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Two-Phase Continuum Mechanics with Mass Transport and Stress

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TWO-PHASE CONTINUUM MECHANICS WITH MASS TRANSPORT AND STRESS.

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1. Introduction.

There are multiphase processes that are essentially isothermal with kinetics driven by mass transport and stress, an example being coarsening or Ostwald ripening, in which a phase, quenched into a metastable state, exibits late-stage kinetics characterized by the dissolution of second-phase domains with large interfacial curvature at the expense of domains with low interfacial curvature. In [1] we developed a continuum-mechanical framework within which such processes can be discussed. We here discuss the results of [1].

We consider a two-phase system consisting of bulk regions separated by a sharp interface endowed with energy and capable of supporting force, following — and in certain respects generalizing — the framework set out in [2-5]. We base our discussion on balance laws for mass and force in conjunction with a version of the second law appropriate to a mechanical system out of equilibrium. We assume that mass transport is characterized by the bulk diffusion of a *single* independent species; we neglect mass diffusion within the interface.

2. Theory without deformation.

We neglect deformation and bulk stress, but allow the diffusion potential (chemical potential) to be discontinuous across the interface. We develop a heirarchy of free-boundary problems at various levels of approximation, framed in terms of the departure $u = \mu - \mu_0$ of the diffusion potential μ from the transition potential μ_0, which is the potential at which the phase change would occur were interfacial structure neglected. For small departures from μ_0 the basic system of equations, neglecting diffusional transients, consists of a PDE in bulk supplemented by three interface conditions. The PDE has the form

$$\operatorname{div} \mathbf{h} = 0, \tag{1}$$

where $\mathbf{h}$, the mass flux, is given by

$$\begin{aligned} \mathbf{h} &= -\mathbf{D}_\alpha \nabla u \qquad \text{in phase } \alpha, \\ \mathbf{h} &= -\mathbf{D}_\beta \nabla u \qquad \text{in phase } \beta, \end{aligned} \tag{2}$$

with $\mathbf{D}_\alpha$ and $\mathbf{D}_\beta$ constant mobility tensors. The first interface condition is balance of mass

$$\mathbf{h}^- \cdot \boldsymbol{\nu} - AV = \mathbf{h}^+ \cdot \boldsymbol{\nu} - BV \equiv J, \tag{3}$$

in which $\mathbf{h}^-$ and $\mathbf{h}^+$, respectively, represent the limits of $\mathbf{h}$ from the α and β phases, A and B are constants representing the density in the α and β phases at the potential μ_0, $\boldsymbol{\nu}$ is the unit normal to the interface directed out of phase α, and V is the normal velocity of the interface. The second interface condition, essentially constitutive, characterizes the net mass flux J *defined* in (3):

$$J = -b_{21}(\boldsymbol{\nu})V - b_{22}(\boldsymbol{\nu})[\mathbf{u}], \tag{4}$$

where $b_{21}(\boldsymbol{\nu})$ and $b_{22}(\boldsymbol{\nu})$ are constitutive moduli, while $[\;]$ (in boldface) denotes the jump across the interface (β minus α). The third interface condition generalizes the classical "Gibbs-Thomson relation" to situations in which the chemical potential is discontinuous across the interface:

$$Bu^+ - Au^- = f(\boldsymbol{\nu})K + \operatorname{div}_\Delta \mathbf{c}(\boldsymbol{\nu}) - b_{11}(\boldsymbol{\nu})V - b_{12}(\boldsymbol{\nu})[\mathbf{u}], \tag{5}$$

where $f(\nu)$ is the interfacial energy,

$$c(\nu) = -\partial_\nu f(\nu) \tag{6}$$

is the surface shear, $b_{11}(\nu)$ and $b_{12}(\nu)$ are constitutive moduli, and $\mathrm{div}_{\mathcal{S}}$ is the surface divergence.

We also establish global growth relations for solutions of the underlying equations. In particular, solutions of the quasi-static equations (1)-(6) consistent with the boundary condition

$$h \cdot n = 0 \quad \text{on} \quad \partial\Omega \tag{7}$$

satisfy

$$\mathrm{vol}(\Omega_\alpha)^{\cdot} = 0, \qquad \Big\{\int_{\mathcal{S}} f(\nu)\,da\Big\}^{\cdot} \le 0. \tag{8}$$

Here $\Omega_\alpha(t)$ is the region occupied by phase α, while $\mathcal{S}(t) = \partial\Omega_\alpha(t)$ represents the interface. The relations (8) yield a formal justification for the statical *Wulff problem,* which, in the present context, is to

$$\textit{minimize} \quad \int_{\mathcal{S}} f(\nu)\,da \tag{9}$$

over all interfaces $\mathcal{S} = \partial\Omega_\alpha$ with $\mathrm{vol}(\Omega_\alpha)$ prescribed.

3. Theory with deformation and bulk diffusion.

We include deformation and stress, but limit our discussion to a continuous potential and to a coherent interface. In addition, we consider only infinitesimal deformations, neglecting inertia. We derive a quasi-static theory analogous to (1)-(6). The bulk equations of this theory are

$$\operatorname{div} T = 0, \qquad \operatorname{div} h = 0 \tag{10}$$

supplemented by (2), where T, the stress, is given by the stress-strain relations

$$\begin{aligned} T &= L_\alpha[E - E_{0\alpha}] \quad \text{in phase } \alpha, \\ T &= L_\beta[E - E_{0\beta}] \quad \text{in phase } \beta, \end{aligned} \tag{11}$$

with L_α and L_β the (constant) elasticity tensors,

$$E = \tfrac{1}{2}(\nabla u + \nabla u^T) \tag{12}$$

the strain tensor, and $E_{0\alpha}$ and $E_{0\beta}$ the (constant) stress-free strains in phases α and β. The corresponding interface conditions are

$$\begin{aligned} \ell u &= [W(E - E_0)] - T\nu\cdot[\nabla u]\nu + f(\nu)K + \operatorname{div}_\mathcal{S} c(\nu) - b(\nu)V, \\ \ell V &= [h]\cdot\nu, \qquad\qquad [T]\nu = 0, \end{aligned} \tag{13}$$

where $W(E - E_0)$ is the strain energy, defined, e.g., in phase α by $\tfrac{1}{2}[E - E_{0\alpha}]\cdot L_\alpha[E - E_{0\alpha}]$, $b(\nu)$ is a constitutive modulus, and ℓ is a constant. We consider solutions of (10)-(13) consistent with (7) and the dead-load condition

$$u^\cdot = 0 \text{ on a portion } U \text{ of } \partial\Omega, \quad Tn = T^*n \text{ on the remainder}, \tag{14}$$

with T^* (=constant) prescribed, where Ω, with outward unit normal n, is the fixed region of space occupied by the body. We prove that such solutions satisfy the global growth relations

$$\begin{aligned} &\operatorname{vol}(\Omega_\alpha)^\cdot = 0, \\ &\Big\{\int_\Omega \{W(E - E_0) - T^*\cdot(E - E_0)\}dv + \int_\mathcal{S} f(\nu)da\Big\}^\cdot \le 0, \end{aligned} \tag{15}$$

relations that suggest the following variational problem: given $\mathrm{vol}(\Omega_\alpha)$ and boundary displacements $\mathbf{g}(\mathbf{x})$ on $\mathcal{U}$,

$$\textit{minimize} \quad \int_\Omega \{W(\mathbf{E}-\mathbf{E}_0)-\mathbf{T}^*\cdot(\mathbf{E}-\mathbf{E}_0)\}\,dv + \int_{\mathcal{S}} f(\mathbf{n})\,da \tag{16}$$

over all interfaces $\mathcal{S}=\partial\Omega_\alpha$ and all displacement fields $\mathbf{u}$ that are continuous across $\mathcal{S}$ and satisfy $\mathbf{u}=\mathbf{g}$ on $\mathcal{U}$. This problem — a natural generalization of the Wulff problem — is purely mechanical: the diffusion potential is not involved.

We also discuss a quasi-linear theory in which the elliptic equations (2), $(10)_2$ are replaced by parabolic equations. This theory leads to the following variational problem, in which the diffusion potential plays an important role:

minimize

$$\mathbf{T}^*\cdot[\mathbf{E}_0]\mathrm{vol}(\Omega_\alpha) + \int_\Omega \{W(\mathbf{E}-\mathbf{E}_0)-\mathbf{T}^*\cdot(\mathbf{E}-\mathbf{E}_0)+Cu^2\}\,dv + \int_{\mathcal{S}} f(\boldsymbol{\nu})\,da \tag{17}$$

subject to

$$-[\Lambda]\mathrm{vol}(\Omega_\alpha) + \int_\Omega \{2Cu+\mathbf{G}\cdot(\mathbf{E}-\mathbf{E}_0)\}\,dv = m_0$$

over all interfaces $\mathcal{S}=\partial\Omega_\alpha$ and all displacement fields $\mathbf{u}$ that are continuous across $\mathcal{S}$ and satisfy $\mathbf{u}=\mathbf{g}$ on $\mathcal{U}$. Here C is a constitutive modulus having values C_α and C_β in phases α and β, while m_0 is a prescribed constant.

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