act within the interface are neglected.

With each motion of the body we associate two force-systems: an *accretive system* consisting of forces that arise in response to the motion of the interface; a *deformational system* consisting of forces related to the gross deformation of the body. Central ingredients of the theory are balance laws for *each* of the two force systems.¹⁸

Let y be a coherent two-phase motion. Then the associated force systems are characterized by the fields:

accretive system

ſ

С	stress		
f	external	interfacial	force

deformational system

S	stress			
b	external	body	force	
g	external	inter	facial	force

C and S are bulk tensor fields, b is a bulk vector field, and f and g are interfacial vector fields. Fix the time, let da and dv represent an area element and a volume element in B away from the interface, and let m denote a unit normal to da. Then Cm da and Sm da represent accretive and deformational forces exerted across da, while b dv represents forces applied by the external world directly to dv. On the other hand, fda and gda represent accretive and deformational forces applied by the external world directly to area elements da on the interface. The external forces generally vanish in problems of interest, but are needed if we are to allow for arbitrary coherent two-phase motions of the body.

The accretive stress C acts in the lattice on the net atomic structure (lattice points plus atoms). This structure undergoes change only at the

¹⁸Cf. [GS], where these balance laws laws are derived as consequences of the invariance of the expended power (Section 5) under changes in observer. This invariance is nonstandard: in addition to the usual spatial observers, who measure the gross velocities of the continuum, [GS] allows for lattice observers, who study the crystal lattice and measure the velocity of the phase interface.

interface; consistent with a constraint of this type, we assume that C is *indeterminate* away from the interface; this indeterminacy obviates the need for an accretive body force (in bulk).

We postulate, for each referential control volume R: an accretive balance¹⁹

and deformational balances (balance of linear and angular momentum)

$$\int \mathbf{Sm} \, d\mathbf{a} + \int \mathbf{b} \, d\mathbf{v} + \int \mathbf{g} \, d\mathbf{a} = \{\int \rho \mathbf{y}^* \, d\mathbf{v}\}^*, \qquad (4.2)$$

$$\partial \mathbf{R} \qquad \mathbf{R} \qquad \mathbf{S} \cap \mathbf{R} \qquad \mathbf{R}$$

$$\int \mathbf{y} \times \mathbf{Sm} \, d\mathbf{a} + \int \mathbf{y} \times \mathbf{b} \, d\mathbf{v} + \int \mathbf{y} \times \mathbf{g} \, d\mathbf{a} = \{\int \mathbf{y} \times \rho \mathbf{y}^* \, d\mathbf{v}\}^*, \qquad (4.3)$$

$$\partial \mathbf{R} \qquad \mathbf{R} \qquad S \cap \mathbf{R} \qquad \mathbf{R}$$

with \mathbf{m} is the outward unit normal to $\partial \mathbf{R}$ (Figure 4a).

Lemma B1 allows us to localize these balance laws to regular interfacial sets, and this in turn leads to the **interfacial force balances**

$$[C]n + f = 0,$$
 $[S]n + g = p$ (4.4)

with \mathbf{p} given by (3.11).

On the other hand, applying (4.1)-(4.3) to referential control volumes R that do not intersect the interface yields the relations

$$Div S + b = \rho y^{\prime \prime}, \qquad Div C = 0$$
(4.5)

in bulk (in B away from the interface) as well as the standard restriction

$$SF^{\mathsf{T}} = F^{\mathsf{T}}S, \tag{4.6}$$

implying the symmetry of the Cauchy stress²⁰ $T = (detF)^{-1}SF^{T}$.

 19 Balance of moments for the accretive system has no relevant consequences within this theory (cf. [GS], eq. $(7.10)_2$). 20 Cf., e.g., Gurtin [1981].



ź

Figure 4a. The accretive and deformational forces on a control volume R. The surface stresses **C** and **S**, neglected here, are considered in Section 10. 5. POWER.

Let \mathbf{y} be a coherent two-phase motion. To write the second law we need a representation for the power expended on an arbitrary referential control volume R.

Deformational forces act in the deformed body as a response to deformation. The stress **S** and the body force **b** act in the bulk material away from the interface and, as is standard, are *conjugate to* (i.e., expend power over) the material velocity \mathbf{y}^* . The external force \mathbf{g} acts at the interface, and we assume that \mathbf{g} is conjugate to the velocity $\overline{\mathbf{v}}$ of the deformed interface.

Accretive forces are associated with the nondeformational kinetics of material points in B, and expend power only at the interface, where the phase i regions $B_i(t)$ undergo change. Thus bulk accretive forces do not expend power, but the external force f, which acts at the interface, does. We assume that f is conjugate to the velocity v at which the interface moves through B.

We therefore write the **power expended** on R in the form

$$\mathcal{P}(\mathbf{R}) = \int \mathbf{Sm} \cdot \mathbf{y}^* d\mathbf{a} + \int \mathbf{b} \cdot \mathbf{y}^* d\mathbf{v} + \int (\mathbf{f} \cdot \mathbf{v} + \mathbf{g} \cdot \overline{\mathbf{v}}) d\mathbf{a}, \qquad (5.1)$$

$$\partial \mathbf{R} \qquad \mathbf{R} \qquad \mathbf{S} \cap \mathbf{R}$$

with **m** the outward unit normal to ∂R . We require that this expression be independent of how we parametrize the interface, and hence independent of the admissible velocity field **v** used to describe its motion. By (3.5), the dependence of (5.1) on **v** is through the term $(\mathbf{f} + \langle \mathbf{F} \rangle^{\mathsf{T}} \mathbf{g}) \cdot \mathbf{v}$ in the last integral. Thus we require that

 $\mathbf{f} + \langle \mathbf{F} \rangle^{\mathsf{T}} \mathbf{g}$ is parallel to \mathbf{n} (5.2)

and, granted this, we may restrict attention to \mathbf{v} and $\mathbf{\bar{v}}$ in the intrinsic forms (3.7).

By Lemma B1, for R_{ϵ} a family of referential control volumes that shrinks to a regular interfacial set. A at time τ ,

$$\mathcal{P}(\mathbf{R}_{\varepsilon}) \rightarrow \int ([\mathbf{Sn} \cdot \mathbf{y}^*] + \mathbf{g} \cdot \bar{\mathbf{v}} + \mathbf{f} \cdot \mathbf{v}) d\mathbf{a}$$
(5.3)
A

at τ , and, by (3.5), (3.7), and (4.4), we can write this integrand in the form

$$-([\mathbf{n}\cdot\mathbf{F}^{\mathsf{T}}\mathbf{S}\mathbf{n}] + [\mathbf{n}\cdot\mathbf{C}\mathbf{n}])\mathbf{\nabla} + \mathbf{p}\cdot\mathbf{\bar{v}}.$$
(5.4)

6. ENERGETICS. DISSIPATION INEQUALITIES.

In this purely mechanical theory the second law is the requirement that the energy increase at a rate not greater than the expended power. Here interfacial energy is neglected; the energy of the system is therefore represented by the **bulk energy** Ψ per unit volume, and the second law takes the form of a global dissipation inequality

$$\left\{ \int (\Psi + \frac{1}{2}\rho |\mathbf{y}^{*}|^{2}) d\mathbf{v} \right\}^{*} \leq \mathcal{P}(\mathbf{R})$$
(6.1)
R

for each referential control volume R, with $\mathcal{P}(R)$ the expended power (5.1).

Using Lemma B1, (3.13), and (5.4), we may localize (6.1) to the interface; the result is

$$(-[\Psi] + [\mathbf{n} \cdot \mathbf{F}^{\mathsf{T}} \mathbf{S} \mathbf{n}] - \mathbf{k} + [\mathbf{n} \cdot \mathbf{C} \mathbf{n}]) \vee \leq 0.$$

Thus, introducing the Eshelby tensor

$$\mathbf{P} = \Psi \mathbf{1} - \mathbf{F}^{\mathsf{T}} \mathbf{S} \tag{6.2}$$

and the accretive tension

$$\Pi = \mathbf{n} \cdot [\mathbf{C}]\mathbf{n}, \tag{6.3}$$

we are led to the interfacial dissipation inequality

$$(\Pi - \mathbf{n} \cdot [\mathbf{P}]\mathbf{n} - \mathbf{k}) \mathbf{V} \leq \mathbf{0}. \tag{6.4}$$

If we consider (6.1) restricted to referential control volumes that do not intersect the interface, we are led, by virtue of $(4.5)_1$, to the requirement that

 $\Psi' \leq \mathbf{S} \cdot \mathbf{F}' \tag{6.5}$

in bulk.

Granted the balance laws for force, the inequalities (6.4) and (6.5) are equivalent to the global dissipation inequality (6.1).

The presence of $\mathbf{n} \cdot [\mathbf{P}]\mathbf{n}$ in the interfacial dissipation inequality will involve this component of $[\mathbf{P}]\mathbf{n}$ in the constitutive theory. On the other hand, for $\mathbf{g}=\mathbf{0}$, the tangential component of $[\mathbf{P}]\mathbf{n}$ is determined by the momentum flow \mathbf{p} : in view of $(3.6)_2$, $(4.4)_2$, and (6.2),

$$(1 - n \otimes n)[P]n = -(1 - n \otimes n)\langle F \rangle^{\mathsf{T}}[Sn] = -(1 - n \otimes n)\langle F \rangle^{\mathsf{T}}p.$$
(6.6)

7. CONSTITUTIVE EQUATIONS.

We assume that the individual phases are homogeneous and elastic, governed by standard constitutive equations

$$\mathbf{S} = \mathbf{\hat{S}}_{i}(\mathbf{F}), \qquad \Psi = \mathbf{\hat{\Psi}}_{i}(\mathbf{F}) \tag{7.1}$$

with²¹

ž

$$\hat{\mathbf{S}}_{i}(\mathbf{F}) = \partial_{\mathbf{F}} \hat{\Psi}_{i}(\mathbf{F}). \tag{7.2}$$

We take Lin⁺ as the domain of the response functions $\hat{\mathbf{S}}_i$ and $\hat{\Psi}_i$, and assume that $\hat{\mathbf{S}}_i$ is consistent with (4.6).

To these equations we adjoin a constitutive equation for the interface giving the accretive tension Π as a function of the normal n, the normal velocity V, and the limiting values F_1 and F_2 of the deformation gradient at the interface:²²

 $\Pi = \hat{\Pi}(\mathbf{z}), \qquad \mathbf{z} = (\mathbf{F}_{1}, \mathbf{F}_{2}, \mathbf{n}, \mathbf{V}).$ (7.3)

The domain of Π is the set Z of all z with $n \in Unit$, $V \in \mathbb{R}$, and $F_1, F_2 \in Lin^+$ with $F_1(1 - n \otimes n) = F_2(1 - n \otimes n)$ (cf. (3.6)₂).

Remark 7.1 (Constitutive Processes). Suppose we are given an arbitrary coherent two-phase motion. Then the constitutive equations may be used to compute a *constitutive process* consisting of z as a *field*, the bulk fields S and Ψ , and the interfacial field Π . The balance laws for force may then be used to compute the accretive stress C and the external forces **b**, **f**, and **g** needed to support the process: (4.4)₂ gives **g**; (4.4)₁,

²¹This restriction is a consequence of the bulk dissipation inequality (6.5). We will postulate rather than prove bulk constitutive restrictions; since they are well known and their proof simple.

 22 Here we use the second law — in the form (6.4) — to suggest which fields should be described by constitutive equations; this is in contrast to the standard procedure of studying balance laws to see where the formal lack of sufficient equations may be compensated for by the introduction of additional constitutive relations. This use of the second law seems to lead — in all classical continuum theories — to the "correct" set of constitutive variables.

(5.2), and (6.3) give f; $(4.5)_1$ gives b; $(4.5)_2$ and (6.3) may be solved (generally not uniquely) for C. The availability of external fields therefore allows us to consider *arbitrary* constitutive processes with the assurance that the balance laws for force are satisfied.

The second law — in the form of the dissipation inequalities (6.4) and (6.5) — remains to be satisfied in all constitutive processes. In view of (7.2), the inequality (6.5) is automatically satisfied; we therefore have only to satisfy the interfacial dissipation inequality (6.4). Let

$$\Phi(\mathbf{z}) = \Pi(\mathbf{z}) - \mathbf{n} \cdot [\mathbf{P}]\mathbf{n} - \mathbf{k}$$
(7.4)

with $\mathbf{n} \cdot [\mathbf{P}]\mathbf{n} + \mathbf{k}$ considered a function of \mathbf{z} by virtue of (3.14) and (6.2); then satisfying (6.4) in all processes is equivalent to satisfying

$$\Phi(\mathbf{z}(\mathbf{X},t)) \vee (\mathbf{X},t) \leq 0$$

in all coherent two-phase motions. By Lemma B2, given an arbitrary value $\mathbf{z}_0 \in \mathbb{Z}$, we can always find a coherent two-phase motion for which $\mathbf{z}(\mathbf{X},t)$ has the value \mathbf{z}_0 at (0,0). We are therefore led to the requirement that $\Phi(\mathbf{z}) \vee \mathbf{v} \leq 0$ for all $\mathbf{z} \in \mathbb{Z}$; hence Φ must have the form

$$\Phi(z) = -\beta V$$

with coefficient β given by a constitutive equation

$$\beta = \hat{\beta}(z) \ge 0. \tag{7.5}$$

Thus

$$\widehat{\Pi}(\mathbf{z}) = \mathbf{n} \cdot [\mathbf{P}] \mathbf{n} + \mathbf{k} - \beta \mathbf{V}, \qquad (7.6)$$

so that the accretive tension is the sum of the normal imbalance in the Eshelby tensor, the relative kinetic energy, and a drag force $-\beta V$, which represents dissipation in the exchange of material between phases. This drag force is the sole source of dissipation in the theory.

The relations $(4.4)_1$, (6.3), and (7.6) yield the **normal accretive** balance

$$\mathbf{n} \cdot [\mathbf{P}]\mathbf{n} + \mathbf{k} = \beta \nabla - \mathbf{f} \cdot \mathbf{n}. \tag{7.7}$$

Note that $\Pi = 0$ when the external forces vanish, a result generally not true when surface stress is included in the theory (cf. (11.10)).

8. EVOLUTION EQUATIONS IN THE ABSENCE OF EXTERNAL FORCES.

Assume now that the external forces vanish. The complete set of interface conditions then consists of the *compatibility conditions*

$$[y^*] = -V[F]n,$$
 $[F](1 - n \otimes n) = 0,$ (8.1)

the deformational force balance

$$[S]n = p, \tag{8.2}$$

and the normal accretive balance²³

$$\mathbf{n} \cdot [\mathbf{P}]\mathbf{n} + \mathbf{k} = \beta \mathbf{V}, \tag{8.3}$$

with

ŧ

$$P = \Psi 1 - F^{T}S, \quad p = -\rho[y^{*}]V, \quad k = \frac{1}{2}\rho[|Fn|^{2}]V^{2}, \quad (8.4)$$

and these with the bulk equations

$$\Psi = \hat{\Psi}_{i}(\mathbf{F}), \qquad \mathbf{S} = \partial_{\mathbf{F}} \hat{\Psi}_{i}(\mathbf{F}), \qquad \operatorname{Div} \mathbf{S} = \rho \mathbf{y}^{**}$$
(8.5)

and appropriate boundary and initial conditions form the free-boundary problem for the mechanical theory.

By (2.2), (3.6)₂, (3.14), and (4.4),

$$\mathbf{n} \cdot [\mathbf{F}^{\mathsf{T}} \mathbf{S}] \mathbf{n} = \langle \mathbf{S} \mathbf{n} \rangle \cdot [\mathbf{F} \mathbf{n}] + \mathbf{p} \cdot \langle \mathbf{F} \mathbf{n} \rangle = \langle \mathbf{S} \rangle \cdot [\mathbf{F}] + \mathbf{k}; \qquad (8.6)$$

thus

$$\mathbf{n} \cdot [\mathbf{P}]\mathbf{n} + \mathbf{k} = [\Psi] - \langle \mathbf{S} \rangle \cdot [\mathbf{F}], \tag{8.7}$$

and we can write the normal accretive balance in the form

²³Proposed by Abeyaratne & Knowles [1990,1991], Truskinovsky [1991].

$$[\Psi] - \langle \mathbf{S} \rangle \cdot [\mathbf{F}] = \beta \mathbf{V}. \tag{8.8}$$

Next, (3.14), (6.6), and (8.3) imply that

ŧ

$$[\mathbf{P}]\mathbf{n} + \langle \mathbf{F} \rangle^{\mathsf{T}} \mathbf{p} = \beta \nabla \mathbf{n}, \tag{8.9}$$

showing that the imbalance in the Eshelby tensor is due entirely to interfacial dissipation and inertia. At equilibrium (8.8) and (8.9) reduce to the standard results

 $[\Psi] - \langle S \rangle \cdot [F] = 0,$ [P]n = 0. (8.10)

B. THEORY WITH INTERFACIAL STRUCTURE.

9. KINEMATICS.

We now augment the notation of Section 3 to include concepts relevant to a discussion of interfacial strain.

Let \mathbf{y} be a coherent two-phase motion. We continue to use the notation of Section 3 for fields such as the deformation gradient \mathbf{F} associated with \mathbf{y} , and we let \mathbf{L} and \mathbf{K} denote the curvature tensor and total curvature for the undeformed interface S(t). (Because of (A5), (A6), and our agreement (3.2), $\mathbf{K} < 0$ for \mathbf{B}_1 a ball.)

The tangential deformation gradient²⁴ $\mathbb{F}(X,t)$, defined at each $X \in S(t)$ by

$$\mathbf{F}(\mathbf{X},t) = \nabla_{\mathbf{S}} \mathbf{y}(\mathbf{X},t), \tag{9.1}$$

is a linear transformation from the tangent plane at $X \in S(t)$ into \mathbb{R}^3 , although $\mathbb{F}(X,t)$ actually maps tangent vectors at $X \in S(t)$ to tangent vectors at $x \in \mathcal{S}(t)$. \mathbb{F} is related to the deformation gradient \mathbb{F} through

$$\mathbf{F} = \mathbf{F}_{\mathbf{i}} \mathbf{1}_{\mathbf{n}} = \langle \mathbf{F} \rangle \mathbf{1}_{\mathbf{n}} \tag{9.2}$$

with $\mathbb{1}_{n}(X,t)$ the inclusion of the tangent plane $n^{\perp}(X,t)$ into \mathbb{R}^{3} (cf. (A1)). Because of the compatibility relation (3.6)₂,

$$[\mathbf{F}] = [\mathbf{F}]\mathbf{n} \otimes \mathbf{n}, \tag{9.3}$$

and, by $(2.2)_2$, the interfacial limits F_i are completely determined by $\langle F \rangle$ and [F]n:

$$\mathbf{F}_{i} = \langle \mathbf{F} \rangle + \frac{1}{2} \delta_{i} ([\mathbf{F}]\mathbf{n}) \otimes \mathbf{n}.$$
(9.4)

Two important identities — valid for \mathbf{v} and $\mathbf{\bar{v}}$ the intrinsic velocity fields (3.7) for S(t) and &(t) — are²⁵

 24 Cf. Gurtin & Murdoch [1974]. Many of the definitions and results that we use can be found there and in Sects. 2.1 and 3.2 of [GS]. 25 Cf. [GS], eq. (3.29).

$$\nabla_{\mathbf{S}} \mathbf{v} = -(\mathbf{n} \otimes \mathbf{n}^{\circ}) \mathbf{1}_{\mathbf{n}} - \nabla \mathbf{L}, \qquad (9.5)$$
$$\nabla_{\mathbf{S}} \mathbf{\bar{v}} = \{ \mathbf{F}_{i}^{\circ} - \mathbf{F}_{i}(\mathbf{n} \otimes \mathbf{n}^{\circ}) \} \mathbf{1}_{\mathbf{n}} - \nabla \mathbf{F}_{i} \mathbf{L},$$

where the superscript "°" represents the normal time derivative (for S) discussed in Appendix A2. The relation $(9.5)_2$ is independent of the phase i, and is therefore valid with \mathbf{F}_i replaced by $\langle \mathbf{F} \rangle$.

Let A(t) be a smoothly evolving subsurface of S(t), with $\Psi(\mathbf{X},t)$ the outward unit normal to the boundary curve $\partial A(t)$. Given any local parametrization $\mathbf{X} = \mathbf{r}(u,t)$ for $\partial A(t)$, $\mathbf{w}(\mathbf{X},t) = (\partial/\partial t)\mathbf{r}(u,t)$ satisfies

$$\mathbf{w} \cdot \mathbf{n} = \mathbf{V}, \qquad \mathbf{w} \cdot \mathbf{V} = \mathbf{V}_{(\partial A) \tan}$$
(9.6)

(cf. (A13)); we will refer to interfacial fields w consistent with (9.6) as admissible velocity fields for ∂A . The interfacial field

$$\overline{\mathbf{w}} = (\mathbf{y}^*)_i + \mathbf{F}_i \mathbf{w} \tag{9.7}$$

then represents a velocity field for the boundary of the deformed surface y(A(t),t). The expression (9.7) is independent of the phase i and hence, by (2.1)₂, may be written in the form:

$$\bar{\mathbf{w}} = \langle \mathbf{y}^* \rangle + \langle \mathbf{F} \rangle \mathbf{w}. \tag{9.8}$$

If we choose $\,{\bf w}\,$ to be the intrinsic velocity $\,{\bf v}_{\partial A}\,$ of $\,\partial A\,$ as defined in (A13), then

$$\mathbf{w} = \mathbf{v} + V_{(\partial A)\tan} \boldsymbol{\mathcal{V}}, \quad \mathbf{\bar{w}} = \mathbf{\bar{v}} + V_{(\partial A)\tan} \langle \mathbf{F} \rangle \boldsymbol{\mathcal{V}}, \quad (9.9)$$

with \mathbf{v} and $\mathbf{\bar{v}}$ the intrinsic velocity fields (3.7).

10. FORCE SYSTEMS.

Ę

Let y be a coherent two-phase motion. Then the associated force systems are characterized by the list of fields described in Section 3 augmented by two interfacial tensor fields:

Caccretive surface stressSdeformational surface stress

Let R be a referential control volume, let

$$A(t) = S(t) \cap R \tag{10.1}$$

denote the portion of the interface in R, and let $\Psi(\mathbf{X},t)$ denote the outward unit normal to the boundary curve $\partial A(t)$. Then $\mathbf{C}\Psi$ and $\mathbf{S}\Psi$ represent accretional and deformational forces, per unit length, applied to R across ∂A .

We postulate, for each referential control volume R: an **accretive balance**

> $\int \mathbf{Cm} d\mathbf{a} + \int \mathbf{f} d\mathbf{a} + \int \mathbf{E} \mathbf{\mathcal{V}} d\mathbf{s} = \mathbf{0}$ (10.2) $\partial \mathbf{R} \qquad \mathbf{A} \qquad \partial \mathbf{A}$

and deformational balances (balance of linear and angular momentum)

 $\int \mathbf{Sm} d\mathbf{a} + \int \mathbf{b} d\mathbf{v} + \int \mathbf{g} d\mathbf{a} + \int \mathbf{S} \mathbf{V} d\mathbf{s} = \{\int \rho \mathbf{y}^* d\mathbf{v}\}^*, \quad (10.3)$ $\partial \mathbf{R} \qquad \mathbf{R} \qquad \mathbf{A} \qquad \partial \mathbf{A} \qquad \mathbf{R}$

 $\int \mathbf{y} \times \mathbf{Sm} \, d\mathbf{a} + \int \mathbf{y} \times \mathbf{b} \, d\mathbf{v} + \int \mathbf{y} \times \mathbf{g} \, d\mathbf{a} + \int \mathbf{y} \times \mathbf{S} \mathbf{V} \, d\mathbf{s} = \{\int \mathbf{y} \times \rho \mathbf{y}^* \, d\mathbf{v}\}^*, \quad (10.4)$ $\partial \mathbf{R} \qquad \mathbf{R} \qquad \mathbf{A} \qquad \partial \mathbf{A} \qquad \mathbf{R}$

with \mathbf{m} the outward unit normal to $\partial \mathbf{R}$ (Figure 4a).

Using the surface divergence theorem (A10) and the argument given in Section 4, we are led to the interfacial force balances (cf. $(3.11)_1$)

$$[C]n + f + Div_{S}C = 0, \quad [S]n + g + Div_{S}S = p, \quad (10.5)$$

and the moment balances²⁶

$$\mathbf{S}^{\mathsf{T}}\mathbf{F}^{\mathsf{T}}\mathbf{n} = \mathbf{0}, \qquad \mathbf{S}\mathbf{F}^{\mathsf{T}} = \mathbf{F}\mathbf{S}^{\mathsf{T}}, \qquad (10.6)$$

asserting that the Cauchy surface stress $T = (\det F)^{-1} SF^T$ is symmetric and tangential.

²⁶Cf. Gurtin & Murdoch [1974], p. 307; [GS], eq. (7.13).

11. POWER.

1

Let R be a referential control volume, with **m** the outward unit normal to ∂R and **V** the outward unit normal to the boundary curve ∂A , $A=S\cap R$. Guided by the discussion preceding (5.1), we assume that the force **CV** is conjugate to (any choice of) admissible velocity **w** for the boundary curve ∂A , while **SV** is conjugate to the corresponding velocity $\overline{\mathbf{w}}$ for the image of ∂A under the motion. Thus, in view of (5.1), we write the **power expended** on R in the form

$$\mathcal{P}(\mathbf{R}) = \int \mathbf{Sm} \cdot \mathbf{y}^* d\mathbf{a} + \int \mathbf{b} \cdot \mathbf{y}^* d\mathbf{v} + \int (\mathbf{f} \cdot \mathbf{v} + \mathbf{g} \cdot \overline{\mathbf{v}}) d\mathbf{a} + \partial \mathbf{R} \qquad \mathbf{R} \qquad \mathbf{A}$$
$$\int (\mathbf{C} \mathbf{V} \cdot \mathbf{w} + \mathbf{S} \mathbf{V} \cdot \overline{\mathbf{w}}) d\mathbf{s}, \qquad (11.1)$$

and require that this expression be independent of both the admissible velocity \mathbf{v} used to describe the motion of the interface and the admissible velocity \mathbf{w} used to describe the motion of the boundary curve ∂A . This requirement leads to (5.2) and to an additional restriction, which we now derive.

The last integral in (11.1) represents the power expended by interfacial stresses; by (9.8) this integral can be written as an accretive part

$$\int (\mathbf{\Box} \boldsymbol{\nu} + \langle \mathbf{F} \rangle^{\mathsf{T}} \mathbf{S} \boldsymbol{\nu}) \cdot \mathbf{w} \, \mathrm{ds}$$
(11.2)
 $\partial \mathbf{A}$

plus a purely deformational part

The stress

$$\mathbf{A} = \mathbf{C} + \langle \mathbf{F} \rangle^{\mathsf{T}} \mathbf{S} \tag{11.3}$$

represents the stress \square due to accretion alone plus the accretive

contribution $\langle F \rangle^T S$ of the deformational stress S. Let \mathbb{A}_{tan} and \mathbb{B} denote the tangential and normal components of \mathbb{A} with respect to the undeformed surface S(t) (cf. (A3)). Since (11.2) is, by hypothesis, independent of the choice of admissible velocity field \mathbf{w} , we may use an argument of [GS]²⁷ to conclude that \mathbb{A}_{tan} is a surface tension σ :

$$\mathbf{A}_{tan} = \sigma \mathbf{1}_{n}. \tag{11.4}$$

Note that, by (A3), (11.3), and (11.4), the tangential and normal components \mathbf{C}_{tan} and \mathbf{C} of the accretive stress are given by

$$\mathbf{C}_{tan} = \sigma \mathbf{1}_{n} - (\mathbf{1} - \mathbf{n} \otimes \mathbf{n}) \langle \mathbf{F} \rangle^{\mathsf{T}} \mathbf{S}, \qquad \mathbf{C} = \mathbf{a} - \mathbf{S}^{\mathsf{T}} \langle \mathbf{F} \rangle \mathbf{n}. \qquad (11.5)$$

We now restrict attention in (11.1) to the intrinsic velocity fields (3.7) and (9.9), so that

$$\mathcal{P}(\mathbf{R}) = \int \mathbf{Sm} \cdot \mathbf{y} \cdot d\mathbf{a} + \int \mathbf{b} \cdot \mathbf{y} \cdot d\mathbf{v} + \int (\mathbf{f} \cdot \mathbf{v} + \mathbf{g} \cdot \overline{\mathbf{v}}) d\mathbf{a} + \partial \mathbf{R} \qquad \mathbf{R} \qquad \mathbf{A}$$
$$\int (\mathbf{C} \mathbf{V} \cdot \mathbf{v} + \mathbf{S} \mathbf{V} \cdot \overline{\mathbf{v}} + \sigma V_{(\partial A) tan}) ds.$$
$$\partial \mathbf{A}$$

The balance laws (10.5) and the identity (A11) yield

$$\int \mathbf{\tilde{L}} \mathbf{\tilde{V}} \cdot \mathbf{v} \, ds = \int \{ \mathbf{\tilde{L}} \cdot \nabla_{S} \mathbf{v} - ([\mathbf{C}]\mathbf{n} + \mathbf{f}) \cdot \mathbf{v} \} \, da,$$

$$\partial A \qquad A$$

$$\int \mathbf{\tilde{S}} \mathbf{\tilde{V}} \cdot \mathbf{v} \, ds = \int \{ \mathbf{\tilde{S}} \cdot \nabla_{S} \mathbf{\tilde{v}} - ([\mathbf{S}]\mathbf{n} + \mathbf{g} - \mathbf{p}) \cdot \mathbf{\tilde{v}} \} \, da$$

$$\partial A \qquad A$$

Thus, by Lemma B1, for R_{ϵ} a family of referential control volumes that shrinks to a regular interfacial set $A_0 = A(\tau)$ at time τ ,

$$\mathcal{P}(\mathbf{R}_{\varepsilon}) \rightarrow \int \mathbf{p} \, \mathrm{da} + \int \sigma V_{(\partial A) \tan} \, \mathrm{ds}$$

$$A_0 \qquad \partial A_0 \qquad (11.6)$$

at τ , where

²⁷Cf. (iii) of the Invariance Lemma given in Appendix C of [GS].

$$\mathbf{p} = [\mathbf{Sn} \cdot \mathbf{y}^*] - [\mathbf{C}]\mathbf{n} \cdot \mathbf{v} - [\mathbf{S}]\mathbf{n} \cdot \bar{\mathbf{v}} + \mathbf{C} \cdot \nabla_{\mathbf{S}} \mathbf{v} + \mathbf{S} \cdot \nabla_{\mathbf{S}} \bar{\mathbf{v}} + \mathbf{p} \cdot \bar{\mathbf{v}}. \quad (11.7)$$

Further, by (A3), (A4), (A6), the fact that L is tangential, the sentence following (9.5), (11.3), (11.4), and (11.5)₂,

$$\begin{split} \mathbf{C} \cdot \nabla_{\mathbf{S}} \mathbf{v} &= -\mathbf{n} \cdot \mathbf{C}_{ext} \mathbf{n}^{\circ} - \nabla \{ \mathbf{K} \sigma - (\langle \mathbf{F} \rangle^{\mathsf{T}} \mathbf{S}) \cdot \mathbf{L} \}, \\ \mathbf{S} \cdot \nabla_{\mathbf{S}} \overline{\mathbf{v}} &= \mathbf{S}_{ext} \cdot \{ \langle \mathbf{F} \rangle^{\circ} - \langle \mathbf{F} \rangle (\mathbf{n} \otimes \mathbf{n}^{\circ}) \} - \nabla (\langle \mathbf{F} \rangle^{\mathsf{T}} \mathbf{S}) \cdot \mathbf{L}, \\ \mathbf{n} \cdot \mathbf{C}_{ext} \mathbf{n}^{\circ} + \mathbf{S}_{ext} \cdot (\langle \mathbf{F} \rangle (\mathbf{n} \otimes \mathbf{n}^{\circ})) = \mathbf{a} \cdot \mathbf{n}^{\circ}, \end{split}$$

and therefore

$$\mathbf{C} \cdot \nabla_{\mathbf{S}} \mathbf{v} + \mathbf{S} \cdot \nabla_{\mathbf{S}} \mathbf{\bar{v}} = -\sigma \mathbf{K} \nabla - \mathbf{B} \cdot \mathbf{n}^{\circ} + \mathbf{S}_{ext} \cdot \langle \mathbf{F} \rangle^{\circ}; \qquad (11.8)$$

thus, using (3.5) and (3.7),²⁸

$$\mathbf{p} = -\sigma \mathbf{K} \nabla - \mathbf{B} \cdot \mathbf{n}^\circ + \mathbf{S}_{ext} \cdot \langle \mathbf{F} \rangle^\circ - ([\mathbf{n} \cdot \mathbf{F}^\mathsf{T} \mathbf{S} \mathbf{n}] + [\mathbf{n} \cdot \mathbf{C} \mathbf{n}]) \nabla + \mathbf{p} \cdot \bar{\mathbf{v}} \qquad (11.9)$$

at τ .

The right side of (11.9) catalogs the manner in which power is expended on the interface: $-\sigma KV$ represents power expended in the creation of new surface, $-\mathbf{E}\cdot\mathbf{n}^\circ$ power expended in changing the orientation of the interface, $\mathbf{E}_{ext}\cdot\langle \mathbf{F}\rangle^\circ$ power expended in stretching the interface, $-([\mathbf{n}\cdot\mathbf{F}^\mathsf{T}\mathbf{Sn}]+[\mathbf{n}\cdot\mathbf{Cn}])V$ power expended in the exchange of material between phases, $\mathbf{p}\cdot\mathbf{\bar{v}}$ power expended by inertial forces.

Note that, since $(1 - n \otimes n) L = L$, we may use (A6), (A9), and $(11.5)_1$ to write the normal component of the accretive force balance $(10.5)_1$ in the form

$$\sigma K + Div_{s} \mathbf{C} - \langle \mathbf{F} \rangle^{\mathsf{T}} \mathbf{S} \cdot \mathbf{L} + \Pi = -\mathbf{f} \cdot \mathbf{n}$$
(11.10)

with $\Pi = \mathbf{n} \cdot [\mathbf{C}]\mathbf{n}$ the accretive tension.

²⁸Cf. (9A) of [GS].

12. ENERGETICS. DISSIPATION INEQUALITIES.

To discuss the energetics of the interface we introduce the interfacial energy ψ , per unit area, which augments the bulk energy Ψ introduced in Section 6. The second law then takes the form of a global dissipation inequality

$$\{ \int (\Psi + \frac{1}{2}\rho|\mathbf{y}^{*}|^{2}) d\mathbf{v} + \int \psi d\mathbf{a} \}^{*} \leq \mathcal{P}(\mathbf{R})$$

$$\mathbf{R} \qquad \mathbf{A}$$

$$(12.1)$$

for each referential control volume R, where $A(t)=S(t)\cap R$, while $\mathcal{P}(R)$ is the power expended (11.1).

If we apply (12.1) to a family of referential control volumes that shrinks to a regular interfacial set $A_0=A(\tau)$ at time τ , and use (A15) and Lemma B1 in conjunction with (3.13), (11.6), and (11.9), we arrive at the inequality

$$\int \{\psi^{\circ} + (\sigma - \psi) K \nabla + \mathbf{b} \cdot \mathbf{n}^{\circ} - \mathbf{S}_{ext} \cdot \langle \mathbf{F} \rangle^{\circ} \} da + A_{0}$$

$$\int (- [\Psi] + [\mathbf{n} \cdot \mathbf{F}^{\mathsf{T}} \mathbf{S} \mathbf{n}] - \mathbf{k} + \Pi) \nabla da + \int (\psi - \sigma) \nabla_{(\partial A) \tan} ds \leq 0$$

$$A_{0} \qquad \partial A_{0}$$

at τ , or equivalently, introducing the Eshelby tensor **P** defined by (6.2),

$$\int \{\psi^{\circ} + (\sigma - \psi) K \nabla + \boldsymbol{B} \cdot \mathbf{n}^{\circ} - \boldsymbol{S}_{ext} \cdot \langle \mathbf{F} \rangle^{\circ} + (\Pi - \mathbf{n} \cdot [\mathbf{P}]\mathbf{n} - \boldsymbol{k}) \nabla \} d\mathbf{a} + A_{0}$$

$$\int (\psi - \sigma) \nabla_{(\partial A) \tan} d\mathbf{s} \leq 0.$$

$$\partial A_{0}$$

$$(12.2)$$

Given an arbitrary time τ and an arbitrary interfacial set A_0 at τ , it is possible to construct a control volume R such that $A_0 = A(\tau)$, and such that $V_{(\partial A)tan}$ is an arbitrary scalar field at $t=\tau$. The coefficient of $V_{(\partial A)tan}$ in (12.2) must therefore vanish, and this yields the standard result

 $\sigma = \psi. \tag{12.3}$

Further, since A is arbitrary, we have the **interfacial dissipation** inequality

$$\psi^{\circ} + \mathbf{a} \cdot \mathbf{n}^{\circ} - \mathbf{S}_{ext} \cdot \langle \mathbf{F} \rangle^{\circ} + (\Pi - \mathbf{n} \cdot [\mathbf{P}]\mathbf{n} - \mathbf{k}) \vee \leq 0.$$
(12.4)

On the other hand, (12.1) applied to referential control volumes that do not intersect the interface yields the bulk dissipation inequality (6.5).

Next, we introduce the interfacial Eshelby tensor

$$\mathbf{P} = \psi \mathbf{1}_{n} - \mathbf{F}^{\mathsf{T}} \mathbf{S} \,. \tag{12.5}$$

Since $(1 - n \otimes n) = 1_n (1_n)^T$, (9.2) yields $(1 - n \otimes n) \langle F \rangle^T = 1_n \mathbb{F}^T$; hence (11.5), (12.3), and (A3) imply that

$$\mathbf{C}_{tan} = \mathbf{P} \tag{12.6}$$

identifying the tangential part of the accretive surface stress as the Eshelby tensor for the interface.

13. CONSTITUTIVE EQUATIONS.

We continue to assume that the bulk material is governed by the constitutive equations (7.1) and (7.2).

To these equations we adjoin constitutive equations for the interface giving the interfacial energy ψ , the deformational surface stress **S**, the normal component²⁹ **C**=**C**^T**n** of the accretive surface stress **C**, and the accretive tension Π as functions of the normal **n**, the normal velocity V, and the limiting values F_1 and F_2 of the deformation gradient at the interface. Coherency requires that the deformation gradients be consistent with $F_1(1-n\otimes n)=F_2(1-n\otimes n)$, a constraint that allows us to choose

$$\mathbf{E} = \langle \mathbf{F} \rangle, \qquad \mathbf{j} = [\mathbf{F}]\mathbf{n} \tag{13.1}$$

as independent variables in place of F_1 and F_2 (cf. (9.4)). We therefore consider constitutive equations of the form:

$$\psi = \hat{\psi}(\mathbf{z}), \quad \mathbf{S} = \hat{\mathbf{S}}(\mathbf{z}), \quad \mathbf{C} = \hat{\mathbf{C}}(\mathbf{z}), \quad \Pi = \hat{\Pi}(\mathbf{z}), \quad (13.2)$$
$$\mathbf{z} = (\mathbf{E}, \mathbf{i}, \mathbf{n}, \mathbf{V})$$

with $\hat{\mathbf{S}}$ consistent with (10.6). The domain of the response functions in (13.2) is the set Z of all \mathbf{z} with $\mathbf{E} \in \mathrm{Lin}^+$, $\mathbf{j} \in \mathbb{R}^3$, $\mathbf{n} \in \mathrm{Unit}$, $\mathbf{V} \in \mathbb{R}$.

Note that, by (11.3), (12.5), and (12.6), the normal component $\mathbf{a} = \mathbf{A}^{\mathsf{T}}\mathbf{n}$ of \mathbf{A} is given by a constitutive equation $\mathbf{a} = \hat{\mathbf{a}}(\mathbf{z})$; and that, by (3.14), (6.2), and (7.1), $\mathbf{n} \cdot [\mathbf{P}]\mathbf{n} + \mathbf{k}$ may also be considered a function of \mathbf{z} .

Remark 13.1 (Constitutive Processes). Suppose we are given an arbitrary coherent two-phase motion. Then the constitutive equations may be used to compute a *constitutive process* consisting of \mathbf{z} as a field, the bulk fields \mathbf{S} and Ψ , and the interfacial fields ψ , \mathbf{S} , \mathbf{C} , and Π . The balance laws for force may then be used to compute the accretive stress \mathbf{C} and the external forces \mathbf{b} , \mathbf{f} , and \mathbf{g} needed to support the process: $(10.5)_2$ gives \mathbf{g} ; $(10.5)_1$, (5.2), and (6.3) give \mathbf{f} ; $(4.5)_1$ gives \mathbf{b} ; $(4.5)_2$ and (6.3) may be solved for \mathbf{C} .

 $^{^{29}}$ The relation (12.6) then yields a corresponding constitutive equation for the tangential part of **C**.

The second law in the form of the interfacial dissipation inequality (12.4) remains to be satisfied in all constitutive processes. We now show — as a consequence of the requirement that all constitutive processes be consistent with (12.4) — that:

(a) The response functions $\hat{\psi}$, $\hat{\mathbf{S}}$, and $\hat{\mathbf{e}}$ are independent of j=[F]n and V; thus ψ , $\hat{\mathbf{S}}$, and $\hat{\mathbf{e}}$ are at most functions of $\mathbf{E} = \langle F \rangle$ and \mathbf{n} :

$$\psi = \hat{\psi}(E,n), \quad \mathbf{S} = \mathbf{S}(E,n), \quad \mathbf{e} = \hat{\mathbf{e}}(E,n). \quad (13.3)$$

(b) The response functions in (13.3) are related through

$$\hat{\mathbf{S}}(\mathbf{E},\mathbf{n})_{\text{ext}} = \partial_{\mathbf{E}}\hat{\boldsymbol{\psi}}(\mathbf{E},\mathbf{n}), \qquad \hat{\mathbf{B}}(\mathbf{E},\mathbf{n}) = -\partial_{\mathbf{n}}\hat{\boldsymbol{\psi}}(\mathbf{E},\mathbf{n}), \qquad (13.4)$$

where $\hat{\mathbf{S}}(\mathbf{E},\mathbf{n})_{ext} = \hat{\mathbf{S}}(\mathbf{E},\mathbf{n})(\mathbb{1}_n)^{\mathsf{T}}$ (cf. (A4)).

(c) The accretive tension has the form

$$\Pi(\mathbf{z}) = \mathbf{n} \cdot [\mathbf{P}] \mathbf{n} + \mathbf{k} - \beta \mathbf{V}$$
(13.5)

with β given by a constitutive equation

$$\boldsymbol{\beta} = \hat{\boldsymbol{\beta}}(\boldsymbol{z}) \ge 0. \tag{13.6}$$

To verify these results we let

$$\Phi(\mathbf{z}) = \widehat{\Pi}(\mathbf{z}) - \mathbf{n} \cdot [\mathbf{P}]\mathbf{n} - \mathbf{k}. \tag{13.7}$$

The requirement that (12.4) hold in all constitutive processes then yields

$$\partial_{\mathbf{v}}\hat{\boldsymbol{\psi}}(\mathbf{z})\boldsymbol{\nabla}^{\circ} + \partial_{\mathbf{j}}\hat{\boldsymbol{\psi}}(\mathbf{z})\cdot\mathbf{j}^{\circ} + [\partial_{\mathbf{n}}\hat{\boldsymbol{\psi}}(\mathbf{z}) + \hat{\boldsymbol{e}}(\mathbf{z})]\cdot\mathbf{n}^{\circ} +$$

$$[\partial_{\mathbf{r}}\hat{\boldsymbol{\psi}}(\mathbf{z}) - \hat{\boldsymbol{s}}(\mathbf{z})_{ext}]\cdot\mathbf{E}^{\circ} + \Phi(\mathbf{z})\boldsymbol{\nabla} \leq 0$$
(13.8)

in all such processes. In view of Lemma B2, given any z_0 in the domain of the response functions, there is a constitutive process such that $z(X,t)=z_0$ at X=0 and t=0, but $E^{\circ}(0,0)$, $j^{\circ}(0,0)$, $n^{\circ}(0,0)$, and $V^{\circ}(0,0)$ are

arbitrary. Thus

$$\partial_{\mathbf{V}}\hat{\boldsymbol{\psi}}(\mathbf{z}) = 0, \quad \partial_{\mathbf{j}}\hat{\boldsymbol{\psi}}(\mathbf{z}) = \mathbf{0}, \quad \hat{\mathbf{a}}(\mathbf{z}) = -\partial_{\mathbf{n}}\hat{\boldsymbol{\psi}}(\mathbf{z}),$$
(13.9)
 $\hat{\mathbf{s}}(\mathbf{z})_{\mathbf{ext}} = \partial_{\mathbf{E}}\hat{\boldsymbol{\psi}}(\mathbf{z}), \quad \Phi(\mathbf{z})\mathbf{V} \leq 0,$

with z an arbitrary element of the domain of the response functions. Thus $\hat{\psi}$ is independent of V and j=[F]n, and (a) and (b) are satisfied. The final result (c) follows, as before, from $(13.9)_5$.

Note that, by (12.3), (12.5), and (13.5), we can write the normal accretive balance (11.10) in the form

$$\mathbf{n} \cdot [\mathbf{P}]\mathbf{n} + \mathbf{k} = -\mathbf{P} \cdot \mathbf{L} - \mathrm{Div}_{\mathbf{S}}\mathbf{C} + \mathbf{\beta} \mathbf{V} - \mathbf{f} \cdot \mathbf{n}, \qquad (13.10)$$

generalizing (7.7) to include interfacial structure.

The results (a) and (b) have important consequences:

(d) The response functions $\hat{\psi}$, $\hat{\mathbf{S}}$, and $\hat{\mathbf{c}}$ depend on $\mathbf{E} = \langle \mathbf{F} \rangle$ through the tangential deformation gradient $\mathbf{F} = \langle \mathbf{F} \rangle \mathbf{1}_n$,

$$\psi = \widetilde{\psi}(\mathbf{F}, \mathbf{n}), \qquad \mathbf{S} = \mathbf{S}(\mathbf{F}, \mathbf{n}), \qquad \mathbf{C} = \mathbf{\widetilde{C}}(\mathbf{F}, \mathbf{n}), \qquad (13.11)$$

with

$$\widetilde{\mathbf{S}}(\mathbf{F},\mathbf{n}) = \partial_{\mathbf{F}}\widetilde{\boldsymbol{\psi}}(\mathbf{F},\mathbf{n}), \quad \widetilde{\mathbf{C}}(\mathbf{F},\mathbf{n}) = -D_{\mathbf{n}}\widetilde{\boldsymbol{\psi}}(\mathbf{F},\mathbf{n}). \quad (13.12)$$

To verify (d), note that $(13.9)_4$ and the sentence following (A1) imply³⁰

$$\partial_{\mathbf{E}}\hat{\psi}(\mathbf{z})\mathbf{n} = \mathbf{0},\tag{13.13}$$

so that, by $(A19)_2$,

$$\partial_{\mathbf{e}}\hat{\psi}(\mathbf{z}) = 0, \qquad \mathbf{e} = \mathbf{E}\mathbf{n} = \langle \mathbf{F} \rangle \mathbf{n}, \qquad (13.14)$$

³⁰Parry [1987], Pitteri [1987], and Podio-Guidugli & Vergara Caffarelli [1990] derive (13.13) as a necessary condition for the statical stability of the interface (cf. Fonseca [1989], Prop. 3.2).

and we may conclude from Lemma A1 that $\hat{\psi}(\mathbf{z}) = \tilde{\psi}(\mathbf{F},\mathbf{n})$. Thus (iii) of Lemma A1 holds, and this result, $(13.9)_4$, and (A4) imply that $\hat{\mathbf{S}}(\mathbf{z}) = \tilde{\mathbf{S}}(\mathbf{F},\mathbf{n})$, and that $(13.12)_1$ is satisfied. Further, by (11.5) and $(13.14)_2$, $\mathbf{z} = \mathbf{c} + \mathbf{S}^{\mathsf{T}}\mathbf{e}$, and this relation, (A19), $(13.9)_3$, and $(13.14)_1$ yield $\hat{\mathbf{c}}(\mathbf{z}) = \tilde{\mathbf{c}}(\mathbf{F},\mathbf{n})$ and $(13.12)_2$. This completes the proof of (d).

ŧ

Remark 13.2. When deciding on possible energies $\hat{\psi}(\mathbf{E},\mathbf{n})$ for an admissible theory, the condition (13.13) is crucial: granted (13.13), the relations (13.4) may be used as *defining relations* for **S** and **E**, and yield (13.11) and (13.12) as consequences.

14. EVOLUTION EQUATIONS IN THE ABSENCE OF EXTERNAL FORCES.

Assume that the external fields vanish. The complete set of interface conditions then consist of 31 the compatibility conditions

$$[y^*] = -V[F]n,$$
 $[F](1 - n \otimes n) = 0,$ (14.1)

the deformational force balance

$$[\mathbf{S}]\mathbf{n} = -\operatorname{Div}_{\mathbf{S}}\mathbf{S} + \mathbf{p}, \qquad (14.2)$$

and the normal accretive balance

$$\mathbf{n} \cdot [\mathbf{P}]\mathbf{n} + \mathbf{k} = -\mathbf{P} \cdot \mathbf{L} - \mathrm{Div}_{\mathrm{S}}\mathbf{C} + \beta \mathrm{V}, \qquad (14.3)$$

with

$$\mathbf{S} = \partial_{\mathbf{F}} \widetilde{\boldsymbol{\psi}}(\mathbf{F}, \mathbf{n}), \qquad \mathbf{C} = -D_{\mathbf{n}} \widetilde{\boldsymbol{\psi}}(\mathbf{F}, \mathbf{n}), \qquad \boldsymbol{\beta} = \hat{\boldsymbol{\beta}}(\mathbf{z}), \qquad (14.4)$$

and with P, p, and \clubsuit given by (8.4). These with the bulk equations

$$\mathbf{S} = \partial_{\mathbf{F}} \Psi_{i}(\mathbf{F}), \qquad \text{Div}\,\mathbf{S} = \rho \mathbf{y}^{**}$$
 (14.5)

and appropriate initial and boundary conditions form the basic freeboundary problem of the theory.

³¹[GS]. For statical situations (14.3) was derived by Leo & Sekerka [1989] (cf. Alexander & Johnson [1985,1986]) as an Euler-Lagrange equation for stable equilibria, while (14.2) was derived by Gurtin & Murdoch [1974]. A counterpart of (14.3) for a rigid system was derived by Gurtin [1988].

15. THEORY WITH BULK DIFFUSION, BUT WITHOUT INERTIA.

We now alter the theory to include mass transport in bulk, neglecting inertia as well as mass transport within the interface. We assume that there are \mathfrak{A} effective³² species of mobile atoms, which we label $\mathfrak{a} = 1, 2, ..., \mathfrak{A}$, and we add to the basic quantities discussed previously the following fields for each species \mathfrak{a} :

ρα	bulk density
h^{α}	diffusive mass flux
μ ^α	chemical potential
Q ^α	external bulk mass supply
d_{α}	external interfacial mass supply

The bulk densities ρ^{α} are atomic or *molar* densities, measured per unit undeformed volume; the diffusive bulk mass fluxes h^{α} are measured in moles per unit undeformed area; Q^{α} and q^{α} , the external supplies of mass of species α to the bulk material and to the interface, respectively, are measured in moles per unit undeformed volume and area.

We assume that the interface is in local equilibrium in the sense that

$$\mu^{a}$$
 is continuous across the interface. (15.1)

We introduce the Gibbs function ω and the associated Eshelby tensor **P**:

$$\omega = \Psi - \Sigma_{\alpha} \rho^{\alpha} \mu^{\alpha}, \qquad (15.2)$$
$$\mathbf{P} = \omega \mathbf{1} - \mathbf{F}^{\mathsf{T}} \mathbf{S},$$

where here and throughout this section Σ_{α} designates the sum over α from 1 to **2**. Since we neglect interfacial mass, the Eshelby tensor for the interface is still given by (12.5).

The basic laws are the force balance relations discussed in Section 10,

37

³²We assume that the atoms of species $a \in \{1, 2, ..., b\}$ lie on lattice points, that the atoms of species $a \in \{b+1, b+2, ..., 2l\}$ are interstitial, that there is an additional mobile species a = 0 whose atoms lie on lattice points, and that all lattice sites are occupied. The constraint $p^{0}+p^{1}+...+p^{b}=$ constant then allows us to omit mention of the species a=0. The chemical potential μ^{α} for $a \in \{1, 2, ..., b\}$ should then be interpreted as $\mu^{\alpha}-\mu^{0}$.

but without inertia, the mass balance

for each species α , and the global dissipation inequality

$$\{ \int \Psi dv + \int \psi da \}^{\bullet} \leq R \qquad S \cap R$$

$$\mathcal{P}(R) + \Sigma_{a} \{ -\int \mu^{a} h^{a} \cdot m da + \int \mu^{a} q^{a} da + \int \mu^{a} Q^{a} dv \}, \quad (15.4)$$

$$\partial R \qquad S \cap R \qquad R$$

with **m** the outward unit normal to ∂R . The requirement that (15.3) and (15.4) hold for all control volumes leads to the identification $\sigma = \psi$, to the bulk relations

$$(\rho^{\alpha})^{\bullet} = -\operatorname{Div} \mathbf{h}^{\alpha} + Q^{\alpha},$$

$$\Psi^{\bullet} - \mathbf{S} \cdot \mathbf{F}^{\bullet} - \Sigma_{\alpha} \{ \mu^{\alpha} (\rho^{\alpha})^{\bullet} - \mathbf{h}^{\alpha} \cdot \nabla \mu^{\alpha} \} \le 0,$$
(15.5)

and to the interface conditions

$$[\rho^{\alpha}] \vee = [\mathbf{h}^{\alpha}] \cdot \mathbf{n} - q^{\alpha}, \qquad (15.6)$$

$$\psi^{\circ} + \mathbf{a} \cdot \mathbf{n}^{\circ} - \mathbf{S}_{ext} \cdot \langle F \rangle^{\circ} + (\Pi - \mathbf{n} \cdot [P]\mathbf{n}) \vee \leq 0,$$

with $\Pi = \mathbf{n} \cdot [\mathbf{C}]\mathbf{n}$ the accretive tension.

Let

$$\rho = (\rho^1, \dots, \rho^{\mathfrak{A}}), \quad \mu = (\mu^1, \dots, \mu^{\mathfrak{A}}), \quad H = (h^1, \dots, h^{\mathfrak{A}}), \quad (15.7)$$

(with H and $\nabla\,\mu$ identified with vectors in $\mathbb{R}^{3\,\mathfrak{A}}$). We consider bulk constitutive equations

$$S = \hat{S}_{i}(F,\rho), \quad \mu = \hat{\mu}_{i}(F,\rho), \quad \Psi = \hat{\Psi}_{i}(F,\rho), \quad (15.8)$$
$$H = -D_{i}(F,\rho)\nabla\mu,$$

for each phase i, with

$$\hat{\mathbf{S}}_{i}(\mathbf{F},\boldsymbol{\rho}) = \partial_{\mathbf{F}}\hat{\Psi}_{i}(\mathbf{F},\boldsymbol{\rho}), \qquad \hat{\mu}_{i}(\mathbf{F},\boldsymbol{\rho}) = \partial_{\boldsymbol{\rho}}\hat{\Psi}_{i}(\mathbf{F},\boldsymbol{\rho}), \qquad (15.9)$$

and with **diffusivity** $D_i(\mathbf{F}, \boldsymbol{\rho})$ (a linear transformation of $\mathbb{R}^{3\mathfrak{A}}$ into itself) compatible with the inequality $\Sigma_{\alpha} \mathbf{h}^{\alpha} \cdot \nabla \mu^{\alpha} \leq 0$.

Regarding the interface, we retain the constitutive relations (13.2), but we allow z to contain the list ρ of densities:

$$z = (E, j, \rho, n, V).$$
 (15.10)

Compatibility with the local dissipation inequality $(15.6)_2$ again leads to the results (13.3) - (13.5), (13.11) and (13.12), but with P as defined in $(15.2)_2$ and z given by (15.10).

The resulting system of equations, 33 in the absence of external fields, consists of the interface conditions (14.1) and

$$[S]n = -Div_{S}S, \qquad [\rho^{\alpha}]V = [h^{\alpha}] \cdot n, \qquad (15.11)$$
$$n \cdot [P]n = -P \cdot L - Div_{S}C + \beta V,$$

the bulk relations

 $Div S = 0, \qquad (\rho^{\alpha})^{\bullet} = -Div h^{\alpha}, \qquad (15.12)$

and the constitutive relations (15.8) and (15.9).

Acknowledgment. This work was supported by the Army Research Office and the National Science Foundation. I acknowledge valuable discussions with Paolo Cermelli, Eliot Fried, Paolo Podio-Guidugli, Perry Leo, Mark Lusk, and Allan Struthers.

³³Cf. Gurtin & Voorhees [1993], who discuss an analogous system appropriate to linear elastic behavior in bulk and no interfacial elasticity.

APPENDIX A. SURFACES.³⁴

A1. SURFACES.

Let Lin(U,W) denote the space of linear transformations from a linear space U into another such space W. It is convenient to write,³⁵ for $n \in Unit$,

$$1_n$$
 = the inclusion of n^{\perp} into \mathbb{R}^3 ; (A1)

 $(1_n)^{\mathsf{T}}$ is then the projection $1 - n \otimes n$ considered as an element of $\operatorname{Lin}(\mathbb{R}^3, n^{\perp})$ rather than $\operatorname{Lin}(\mathbb{R}^3, \mathbb{R}^3)$.

Let Γ be a smooth surface, in \mathbb{R}^3 , oriented by a choice of unit normal field **n**. A superficial scalar (vector) field for Γ is a scalar (vector) field on Γ . A tangential vector field is a superficial vector field **c** with values $\mathbf{C}(\mathbf{x}) \in \mathbf{n}(\mathbf{x})^{\perp}$. A superficial tensor field is a field **c** on Γ whose values $\mathbf{C}(\mathbf{x})$ are linear transformations from the tangent space $\mathbf{n}(\mathbf{x})^{\perp}$ into \mathbb{R}^3 ; a tangential tensor field is a superficial tensor field **c** whose values satisfy $\mathbf{C}(\mathbf{x})\mathbf{a}\in\mathbf{n}(\mathbf{x})^{\perp}$ for each $\mathbf{a}\in\mathbf{n}(\mathbf{x})^{\perp}$. Each superficial tensor field **c** admits the unique decomposition

$$\mathbf{C} = \mathbf{C}_{tan} + \mathbf{n} \otimes \mathbf{C}, \tag{A2}$$

with \mathbf{C}_{tan} a tangential tensor field and \mathbf{c} a tangential vector field; in fact,

$$\mathbf{C}_{tan} = (1 - n \otimes n) \mathbf{C}, \qquad \mathbf{C} = \mathbf{C}^{\mathsf{T}} n; \tag{A3}$$

we refer to \mathbf{C}_{tan} and \mathbf{C} as the tangential and normal³⁶ components of \mathbf{C} with respect to the interface Γ .

We use the term tensor field (as opposed to superficial tensor field) on Γ to denote a field H on Γ with values $H(\mathbf{x}) \in \operatorname{Lin}(\mathbb{R}^3, \mathbb{R}^3)$. A tensor field H on Γ is easily transformed to a superficial tensor field by postmultiplication with 1_n , since $H1_n$ is a superficial tensor field. Here

³⁵For A a subset of B, the inclusion of A into B is the mapping $\iota: A \to B$ that assigns to each $a \in A$ the same element $\iota(a)=a$ considered as a member of B.

³⁴Cf. Sect. 2 of [GS].

³⁶**C**, a tangential vector field, represents the normal component of **C**, since $(n \otimes C)(\mathbf{x}, t)$ in (A2) maps tangent vectors at $\mathbf{x} \in \Gamma(t)$ to normal vectors.

 1_n is the field $\mathbf{x} \mapsto 1_{n(\mathbf{x})}$ with $1_{n(\mathbf{x})}$ the inclusion of the tangent space $n(\mathbf{x})^{\perp}$ at $\mathbf{x} \in \Gamma$ into \mathbb{R}^3 . In the same spirit, we define the extension \mathbb{H}_{ext} of a superficial tensor field \mathbb{H} by

$$\mathbb{H}_{\text{ext}} = \mathbb{H}(\mathbb{1}_n)^{\mathsf{T}}; \tag{A4}$$

 $\mathbb{H}_{ext}(\mathbf{x}) \in \operatorname{Lin}(\mathbb{R}^3, \mathbb{R}^3)$, so that \mathbb{H}_{ext} is a tensor field on Γ .

We write ∇_{Γ} for the surface gradient on Γ and div_{Γ} for the surface divergence on Γ . The tangential tensor field

$$\mathbf{L} = -\nabla_{\Gamma} \mathbf{n} \tag{A5}$$

is the **curvature tensor**; its trace

$$K = tr \mathbf{L} = \mathbf{1}_{n} \cdot \mathbf{L}$$
(A6)

is the **total curvature** (twice the mean curvature). The curvature tensor is tangential, so that

$$\mathbf{L}^{\mathsf{T}}\mathbf{n} = \mathbf{0},\tag{A7}$$

and symmetric in the sense that $L_{ext} = (L_{ext})^T$, or equivalently,

$$L(\mathbf{1}_n)^{\mathsf{T}} = \mathbf{1}_n L^{\mathsf{T}}.$$
 (A8)

Let **C** be a superficial tensor field. The following identity will be useful:

$$\mathbf{n} \cdot \operatorname{div}_{\Gamma} \mathbf{C} = \mathbf{C}_{\operatorname{tan}} \cdot \mathbf{L} + \operatorname{div}_{\Gamma} \mathbf{C}$$
(A9)

with \mathbf{C}_{tan} and \mathbf{C} the tangential and normal components of \mathbf{C} .

Let A denote a smooth subsurface of Γ , and let $\Psi(\mathbf{x})$ denote the **outward unit normal** to the boundary curve ∂A , so that $\Psi(\mathbf{x})$ is tangent to Γ at each $\mathbf{x} \in \partial A$. Let \mathbf{C} be a superficial tensor field, \mathbf{C} a tangential vector field. We will use the surface divergence theorem

$$\int \mathbf{C} \cdot \mathbf{\nu} ds = \int di \mathbf{v}_{\Gamma} \mathbf{C} da, \qquad \int \mathbf{C} \mathbf{\nu} ds = \int di \mathbf{v}_{\Gamma} \mathbf{C} da, \qquad (A10)$$

$$\partial A \qquad A \qquad \partial A \qquad A$$

as well as the integral identities

$$\int \mathbf{C} \boldsymbol{\mathcal{V}} \cdot \mathbf{p} \, ds = \int \{ \mathbf{C} \cdot \nabla_{\Gamma} \mathbf{p} + \mathbf{p} \cdot \operatorname{div}_{\Gamma} \mathbf{C} \} \, da,$$

$$\partial A \qquad A \qquad (A11)$$

$$\int \mathbf{p} \mathbf{C} \cdot \boldsymbol{\mathcal{V}} \, ds = \int \{ \mathbf{C} \cdot \nabla_{\Gamma} \mathbf{p} + \mathbf{p} \, \operatorname{div}_{\Gamma} \mathbf{C} \} \, da \qquad (A11)$$

$$\partial A \qquad A \qquad A \qquad (A11)$$

with p a superficial vector field and p a superficial scalar field.

A2. SMOOTHLY EVOLVING SURFACES.³⁷

Let $\Gamma(t)$ ($t\in T\subset \mathbb{R}$) be a smoothly evolving surface. Superficial and tangential fields for $\Gamma(t)$ ($t\in T$) are functions of $\mathbf{x}\in\Gamma(t)$ and $t\in T$, but are superficial or tangential with respect to $\Gamma(t)$ at each t. Similarly, ∇_{Γ} and div_{Γ} denote the surface gradient and surface divergence on $\Gamma(t)$ for fixed t; $\mathbf{n}(\mathbf{x},t)$ is the (orienting) unit normal to $\Gamma(t)$; $V(\mathbf{x},t)$, $K(\mathbf{x},t)$, and $\mathbf{L}(\mathbf{x},t)$ are the normal velocity, total curvature, and curvature tensor for $\Gamma(t)$.

We write φ° for the normal time-derivative of a scalar, vector, or tensor field φ on Γ (the derivative following the normal trajectories of the surface). We then have the identity

$$\mathbf{n}^{\circ} = -\nabla_{\Gamma} \mathbf{V}. \tag{A12}$$

Let A(t) denote a smoothly evolving subsurface of $\Gamma(t)$, and let $\Psi(\mathbf{x},t)$ denote the **outward unit normal** to the boundary curve $\partial A(t)$, so that $\Psi(\mathbf{x},t)$ is *tangent* to A(t) at each $\mathbf{x} \in \partial A(t)$. The motion of $\partial A(t)$ may be characterized intrinsically by the velocity field

$$\mathbf{v}_{\partial A} = \mathbf{V}\mathbf{n} + \mathbf{V}_{(\partial A)\tan} \boldsymbol{\mathcal{V}}, \tag{A13}$$

where $V_{(\partial A)tan}$, the **tangential edge velocity** of A(t), is the velocity of ∂A in the direction of the normal \mathbf{V} : for $\mathbf{x} = \mathbf{r}(\mathbf{u}, t)$ a local parametrization $\frac{3^7}{\text{Cf. Sect. 2.2 of [GS], where the term smoothly propagating surface is used.}$

42

of $\partial A(t)$, $V_{(\partial A)tan}(\mathbf{x},t) = \mathbf{v}(\mathbf{x},t) \cdot (\partial/\partial t)\mathbf{r}(u,t)$. We will refer to $\mathbf{v}_{\partial A}$ as the intrinsic velocity of ∂A .

For ϕ a superficial scalar field, we write

$$\begin{cases} \int \varphi da \}^{\bullet}(t) = (d/dt) \{ \int \varphi(\mathbf{x}, t) da(\mathbf{x}) \}. \\ A & A(t) \end{cases}$$
(A14)

The following identity will be useful:³⁸

$$\{\int \varphi da\}^{\bullet} = \int (\varphi^{\circ} - \varphi KV) da + \int \varphi V_{(\partial A)tan} ds.$$
(A15)
A A ∂A

A3. INTERFACE RESPONSE FUNCTIONS.

In discussing interfaces we will consider functions

 $\varphi(\mathbf{E},\mathbf{n})$

with domain $Lin^+ \times Unit$, where **n** is the interface normal, while **E** is the deformation gradient of one of the phases at the interface, or the average value of the deformation gradient at the interface.

Given $n \in Unit$, a tensor $E \in Lin^+$ admits the unique decomposition

$$\mathbf{E} = \mathbf{E} (\mathbf{1}_{\mathbf{n}})^{\mathsf{T}} + \mathbf{e} \otimes \mathbf{n}, \quad \mathbf{E} \in \operatorname{Lin}(\mathbf{n}^{\perp}, \mathbb{R}^3), \quad \mathbf{e} \in \mathbb{R}^3, \quad (A16)$$

with

$$\mathbf{E} = \mathbf{E}\mathbf{1}_{\mathbf{n}}, \quad \mathbf{e} = \mathbf{E}\mathbf{n}. \tag{A17}$$

The decomposition (A16) allows us to consider $\varphi(\mathbf{E},\mathbf{n})$ as a function

$$\widetilde{\varphi}(\mathbf{E},\mathbf{e},\mathbf{n}) = \varphi(\mathbf{E}(\mathbf{1}_{n})^{\mathsf{T}} + \mathbf{e} \otimes \mathbf{n},\mathbf{n})$$
(A18)

of the "components" \mathbb{E} and \mathbf{e} . The partial derivatives $\partial_{\mathbf{E}} \varphi(\mathbf{E}, \mathbf{n}) \in \operatorname{Lin}(\mathbf{n}^{\perp}, \mathbb{R}^{3})$ and $\partial_{\mathbf{e}} \varphi(\mathbf{E}, \mathbf{n}) \in \mathbb{R}^{3}$ are then the corresponding partial ³⁸Cf. Petryk & Mroz [1986]; Gurtin, Struthers & Williams [1989]; Estrada & Kanwal [1991]; Jaric [1991]. derivatives of $\tilde{\varphi}(\mathbf{E}, \mathbf{e}, \mathbf{n})$. In addition, we write $D_n \varphi(\mathbf{E}, \mathbf{n}) \in \mathbf{n}^{\perp}$ for the partial derivative with respect to **n** following the interface.³⁹ We then have the identities:⁴⁰

$$\partial_{\mathbf{E}} \varphi(\mathbf{E}, \mathbf{n}) = \partial_{\mathbf{E}} \varphi(\mathbf{E}, \mathbf{n}) \mathbf{1}_{\mathbf{n}},$$

$$\partial_{\mathbf{e}} \varphi(\mathbf{E}, \mathbf{n}) = \partial_{\mathbf{E}} \varphi(\mathbf{E}, \mathbf{n}) \mathbf{n},$$

$$D_{\mathbf{n}} \varphi(\mathbf{E}, \mathbf{n}) = \partial_{\mathbf{n}} \varphi(\mathbf{E}, \mathbf{n}) + \partial_{\mathbf{E}} \varphi(\mathbf{E}, \mathbf{n})^{\mathsf{T}} \mathbf{e} - \mathbf{E}^{\mathsf{T}} \partial_{\mathbf{e}} \varphi(\mathbf{E}, \mathbf{n}).$$
(A19)

Lemma A1. The following are equivalent:

- (i) $\partial_{\mathbf{e}} \varphi(\mathbf{E}, \mathbf{n}) = \mathbf{0}$ for all (\mathbf{E}, \mathbf{n}) ;
- (ii) $\widetilde{\phi}(\textbf{E},\textbf{e},\textbf{n})$ is independent of e;
- (iii) $\partial_{\mathbf{E}} \varphi(\mathbf{E}, \mathbf{n}) (\mathbf{1}_{\mathbf{n}})^{\mathsf{T}} = \partial_{\mathbf{E}} \varphi(\mathbf{E}, \mathbf{n})$ for all (\mathbf{E}, \mathbf{n}) .

 $^{3\,9}$ Cf. eqt. (2.48) of [GS]. $^{4\,0}$ Cf. Lemma 2D of [GS] for (A19) and Lemma (2E) for Lemma A1.

APPENDIX B. LOCALIZATION AND VARIATION LEMMAS.

The next definition and lemma use the notation and terminology of Section 2, with $\Omega = \{\Omega(t), \Omega_1(t), \Omega_2(t); t \in T\}$ the underlying evolving twophase region. Given a family Q_{ε} ($0 < \varepsilon < \varepsilon_0$) of sets and a set A, we write $Q_{\varepsilon} \rightarrow A$ as $\varepsilon \rightarrow 0$ if the family Q_{ε} nests as $\varepsilon \rightarrow 0$ with A as its intersection. We say that A is a regular interfacial set at time τ if A is the intersection of $\Gamma(\tau)$ with a closed ball. We say that a family R_{ε} ($0 < \varepsilon < \varepsilon_0$) of control volumes shrinks to A at time τ if:

(i) τ is a regular time for R_{ϵ} for all ϵ ;

(ii) $A=R_{\varepsilon}\cap\Gamma(\tau)$ for all ε ;

(iii)
$$R_{\epsilon} \rightarrow A$$
 as $\epsilon \rightarrow 0$.

Given a regular interfacial set A at τ , it is possible to construct a family R_r of control volumes that shrinks to A at τ .

Let φ be a bulk scalar field and let D(t) be a (possibly) timedependent region in $\Omega(t)$. Then we write

Lemma B1 (Localization Lemma). Choose a time τ , let R_{ε} be a family of control volumes that shrinks to a regular interfacial set A at τ , and let \mathbf{m}_{ε} denote the outward unit normal to ∂R_{ε} . Then given a bulk scalar field φ and a bulk tensor field S, we have the following limits at time τ as $\varepsilon \rightarrow 0$:

$$\begin{array}{cccc} (d/dt) \{ \int \varphi \, dv \} &\to - \int [\varphi] \vee da, & (d/dt) \{ \int \varphi \, dv \} \to -\delta_i \int \varphi_i \vee da, & (B1) \\ R_{\epsilon} & A & \Omega_i \cap R_{\epsilon} & A \\ \\ \int \mathbf{Sm}_{\epsilon} \, da &\to & \int [\mathbf{S}] \mathbf{n} \, da, & \int \mathbf{Sm}_{\epsilon} \, da &\to & \delta_i \int \mathbf{S}_i \mathbf{n} \, da, & (B2) \\ \partial R_{\epsilon} & A & \Omega_i \cap (\partial R_{\epsilon}) & A \end{array}$$

with $\delta_i = (-1)^i$. (A similar expression holds for vector fields.)

Lemma B2 (Variation Lemma for Coherent Motions). There is a coherent two-phase motion y such that $0 \in S(0)$ and such that the following fields have arbitrarily preassigned values at (0,0):

$$E = \langle F \rangle$$
, $j = [F]n$, n , V , E° , j° , n° , V° . (B3)

Proof (sketch). Choose the body B to be \mathbb{R}^3 . Let n and Z be arbitrary smooth functions of time with $n(t)\in Unit$ and $Z(t)\in \mathbb{R}^3$ at each t, and with Z(0)=0. Further, let S(t) be the plane through Z(t) with normal n(t), and let

$$B_{1}(t) = \{ X : (X - Z(t)) \cdot n(t) \le 0 \},\$$

$$B_{2}(t) = \{ X : (X - Z(t)) \cdot n(t) \ge 0 \}.\$$

Let E_0 and j_0 be arbitrary smooth functions of time with $E_0(t) \in Lin^+$ and $j_0(t) \in \mathbb{R}^3$ at each t, and let

 $\mathbf{y}(\mathbf{X},t) = \mathbf{F}(\mathbf{X},t)\mathbf{X},$

for all $\mathbf{X} \in \mathbb{R}^3$ and $t \in \mathbb{R}$, where

$$\mathbf{E}_{0}(t) - \frac{1}{2}\mathbf{j}_{0}(t) \otimes \mathbf{n}(t), \quad \mathbf{X} \in \mathbf{B}_{1}(t)$$
$$\mathbf{F}(\mathbf{X},t) = \mathbf{E}_{0}(t) + \frac{1}{2}\mathbf{j}_{0}(t) \otimes \mathbf{n}(t), \quad \mathbf{X} \in \mathbf{B}_{2}(t).$$

Then **y** is a coherent two-phase motion. Moreover, we may choose the functions **n** and **Z** such that **n**, V, **n**°, and V° have arbitrarily preassigned values at (0,0); and we may choose the functions E_0 and j_0 such that $E=\langle F \rangle$, j=[F]n, E° , and j° have arbitrarily preassigned values at (0,0). \Box

REFERENCES.

j. ₹

- [1878] Gibbs, J. W., On the equilibrium of hetrogeneous substances, Trans.
 Connecticut Acad. 3, 108-248 (1878). Reprinted in: *The Scientific* Papers of J. Willard Gibbs, vol. 1, Dover, New York (1961).
- [1952] Brooks, H., Theory of internal boundaries, in: Metal Interfaces, Am. Soc. Metals, Cleveland Press.
- [1974] Gurtin, M. E. & I. Murdoch, A continuum theory of elastic material surfaces, Arch. Rational Mech. Anal., **57**, 291–323.
- [1974] Robin, P.-Y. F., Thermodynamic equilibrium across a coherent interface in a stressed crystal, Am. Min. **59**, 1286-1298.
- [1975] Eshelby, J. D., The elastic energy-momentum tensor, J. Elasticity 5, 321-335.
- [1978] Larché, F. C. & J. W. Cahn, A linear theory of thermochemical equilibrium of solids under stress, Act. Metall. **26**, 1579–1589.
- [1980] Cahn, J. W., Surface stress and the chemical equilibrium of small crystals. 1. The case of the isotropic surface, Act. Metall. 28, 1333– 1338.
- [1981] Gurtin, M. E., An Introduction to Continuum Mechanics, Academic Press, New York.
- [1981] Mullins, W. W., On the validity of the Onsager reciprocal relations, in Proc. Int. Conf. Solid-Solid Phase Transitions (ed. H. I. Aronson, D. E. Laughlin, R. F. Sekerka and C. M. Wayman), TMS-AIME, Warrandale, Pa.
- [1982] Cahn, J. W. & F. C. Larché, Surface stress and the chemical equilibrium of small crystals. 2. Solid particles embedded in a solid matrix, Act. Metall. 30, 51–56.
- [1984] Mullins, W. W., Thermodynamic equilibrium of a crystalline sphere in a fluid, J. Chem. Phys. **81**, 1436–1442.
- [1985] Alexander, J. I. D. & W. C. Johnson, Thermomechanical equilibrium solid-fluid systems with curved interfaces, J. Appl. Phys. 58, 816-824.
- [1985] Larché, F. C. & J. W. Cahn, The interaction of composition and stress in crystalline solids, Act. Metall. **33**, 331–357.
- [1986] Petryk, H. & Z. Mroz, Z., Time derivatives of integrals and functionals defined on varying volume and surface domains, Arch.

47

Mech. **38**, 697-724.

ŧ

- [1986] Johnson W. C. & J. I. D. Alexander, Interfacial conditions for thermomechanical equilibrium in two-phase crystals, J. Appl. Phys. 59, 2735-2746.
- [1987] Parry, G. P., On shear bands in unloaded crystals, Preprint.
- [1987] Pitteri, M., On 1- and 3-dimensional models in "non-convex" elasticity, Preprint.
- [1988] Gurtin, M. E., Multiphase thermomechanics with interfacial structure. 1. Heat conduction and the capillary balance law, Arch. Rational Mech. Anal., 104, 185-221.
- [1989] Fonseca, I., Interfacial energy and the Maxwell rule, Arch. Rational Mech. Anal., **106**, 63-95.
- [1989] Gurtin, M. E., A. Struthers, & W. O. Williams, A transport theorem for moving interfaces, Quart. Appl. Math., 47, 773-777.
- [1989] Leo, P. H. & R. F. Sekerka, The effect of surface stress on crystalmelt and crystal-crystal equilibrium, Act. Metall. **37**, 3119-3138.
- [1990] Abeyaratne, R. & J. K. Knowles, On the driving traction acting on a surface of strain discontinuity in a continuum, J. Mech. Phys. Solids, 38, 345-360.
- [1990] Gurtin, M. E. & A. Struthers, Multiphase thermomechanics with interfacial structure. 3. Evolving phase boundaries in the presence of bulk deformation, Arch. Rational Mech. Anal. 112, 97-160.
- [1990] Podio-Guidugli P. & G. Vergara Caffarelli, Surface interaction potentials in elasticity, Arch. Rational Mech. Anal. **109**, 343-383.
- [1991] Abeyaratne, R. & J. K. Knowles, Kinetic relations and the propagation of phase boundaries in elastic solids, Arch. Rational Mech. Anal., 114, 119–154.
- [1991] Estrada, R. & R. P. Kanwal, Non-classical derivation of the transport theorems for wave fronts, J. Math. Anal. Appl., 159, 290-297.
- [1991] Gurtin, M. E., On thermodynamical laws for the motion of a phase interface, Zeit. angew. Math. Phys., 42, 370–388.
- [1991] Jaric, J. P., On a transport theorem for moving interfaces, Preprint.
- [1991] Truskinovsky, L., Kinks versus shocks, in *Shock Induced Transitions and Phase Structures in General Media* (ed. R. Fosdick,

- E. Dunn and M. Slemrod), Springer-Verlag, Berlin.
- [1992] Pfenning, N. M. & W. O. Williams, On non-material surfaces with structure, Quart. Appl. Math., Forthcoming.
- [1993] Gurtin, M. E. & P. W. Voorhees, The continuum mechanics of two-phase systems with mass transport and stress, Proc. Roy. Soc., Forthcoming.

Department of Mathematics Carnegie Mellon University Pittsburgh, PA

.....

Center for Nonlinear Analysis Report Series

Nonlinear Analysis Series

No.

. ,

.

.

~

91-NA-001	[]	Lions, P.L., Jacobians and Hardy spaces, June 1991
91-NA-002	[]	Giga, Y. and Soto, MH., Generalized interface evolution with the Neumann boundary condition, July 1991
91-NA-003	[]	Soner, H.M. and Souganidis, P.E., Uniqueness and singularities of cylindrically symmetric surfaces moving by mean curvature, July 1991
91-NA-004	[]	Coleman, B.D., Marcus, M. and Mizel, V.J., On the Thermodynamics of periodic phases, August 1991
91-NA-005	[]	Gurtin, M.E. and Podio-Guidugli, P., On the formulation of mechanical balance laws for structured continua, August 1991
91-NA-006	[]	Gurtin, M.E. and Voorhees, P., Two-phase continuum mechanics with mass transport and stress, August 1991
91-NA-007	[]	Fried, E., Non-monotonic transformation kinetics and the morphological stability of phase boundaries in thermoelastic materials, September 1991
91-NA-008	[]	Gurtin, M.E., Evolving phase boundaries in deformable continua, September 1991
91-NA-009	[]	Di Carlo, A., Gurtin, M.E., and Podio-Guidugli, P., A regularized equation for anisotropic motion-by-curvature, September 1991
91-NA-010	[]	Kinderlehrer, D. and Ou, B., Second variation of liquid crystal energy at x/lxl, August 1991
91-NA-011	[]	Baughman, L.A. and Walkington, N., Co-volume methods for degenerate parabolic problems, August 1991
91-NA-012	[]	James, R.D. and Kinderlehrer, D., Frustration and microstructure: An example in magnetostriction, November 1991
91-NA-013	[]	Angenent, S.B. and Gurtin, M.E., Anisotropic motion of a phase interface, November 1991

92-NA-001	[]	Nicolaides, R.A. and Walkington, N.J., Computation of microstructure utilizing Young measure representations, January 1992
92-NA-002	[]	Tartar, L., On mathematical tools for studying partial differential equations of continuum physics: H-measures and Young measures, January 1992
92-NA-003	[]	Bronsard, L. and Hilhorst, D., On the slow dynamics for the Cahn- Hilliard equation in one space dimension, February 1992
92-NA-004	[]	Gurtin, M.E., Thermodynamics and the supercritical Stefan equations with nucleations, March 1992
92-NA-005	[]	Antonic, N., Memory effects in homogenisation linear second order equation, February 1992
92-NA-006	[]	Gurtin, M.E. and Voorhees, P.W., The continuum mechanics of coherent two-phase elastic solids with mass transport, March 1992
92-NA-007	[]	Kinderlehrer, D. and Pedregal, P., Remarks about gradient Young measures generated by sequences in Sobolev spaces, March 1992
92-NA-008	[]	Workshop on Shear Bands, March 23-25, 1992 (Abstracts), March 1992
92-NA-009	[]	Armstrong, R. W., Microstructural/Dislocation Mechanics Aspects of Shear Banding in Polycrystals, March 1992
92-NA-010	[]	Soner, H. M. and Souganidis, P. E., Singularities and Uniqueness of Cylindrically Symmetric Surfaces Moving by Mean Curvature, April 1992
92-NA-011	[]	Owen, David R., Schaeffer, Jack, andWang, Keming, A Gronwall Inequality for Weakly Lipschitzian Mappings, April 1992
92-NA-012	[]	Alama, Stanley and Li, Yan Yan, On "Multibump" Bound States for Certain Semilinear Elliptic Equations, April 1992
92-NA-013	[]	Olmstead, W. E., Nemat-Nasser, S., and Li, L., Shear Bands as Discontinuities, April 1992
92-NA-014	[]	Antonic, N., H-Measures Applied to Symmetric Systems, April 1992
92-NA-015	[]	Barroso, Ana Cristina and Fonseca, Irene, Anisotropic Singular Perturbations - The Vectorial Case, April 1992
92-NA-016	[]	Pedregal, Pablo, Jensen's Inequality in the Calculus of Variations , May 1992
92-NA-017	[]	Fonseca, Irene and Muller, Stefan, Relaxation of Quasiconvex Functionals in BV($\Omega, \Re P$) for Integrands $f(x, u, \nabla u)$, May 1992

: / /

· • •

-

•

-

. .

.

92-NA-018	[]	Alama, Stanley and Tarantello, Gabriella, On Semilinear Elliptic Equations with Indefinite Nonlinearities, May 1992
92-NA-019	[]	Owen, David R., Deformations and Stresses With and Without Microslip, June 1992
92-NA-020	[]	Barles, G., Soner, H. M., Souganidis, P. E., Front Propagation and Phase Field Theory, June 1992
92-NA-021	[]	Bruno, Oscar P. and Reitich, Fernando, Approximation of Analytic Functions: A Method of Enhanced Convergence, July 1992
92-NA-022	[]	Bronsard, Lia and Reitich, Fernando, On Three-Phase Boundary Motion and the Singular Limit of a Vector-Valued Ginzburg- Landau Equation, July 1992
92-NA-023	[]	Cannarsa, Piermarco, Gozzi, Fausto and Soner, H.M., A Dynamic Programming Approach to Nonlinear Boundary Control Problems of Parabolic Type, July 1992
92-NA-024	[]	Fried, Eliot and Gurtin, Morton, Continuum Phase Transitions With An Order Parameter; Accretion and Heat Conduction, August 1992
92-NA-025	[]	Swart, Pieter J. and Homes, Philip J., Energy Minimization and the Formation of Microstructure in Dynamic Anti-Plane Shear, August 1992
92-NA-026	[]	Ambrosio, I., Cannarsa, P. and Soner, H.M., On the Propagation of Singularities of Semi-Convex Functions, August 1992
92-NA-027	[]	Nicolaides, R.A. and Walkington, Noel J., Strong Convergence of Numerical Solutions to Degenerate Varational Problems, August 1992
92-NA-028	[]	Tarantello, Gabriella, Multiplicity Results for an Inhomogenous Neumann Problem with Critical Exponent, August 1992
92-NA-029	[]	Noll, Walter, The Geometry of Contact, Separation, and Reformation of Continous Bodies, August 1992
92-NA-030	[]	Brandon, Deborah and Rogers, Robert C., Nonlocal Superconductivity, July 1992
92-NA-031	[]	Yang, Yisong, An Equivalence Theorem for String Solutions of the Einstein-Matter-Gauge Equations, September 1992
92-NA-032	[]	Spruck, Joel and Yang, Yisong, Cosmic String Solutions of the Einstein-Matter-Gauge Equations, September 1992
92-NA-033	[]	Workshop on Computational Methods in Materials Science (Abstracts), September 16-18, 1992.

~

a fat a 🌗 e 🤷

-

~

•

.



- 92-NA-034 [] Leo, Perry H. and Herng-Jeng Jou, Shape evolution of an initially circular precipitate growing by diffusion in an applied stress field, October 1992
- 92-NA-035 [] Gangbo, Wilfrid, On the weak lower semicontinuity of energies with polyconvex integrands, October 1992
- 92-NA-036 [] Katsoulakis, Markos, Kossioris, Georgios T. and Retich, Fernando, Generalized motion by mean curvature with Neumann conditions and the Allen-Cahn model for phase transitions, October 1992
- 92-NA-037 [] Kinderlehrer, David, Some methods of analysis in the study of microstructure, October 1992
- 92-NA-038 [] Yang, Yisong, Self duality of the Gauge Field equations and the Cosmological Constant, November 1992
- 92-NA-039 [] Brandon, Deborah and Rogers, Robert, Constitutive Laws for Pseudo-Elastic Materials, November 1992
- 92-NA-040 [] Leo, P. H., Shield, T. W., and Bruno, O. P., Transient Heat Transfer Effects on the Pseudoelastic Behavior of Shape-Memory Wires, November 1992
- 92-NA-041 [] Gurtin, Morton E., The Dynamics of Solid-Solid Phase Transitions 1. Coherent Interfaces, November 1992

Stochastic Analysis Series

- 91-SA-001 [] Soner, H.M., Singular perturbations in manufacturing, November 1991
 91-SA-002 [] Bridge, D.S. and Shreve, S.E., Multi-dimensional finite-fuel singular stochastic control, November 1991
- 92-SA-001 [] Shreve, S. E. and Soner, H. M., Optimal Investment and Consumption with Transaction Costs, September 1992