Evolving phase boundaries in deformable continua

Morton E. Gurtin
Carnegie Mellon University
NOTICE WARNING CONCERNING COPYRIGHT RESTRICTIONS:
The copyright law of the United States (title 17, U.S. Code) governs the making
of photocopies or other reproductions of copyrighted material. Any copying of this
document without permission of its author may be prohibited by law.
Evolving Phase Boundaries in Deformable Continua

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

Research Report No. 91-NA-008

September 1991
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 \( F \), the normal \( n \) 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 \( F \) at most through the tangential deformation gradient \( \tilde{F} \); in fact, the energy

\[
\psi = \tilde{\psi}(F, n)
\]

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

\[
S = \partial_F \tilde{\psi}(F, n), \quad c = -D_n \tilde{\psi}(F, n),
\]

in which \( S \) is the deformational (Piola-Kirchhoff) surface stress, \( c \) is the normal accretive stress, \( \partial_F \) 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 thermodynamics is an explicit expression for the normal attachment force \( \pi \):

\[
\pi = k + \Psi + bv, \quad b = \tilde{b}(F, n, v, z) \geq 0,
\]

where \( \Psi \) 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

\[ \text{div}_S S + (S_2 - S_1)n = \rho v(v_1 - v_2), \]

\[ \Psi_1 - \Psi_2 = (S_1 n) \cdot (F_1 n) - (S_2 n) \cdot (F_2 n) - k - g - bv, \]

with

\[ k = \frac{1}{2} \rho v^2 \{|F_1 n|^2 - |F_2 n|^2\}, \]

\[ g = -\psi \kappa - \text{div}_S \varepsilon + (F^T S) \cdot L. \]

The subscripts 1 and 2 denote the two phases: \( \Psi_1 \) and \( \Psi_2 \) are the bulk energies per unit reference volume; \( S_1 \) and \( S_2 \) are the bulk Piola-Kirchhoff stresses; \( F_1 \) and \( F_2 \) are the bulk deformation gradients; \( v_1 \) and \( v_2 \) are the material velocities; \( \rho \) is the reference density. The remaining quantities concern the interface: \( L \) is the curvature tensor with \( \kappa \), its trace, the total curvature; \( \text{div}_S \) is the surface divergence.

SIMPLIFIED EQUATIONS. 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

\[
\begin{align*}
(\text{phase 1}) & \quad c_1^2 u_{xx} = u_{tt}, \quad \sigma = \beta_1 u_x, \quad \psi = \frac{1}{2} \beta_1 u_x^2 \\
(\text{phase 2}) & \quad c_2^2 u_{xx} = u_{tt}, \quad \sigma = \sigma_0 + \beta_2 u_x, \quad \psi = \psi_0 + \sigma_0 u_x + \frac{1}{2} \beta_2 u_x^2
\end{align*}
\]

and the interface conditions

\[
[\sigma] = -\rho v[u_1], \quad [u_1] = -v[u_x], \quad [\psi] = \langle \sigma \rangle [u_x] + bv,
\]

where \( c_i^2 = \beta_i/\rho \) with \( \beta_i \) the elastic moduli; \( \sigma_0 \) and \( \psi_0 \) are constants; \( [\cdot] \) denotes the jump across the interface; \( \langle \cdot \rangle \) 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 \( (S = 0, c = 0, \psi = 0) \): (4)\(_1\) is a standard shock relation; (4)\(_2\) (with \( b \neq 0 \)) was established by Abeyaratne and Knowles [7] and Truskinovskiy [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 $T(x, y, t)$ the basic equations are the bulk equations

(phase 1) \[ s_1^2 \Delta u = u_{tt}, \quad T = \mu_1 \nabla u, \quad \psi = \frac{1}{2} \mu_1 |\nabla u|^2 \]

(phase 2) \[ s_2^2 \Delta u = u_{tt}, \quad T = T_0 + \mu_1 \nabla u, \quad \psi = \psi_0 + T_0 \cdot \nabla u + \frac{1}{2} \mu_2 |\nabla u|^2 \]

and the interface conditions

\[
[T] \cdot n = \rho v^2 [\nabla u] \cdot n, \quad [u_t] = -v [\nabla u] \cdot n, \\
[\psi] = (T) \cdot n ([\nabla u] \cdot n) + b v,
\]

where $\Delta$ is the laplacian; $s_i^2 = \mu_i/\rho$ with $\mu_i$ the shear moduli; $T_0$ and $\psi_0$ are constants.

Acknowledgment. The research discussed here was supported by the Army Research Office and the National Science Foundation.

REFERENCES

Nonlinear Analysis Series

No.

91-NA-001  [ ]  Lions, P.L., Jacobians and Hardy spaces, June 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-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-010  [ ]  Kinderlehrer, D. and Ou, B., Second variation of liquid crystal energy at \( \frac{x}{|x|} \), August 1991


91-NA-012  [ ]  James, R.D. and Kinderlehrer, D., Frustration and microstructure: An example in magnetostriction, November 1991

92-NA-001 [ ] Nicolaides, R.A. and Walkington, N.J., Computation of microstructure utilizing Young measure representations, 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-007 [ ] Kinderlehrer, D. and Pedregal, P., Remarks about gradient Young measures generated by sequences in Sobolev spaces, 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-012 [ ] Alama, Stanley and Li, Yan Yan, On "Multibump" Bound States for Certain Semilinear Elliptic Equations, 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(Ω,RP) for Integrands f(x,u,∇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-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-028 [ ] Tarantello, Gabriella, Multiplicity Results for an Inhomogenous Neumann Problem with Critical Exponent, August 1992


92-NA-030 [ ] Brandon, Deborah and Rogers, Robert C., Nonlocal Superconductivity, July 1992


92-NA-032 [ ] Spruck, Joel and Yang, Yisong, Cosmic String Solutions of the Einstein-Matter-Gauge Equations, September 1992

<table>
<thead>
<tr>
<th></th>
<th>Title</th>
</tr>
</thead>
<tbody>
<tr>
<td>92-NA-034</td>
<td>Leo, Perry H. and Herng-Jeng Jou, <em>Shape evolution of an initially circular precipitate growing by diffusion in an applied stress field</em>, October 1992</td>
</tr>
<tr>
<td>92-NA-036</td>
<td>Katsoulakis, Markos, Kossioris, Georgios T. and Retich, Fernando, <em>Generalized motion by mean curvature with Neumann conditions and the Allen-Cahn model for phase transitions</em>, October 1992</td>
</tr>
<tr>
<td>92-NA-038</td>
<td>Yang, Yisong, <em>Self duality of the Gauge Field equations and the Cosmological Constant</em>, November 1992</td>
</tr>
</tbody>
</table>

**Stochastic Analysis Series**

<table>
<thead>
<tr>
<th></th>
<th>Title</th>
</tr>
</thead>
</table>