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Evolving Phase Boundaries in Deformable Continua

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ABSTRACT. Recently, Gurtin and Struthers [2] developed a dynamical theory of phase transitions in crystal-crystal systems in which the interface is sharp, coherent, and endowed with energy, entropy, and superficial force. A fundamental conceptual ingredient of the theory is the use of three force systems: *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. Here I will discuss the main results of the theory, which are constitutive equations and balance laws for the interface.

CONSTITUTIVE THEORY. The surface energy and the accretive and deformational surface stresses are allowed to depend on the bulk deformation gradient $\mathbf{F}$, the normal $\mathbf{n}$ to the interface, the normal speed v of the interface, and a list z of subsidiary variables of lesser importance. It follows, as a consequence of thermodynamic admissibility, 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 $\boldsymbol{F}$; in fact, the energy

$$\psi = \hat{\psi}(\boldsymbol{F}, \mathbf{n}) \tag{1}$$

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

$$\boldsymbol{S} = \partial_{\boldsymbol{F}}\hat{\psi}(\boldsymbol{F}, \mathbf{n}), \qquad \boldsymbol{c} = -D_{\mathbf{n}}\hat{\psi}(\boldsymbol{F}, \mathbf{n}), \tag{2}$$

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

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

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[1]

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

with

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

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

SIMPLIFIED EQUATIONS.[2] 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[3] the bulk equations

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

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

and the interface conditions

$$
\begin{aligned} [\sigma] = -\rho v[u_t], \qquad [u_t] = -v[u_x], \\ [\psi] = \langle\sigma\rangle[u_x] + bv, \end{aligned}
$$

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.

---

[1] For statical situations: $(4)_1$ was derived by Gurtin and Murdoch [6] as a consequence of balance of forces; $(4)_2$ and its counterpart for crystal-melt interactions were derived by Leo and Sekerka [5] (cf. Johnson and Alexander [3,4]) as Euler-Lagrange equations for stable equilibria. In the absence of surface stress and surface energy ($\boldsymbol{S} = 0, \boldsymbol{c} = 0, \psi = 0$): $(4)_1$ is a standard shock relation; $(4)_2$ (with $b \neq 0$) was established by Abeyaratne and Knowles [7] and Truskinovsky [11]. Counterparts of (4) for a rigid crystal in an inviscid melt were derived in [8]; an analog of $(4)_2$ for a rigid system was given in [1].

[2] Cf. [9]

[3] Cf. Abeyaratne and Knowles [10], whose treatment is slightly different.

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

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

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

and the interface conditions

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

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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