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DYNAMICS OF EVOLVING PHASE BOUNDARIES IN DEFORMABLE CONTINUA

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Introduction.

Recent studies of Gurtin [8, 9, 10], Angenent and Gurtin [4], and Gurtin and Struthers [15] form an investigation whose goal is a *nonequilibrium* thermomechanics of two-phase continua in which the interface is sharp and endowed with energy, entropy and superficial force. In all of these studies except the last the crystal is *rigid*, an assumption that forms the basis for a large class of problems discussed by material scientists, but there are situations in which deformation is the paramount concern, examples being shock-induced transformations and mechanical twinning. Here I discuss the results of Gurtin and Struthers,(1) who consider *deformable* crystal-crystal systems with coherent interface.

(1) This study was motivated by papers of Cahn [5], Mullins [18,19], Cahn and Larche [6], Alexander and Johnson [3,16], and Leo and Sekerka [17], all of whom consider deformable media and derive equilibrium balance laws for the interface as Euler-Lagrange equations for a global Gibbs function to be stationary.

Force Systems. Energy. Invariance.

One of the chief differences between theories involving phase transitions and the more classical theories of continuum mechanics is the presence of *accretion*, the creation and deletion of material points as the phase interface moves relative to the underlying material, and the interplay between accretion and deformation leads to conceptual difficulties. Three force systems are needed:(2) *deformational forces* that act in response to the motion of material points; *accretive forces* that act within the crystal lattice to drive the crystallization process; *attachment forces* associated with the attachment and release of atoms as they are exchanged between phases.

Because of the nonclassical nature of these force systems, it is not at all clear whether there should be additional balance laws, let alone what they should be and how they should relate to the classical momentum balance laws. For that reason *most considerations of this nature are based on invariance*. A new idea, that of *lattice observers*, is introduced: these observers study the crystal lattice and measure the velocity of the accreting crystal surface; they act in addition to the standard *spatial observers*, who measure the gross velocities of the continuum.

The work [15] is devoted entirely to the physics of the phase interface,(3) and for that reason infinitesimally thin control volumes are used; such control volumes contain a portion of the interface plus the immediately adjacent bulk material. A basic ingredient of the theory is the *mechanical production* (the outflow of kinetic energy minus the expended power) associated with a control volume. The first law of thermodynamics requires that this production be balanced by the addition of heat and by changes in the internal energy; since heat and energy are invariant quantities, it seems reasonable to presume

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(2) That more than one force system is needed is clear from a discussion of Cahn [5], who writes: "solid surfaces can have their physical area changed in two ways, either by creating or destroying surface without changing surface structure and properties per unit area, or by an elastic strain ...... along the surface keeping the number of surface lattice sites constant while changing the form, physical area and properties" (cf. Gibbs [7] pp. 314 – 331).

(3) The basic equations satisfied by the bulk material are the standard equations of a one-phase material and can be found, e.g., in [11].

that the mechanical production itself be invariant. This invariance is used to derive several important results: invariance under changes in the kinetic description of the interface reduces the tangential part of the total accretive stress to a *surface tension*; invariance under changes in spatial and lattice observer yields the mechanical balance laws of the theory. This latter use of invariance is highly nontrivial; it not only leads to the expected mementum balance laws for the surface, it leads to *additional force and moment balance laws for the accretive system*.

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

Constitutive theory.

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

$$(1)\qquad \psi = \widehat{\psi}(\mathsf{F}, \mathbf{n})$$

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

$$(2)\qquad \mathbf{S} = \partial_{\mathsf{F}}\widehat{\psi}(\mathsf{F}, \mathbf{n}), \qquad \mathbf{c} = -D_{\mathbf{n}}\widehat{\psi}(\mathsf{F}, \mathbf{n}),$$

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

$$\pi = k + \Psi + bv, \qquad b = \hat{b}(\mathbf{F}, \mathbf{n}, v, \mathbf{z}) \geq 0, \tag{3}$$

where Ψ is the difference in bulk energies, while k is related to changes in momentum and kinetic energy across the interface. These results imply that the sole source of dissipation is the exchange of atoms between phases, with bv^2 the dissipation per unit interfacial area.

Interface conditions.

The system of constitutive equations and balance laws combine to give the interface conditions(4)

$$\begin{aligned} &div_{\mathcal{S}}\mathbf{S} + (\mathbf{S}_2 - \mathbf{S}_1)\mathbf{n} = \rho v(\mathbf{v}_1 - \mathbf{v}_2), \\ &\Psi_1 - \Psi_2 = (\mathbf{S}_1\mathbf{n}) \cdot (\mathbf{F}_1\mathbf{n}) - (\mathbf{S}_2\mathbf{n}) \cdot (\mathbf{F}_2\mathbf{n}) - k - g - bv, \end{aligned} \tag{4}$$

with

$$\begin{aligned} k &= \frac{1}{2}\rho v^2\{|\mathbf{F}_1\mathbf{n}|^2 - |\mathbf{F}_2\mathbf{n}|^2\} \\ g &= -\psi\kappa - div_{\mathcal{S}}\mathbf{c} + (\mathbf{F}^T\mathbf{S}) \cdot \mathbf{L}. \end{aligned} \tag{5}$$

The subscripts 1 and 2 denote the two phases: Ψ_1 and Ψ_2 are the bulk energies per unit reference volume; $\mathbf{S}_1$ and $\mathbf{S}_2$ are the bulk Piola-Kirchhoff stresses; $\mathbf{F}_1$ and $\mathbf{F}_2$ are the bulk deformation gradients; $\mathbf{v}_1$ and $\mathbf{v}_2$ are the material velocities; ρ is the reference

(4) For statical situations: $(4)_1$ was derived by Gurtin and Murdoch [14] as a consequence of balance of forces; $(4)_2$ and its counterpart for crystal-melt interactions were derived by Leo and Sekerka [17] (cf. Johnson and Alexander [3,16]) as Euler-Lagrange equations for stable equilibria. In the absence of surface stress and surface energy ($\mathbf{S} = 0, \mathbf{c} = 0, \psi = 0$): $(4)_1$ is a standard shock relation; $(4)_2$ (with $b \neq 0$) was established by Abeyaratne and Knowles [2] and Truskinovsky [20]. Counterparts of (4) for a rigid crystal in an inviscid melt were derived in [17]; an analog of $(4)_2$ for a rigid system was given in [10].

density. The remaining quantities concern the interface: **L** is the curvature tensor with κ, its trace, the total curvature; $div_{\mathcal{S}}$ is the surface divergence.

The theory of [15] is generalized to include thermal influences, but I will not discuss these results here.

Simplified equations(5).

Assume that both phases are isotropic with *linearized* stress-strain relations in each phase, and neglect all interfacial terms with the exception of the dissipative term bv in (4). Then for *longitudinal motions* with scalar displacement $u(x,t)$ and scalar tensile stress $\sigma(x,t)$ the basic equations are(6) the bulk equations

$$(phase\ 1) \qquad c_1^2 u_{xx} = u_{tt}, \quad \sigma = \beta_1 u_x, \quad \psi = \frac{1}{2}\beta_1 u_x^2$$

$$(phase\ 2) \qquad c_2^2 u_{xx} = u_{tt}, \quad \sigma = \sigma_0 + \beta_2 u_x, \quad \psi = \psi_0 + \sigma_0 u_x + \frac{1}{2}\beta_2 u_x^2$$

and the interface conditions

$$[\sigma] = -\rho v[u_t], \qquad [u_t] = -v[u_x],$$
$$[\psi] = \langle\sigma\rangle[u_x] + bv,$$

where $c_i^2 = \beta_i/\rho$ with β_i the elastic moduli; σ_0 and ψ_0 are constants; [ ] denotes the jump across the interface; $\langle\rangle$ designates the average interfacial value.

For *antiplane shear* with scalar displacement $u(x,y,t)$ and shear-stress vector $\mathbf{T}(x,y,t)$ the basic equations are the bulk equations

$$(phase\ 1) \qquad s_1^2\Delta u = u_{tt}, \mathbf{T} = \mu_1\nabla u, \qquad \psi = \frac{1}{2}\mu_1|\nabla u|^2$$

$$(phase\ 2) \quad s_2^2\Delta u = u_{tt}, \quad \mathbf{T} = \mathbf{T}_0 + \mu_1\nabla u, \ \psi = \psi_0 + \mathbf{T}_0\cdot\nabla u + \frac{1}{2}\mu_2|\nabla u|^2$$

(5) Cf. [13]
(6) Cf. Abeyaratne and Knowles [2], whose treatment is slightly different.

and the interface conditions

$$[\mathbf{T}]\cdot\mathbf{n} = \rho v^2[\nabla u]\cdot\mathbf{n}, \qquad [u_t] = -v[\nabla u]\cdot\mathbf{n}\,,$$
$$[\psi] = \langle\mathbf{T}\rangle\cdot\mathbf{n}([\nabla u]\cdot\mathbf{n}) + bv\,,$$

where Δ is the laplacian; $s_i^2 = \mu_i/\rho$ with μ_i the shear moduli; $\mathbf{T}_0$ and ψ_0 are constants.

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