ON THE CONTINUUM MECHANICS OF THE MOTION OF A PHASE INTERFACE

by

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

Research Report No. 90-69

January 1990

ON THE CONTINUUM MECHANICS OF THE MOTION OF A PHASE INTERFACE

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

Presented at the Seventh Army Conference on Applied Mathematics and Computing, West Point, June, 1989

ON THE CONTINUUM MECHANICS OF THE MOTION OF A PHASE INTERFACE[1]

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

ABSTRACT. A recent series of papers [G,AG,GS] began an investigation whose goal is a thermomechanics of two-phase continua based on Gibbs's notion of a sharp phase-interface endowed with thermomechanical structure. In [G] a new balance law, balance of capillary forces, was introduced and then applied in conjunction with suitable statements of the first two laws of thermodynamics; the chief results are thermodynamic restrictions on constitutive equations, exact and approximate free-boundary conditions at the interface, and a heirarchy of free-boundary problems. [AG] applied this theory to perfect conductors, in which the underlying equations reduce to a single evolution equation for the interface. [G] and [AG] were limited to rigid systems; [GS] extends the theory to include bodies that deform as they solidify or melt. These theories involve several new concepts, examples being: the creation of new material points; work intrinsic to a moving interface; the formulation of conservation laws for a moving interface. Here I shall discuss some of the new ideas involved in [GS].

MECHANICS AND ENERGETICS OF DEFORMING, ACCRETING CRYSTALS. In [GS],[2] the body, ostensibly a crystal, is allowed:

[1]Supported by the U. S. Army Research Office.

[2][GS] was motivated by studies of Leo and Sekerka [LS], Alexander and Johnson [AJ,JA], and Larche and Cahn [LC], which derive *equilibrium* relations for the crystal surface as Euler-Lagrange equations corresponding to a stationary global Gibbs function. Such derivations are appropriate to statics but tend to obscure the fundamental nature of balance laws as *basic axioms* in any dynamical framework which includes inertia and dissipation.

(i) to crystallize through the addition or deletion of material points at the crystal surface, a process termed *accretion;*
(ii) to *deform.*

In conjunction with these kinematical processes, *two distinct force systems are introduced:*

(i) a system of *accretive forces* which acts within the crystal lattice to drive the crystallization process;
(ii) a system of *deformational forces* to be identified with the more or less standard forces that act in response to the local motion of material points.

Because of the nonclassical nature of accretive forces, it is not at all clear that there should be an accompanying balance law, let alone what it should be and how it should relate to the deformational system. For that reason the underlying mechanical balance laws are derived from the requirement that the *mechanical production* - the rate of kinetic energy minus the rate of working - be independent of the observer. Here it is necessary to introduce a new idea, that of a *lattice observer:* in addition to the standard observer who measures the gross velocities of the continuum, *there is a second observer,*[3] *who studies the lattice and measures the velocity of the accreting crystal surface.* This proceedure leads, not only to the "standard" balance laws for linear and angular momentum, but to new laws expressing balance of (micro)forces and (micro)moments within the crystal lattice at the crystal surface.

One of the chief differences between theories involving phase transitions and the more classical theories of continuum mechanics is the creation and deletion of material points as the phase interface moves relative to the underlying material. We associate with this process internal forces whose working provides an outflow of "mechanical energy" associated with the attachment and release of atoms as they are exchanged between phases. We write an energy balance relating these internal forces, the forces

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

described previously, and the bulk energy of the two phases at the crystal surface.

COHERENT CRYSTAL-CRYSTAL INTERACTIONS. To illustrate the results of the general theory,[4] consider an isothermal crystal-crystal interaction,[5] in which the environment consists of a second solid phase of the crystal material, and in which the reference lattices can be chosen to match exactly at the interface, even though the states of stress and deformation will generally differ across the interface. For such an interface **balance of linear momentum** has the form

$$\mathrm{div}_{\mathcal{S}}\,\mathbb{S} + (\mathbf{S}_\beta - \mathbf{S}_\alpha)\mathbf{n} = \rho v(\mathbf{v}_\alpha - \mathbf{v}_\beta), \qquad \text{(LM)}$$

while the accretive laws for force and energy may be combined to form a single **accretive balance law**

$$\begin{aligned} \Psi_\beta - \Psi_\alpha \;=\; & (\mathbf{S}_\beta \mathbf{n})\cdot(\mathbf{F}_\beta \mathbf{n}) - (\mathbf{S}_\alpha \mathbf{n})\cdot(\mathbf{F}_\alpha \mathbf{n}) + \\ & \tfrac{1}{2}\rho v^2\{|\mathbf{F}_\alpha \mathbf{n}|^2 - |\mathbf{F}_\beta \mathbf{n}|^2\} + \\ & \pi - \sigma\kappa - \mathrm{div}_{\mathcal{S}}\,\mathbb{C} + (\mathbf{F}^{\mathrm{T}}\mathbb{S})\cdot\mathbb{L}. \end{aligned} \qquad \text{(AB)}$$

Here α and β identify the two phases; $\mathbf{S}$, $\mathbf{v}$, Ψ, and $\mathbf{F}$ (appropriately labelled) designate the bulk Piola-Kirchhoff stress, the bulk velocity, the bulk free energy, and the bulk deformation gradient; ρ is the common referential density of the two phases; σ, $\mathbb{S}$, $\mathbb{C}$ and π are the surface tension, the interfacial Piola-Kirchhoff stress, the accretive shear, and the normal attachment force; $\mathbf{n}$ is the outward unit normal to phase α; v, $\mathbb{L}$, κ, and $\mathrm{div}_{\mathcal{S}}$ are the normal velocity, the curvature tensor, twice the mean curvature, and the surface divergence for the interface.

The balance laws (LM) and (AB) are general relations, independent of the particular material under consideration. [GS] gives a thermodynamic argument in support of the interfacial

[4] [GS] also derives equations for a solid crystal in a liquid melt.

[5] Cf. Larche and Cahn [LC].

constitutive equations

$$\begin{aligned} \sigma &= \hat{\psi}(\mathbb{F},\mathbf{n}), \\ \mathbb{S} &= \partial_{\mathbb{F}}\hat{\psi}(\mathbb{F},\mathbf{n}), \\ \mathbf{c} &= -D_{\mathbf{n}}\hat{\psi}(\mathbb{F},\mathbf{n}), \\ \pi &= \beta(\mathbb{F},\mathbf{n})v, \end{aligned} \qquad \text{(CE)}$$

where $\hat{\psi}(\mathbb{F},\mathbf{n})$ is a constitutive function for the interfacial free energy, $\mathbb{F}$ is the tangential deformation gradient, $D_{\mathbf{n}}$ is the derivative with respect to $\mathbf{n}$ following the interface, and $\beta(\mathbb{F},\mathbf{n}) \geq 0$ is a material function.

Note added: The accretive balance law (AB), for the special case in which $\sigma = 0$, $\mathbb{S} = 0$, $\mathbf{c} = 0$, $\pi = \beta v$, was discovered independently and earlier by Abeyaratne and Knowles (On the driving traction on the surface of a strain discontinuity, Forthcoming).

REFERENCES.

[AG] Angenent, S. and M. E. Gurtin, Multiphase thermomechanics with interfacial structure. 2. Evolution of an isothermal interface. Arch. Rational Mech. Anal., forthcoming.

[AJ] Alexander, J. I. D. and W. C. Johnson, Thermomechanical equlibrium in solid-fluid systems with curved interfaces. J. Appl. Phys. **58**, 816-824 (1985).

[G] Gurtin, M. E., Multiphase thermomechanics with interfacial structure. 1. Heat conduction and the capillary balance law. Arch. Rational Mech. Anal. **104**, 195-221 (1988).

[GS] Gurtin, M. E. and A. Struthers, Multiphase thermomechanics with interfacial structure. 3. Evolving phase boundaries in the presence of bulk deformation, In preparation.

[JA] Johnson, W. C. and J. I. D. Alexander, Interfacial conditions for thermomechanical equlibrium in two phase crystals. J. Appl. Phys. **59**, 2735-2746 (1986).

[LC] Larche, F. C. and J. W. Cahn, Thermomechanical equilibrium of multiphase solids under stress, Acta Met. **26**, 1579-1589 (1978).

[LS] Leo, P. H. and R. F. Sekerka, The effect of surface stress on crystal-melt and crystal-crystal equilibrium, forthcoming.