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PLANAR MOTION OF AN ANISOTROPIC INTERFACE

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1. BACKGROUND. THE ANISOTROPIC EVOLUTION EQUATION

There are situations of interest for which the motion of a phase interface is essentially independent of the behavior of the corresponding bulk phases. One of the first to model such motions was Mullins [Mu], who introduced the *curve-shortening equation*

$$V = K \tag{1}$$

to study the *planar* motion of grain boundaries. Here V is the normal velocity, with positive normal-direction outward from the boundary $\partial\Omega$ of the grain $\Omega = \Omega(t)$, and K is the curvature, with $K < 0$ when $\partial\Omega$ is a circle. The curve-shortening equation is a parabolic PDE with a large literature (cf. Brakke [Br], Sethian [Se], Abresch and Langer [AL], Gage and Hamilton [GH], Grayson [Gr], Osher and Sethian [OS], Evans and Spruck [ES1-3], Chen, Giga, and Goto [CGG], Giga and Sato [GS], Almgren, Taylor, and Wang [ATW], Taylor, Cahn, and Handwerker [TCH]). As shown by Gage and Hamilton [GH] and Grayson [Gr], a boundary curve with evolution governed by (1), and of arbitrary initial shape, shrinks to a point in finite time, with asymptotic shape a circle.

The curve-shortening equation also arises as an approximation to the Landau-Ginzburg equation, a result established formally by Allen and Cahn [AC] and Rubinstein, Sternberg, and Keller [RSK], and then rigorously by Barles, Soner, and Souganides [BSS], Evans, Soner, and Souganides [ESS], Chen [Ch], and DeMottoni and Schatzman [DS].

Mullins's theory was generalized by Gurtin [Gl] and Angenent and Gurtin [AG1] to include anisotropy and the possibility of a difference in bulk energies between phases. The resulting equation is

$$b(e)V \ll g(e)K - U, \tag{2}$$

where ©, the normal-angle, is the counterclockwise angle from a fixed axis to the outward normal of dQ. Here

$$g(e) - f(e) + f'(e) \tag{3}$$

with $f(©)>0$ the interfacial energy; U is the relative energy of the material in Q; and $b(©)>0$, the kinetic modulus, is a material function. The presence of the angle *B* reflects anisotropy, and the particular form in which f appears in (3) is a consequence of thermodynamics. In fact, a consequence of (2) and (3) is the thermodynamic inequality

$$(d/dt)\{\int_{\partial Q(t)} f(e)ds + U\,\mathrm{area}(Q(t))\} \leq -\int_{\partial Q(t)} b(e)V^2 ds, \tag{4}$$

showing that $b(e)V^2$ represents the rate of energy dissipation, per unit length.

In writing (2) we have neglected the dependence of b(e) on V, a dependence not ruled out by thermodynamics and considered important by material scientists (Owen, Schoen, and Srinivasan [OSS], Hillert [Hi]). The behavior of (2) with b(e) replaced by $b(©,V)>0$ remains an open problem.

2. BACKWARD PARABOLICITY. CORNERS, FACETS, AND WRINKLINGS

When

$$g(e) > 0, \tag{5}$$

(2) is parabolic, and the underlying behavior, which is not much different than that for V=K, is well understood (Angenent [Ag], Chen, Giga, and Goto

[CGG], Soner [So], Barles, Soner, and Souganidis [BSS]). What makes (2) nonstandard is the possibility of interfacial energies that satisfy

$$g(\theta) < 0 \tag{6}$$

for certain ranges of the angle θ, for in these ranges the evolution equations are *backward parabolic*. Such energies are not mathematical curiosities: material scientists give strong arguments in support of interfacial energies that satisfy $g(\theta)<0$ for some values of θ (Gjostein [Gj], Cahn and Hoffman [CH]).

Let

$$N(\theta) = (\cos\theta,\sin\theta), \quad T(\theta) = (\sin\theta,-\cos\theta), \tag{7}$$

so that T and N represent a unit tangent and normal to the interface when θ is its normal-angle. In analyzing energies with backward-parabolic angle-intervals an important concept is the **Frank diagram** $\mathcal{F}$, which is the polar diagram of $f(\theta)^{-1}$ (the curve defined in polar coordinates (r,θ) by $r = f(\theta)^{-1}$); $\mathcal{F}$ is locally strictly convex where $g(\theta) > 0$ and locally strictly concave where $g(\theta) < 0$. The importance of the Frank diagram becomes evident when one considers the homogeneous extension $\tilde{f}$ of f to $\mathbb{R}^2\backslash\{0\}$: $\tilde{f}(\alpha N(\theta)) = \alpha f(\theta)$ for all angles θ and all $\alpha > 0$. Then $\mathcal{F}$ is the one-level set of $\tilde{f}$, so that convexity properties of $\tilde{f}$ are related to those of $\mathcal{F}$. In particular, $\tilde{f}$ is convex if and only if the region enclosed by $\mathcal{F}$ is convex. Further,

$$g(\theta) = T(\theta)\cdot[\nabla\nabla\tilde{f}(N(\theta))]T(\theta), \tag{8}$$

which, to some extent, explains the form of (3).

A method of overcoming (6), introduced by Angenent and Gurtin [AG1], is to allow the interface to contain corners (jumps in angle) that exclude the backward-parabolic ranges of θ. In the presence of a corner the evolution equation (2) does not by itself characterize the motion of the interface; there is an additional condition requiring that the *capillary force*

$$C(\theta) = f(\theta)T(\theta) + f'(\theta)N(\theta) \quad \text{is continuous.} \tag{9}$$

Thus for a corner corresponding to an angle jump from θ_1 to θ_2 we must have

$$C(\theta_1) = C(\theta_2), \tag{10}$$

which has an important consequence: the tangent line to $\mathcal{F}$ at θ_1 is also a tangent line to $\mathcal{F}$ at θ_2; that is, θ_1 and θ_2 must be angles of bitangency for the Frank diagram [AG1].

Let $\mathcal{C}(\mathcal{F})$ denote the convexification of $\mathcal{F}$ (the boundary of the convex hull of $\mathcal{F}$), and let $F(\theta)$, the *convexified energy*, denote the energy whose Frank diagram is $\mathcal{C}(\mathcal{F})$, so that $f(\theta) \geq F(\theta)$. Then angles θ with $f(\theta) = F(\theta)$ satisfy $g(\theta) \geq 0$; we refer to such angles as *globally stable;* we refer to angles θ with $f(\theta) > F(\theta)$ as *globally unstable;* and we refer to each maximal interval (θ_1,θ_2) of angles θ with $f(\theta) > F(\theta)$ as a *globally unstable angle-interval.* Then each globally unstable angle-interval (θ_1,θ_2) has θ_1 and θ_2 as angles of bitangency for $\mathcal{F}$ and hence as admissible angles for a corner.

Wrinklings consisting of facets with normal angle θ_1 alternating with facets of normal angle θ_2 are solutions of (2) and (9) provided the θ_1 and θ_2 facets evolve according to $V = -U/b(\theta_1)$ and $V = -U/b(\theta_2)$, respectively. Such wrinklings evolve as a rigid body with velocity ω defined by

$$\omega \cdot N(\theta_1) = -b(\theta_1)^{-1}U, \quad \omega \cdot N(\theta_2) = -b(\theta_2)^{-1}U \tag{11}$$

[AG1]. One also has the possibility of solutions involving curved sections with globally stable normal angles separated by wrinklings.

Local well-posedness of evolutions consistent with (2) and (9) — ensuing from initial curves consisting of globally stable sections separated by appropriate corners — is established by Angenent and Gurtin [AG2].

A limitation of the procedure described above is that it is inapplicable for an initial curve $\partial\Omega(0)$ with globally unstable normal angles. The next section confronts this difficulty.

3. RELAXED EQUATION FOR INITIAL DATA WITH GLOBALLY UNSTABLE NORMAL ANGLES

Consider an initial curve $\partial\Omega(0)$ that has normal angles in a globally unstable interval (θ_1,θ_2). We formally consider Γ as being infinitesimally wrinkled, with each infinitesimal facet having either θ_1 or θ_2 as normal angle, an idea due to Cahn and Taylor (private communication with the author in 1990). The expansion

$$N(\theta) = \mu_1(\theta)N(\theta_1) + \mu_2(\theta)N(\theta_2), \qquad \theta\epsilon(\theta_1,\theta_2), \tag{12}$$

then defines, for each i, the density $\mu_i(\theta)$ of θ_i-facets at any point of Γ with normal angle θ, with $\mu_i(\theta)$ measured per unit length of Γ.

The use of infinitesimal wrinklings is formally equivalent to replacing the interfacial energy $f(\theta)$ by the convexified energy $F(\theta)$, since

$$F(\theta) = \mu_1(\theta)f(\theta_1) + \mu_2(\theta)f(\theta_2), \qquad \theta\epsilon(\theta_1,\theta_2). \tag{13}$$

A further reason for the use of such wrinklings is that the initially wrinkled curve is more stable than the original curve:

$$\int_{\partial\Omega(0)} F(\theta)ds \le \int_{\partial\Omega(0)} f(\theta)ds. \tag{14}$$

If we allow $\partial\Omega(t)$ to infinitesimally wrinkle in the same manner, we are led to the conclusion that the effective interfacial energy for the evolution should be $F(\theta)$, so that the *effective energy modulus* is given by

$$G(\theta) = F(\theta) + F''(\theta). \tag{15}$$

The next question we must answer is: What is an appropriate kinetic modulus for the infinitesimally wrinkled curve? As noted in the paragraph containing (11), if $\Gamma(t)$ is a finite wrinkling whose facets have θ_1 and θ_2 as normal angles, then $\Gamma(t)$ evolves as a rigid body with constant velocity ω (although $\Gamma(t)$ may shrink or grow tangentially). Since ω depends on

the particular wrinkling only through θ_1 and θ_2, it seems reasonable to suppose that *infinitesimal wrinklings* with θ_1 and θ_2 as normal angles also evolve with rigid velocity ω, a supposition equivalent to replacing the kinetic modulus $b(\theta)$ between θ_1 and θ_2 by an effective modulus $B(\theta)$ that agrees with $b(\theta)$ at θ_1 and θ_2 and has polar diagram between θ_1 and θ_2 a straight line:

$$B(\theta)^{-1} = \mu_1(\theta)b(\theta_1)^{-1} + \mu_2(\theta)b(\theta_2)^{-1} \qquad (16)$$

We are therefore led to an *effective kinetic modulus* $B(\theta)$ for all θ: $B(\theta)>0$ is continuous; $B(\theta)=b(\theta)$ for all globally stable angles θ; the polar diagram of $B(\theta)$ is a straight line over angle intervals with $f(\theta)>F(\theta)$.

This procedure, introduced by Gurtin [G2], yields a *relaxed evolution equation*

$$B(\theta)V = G(\theta)K - U \qquad (17)$$

with B and G the effective moduli corresponding to f and g. It is important to note that:

(a) The relaxed equation coincides with the original equation (2) at globally stable angles θ.

(b) Because of the construction of $G(\theta)$, no matter how smooth $f(\theta)$ is, $G(\theta)$ *will generally be discontinuous* whenever the angle θ changes from globally stable to globally unstable; this property of $G(\theta)$ renders the relaxed evolution equation nonstandard.

(c) $G(\theta)=0$ whenever θ is globally unstable, so that (17) degenerates to hyperbolic at globally unstable angles.

The relaxed evolution equation (17) is studied by Gurtin, Soner, and Souganides [GSS]; their main results are a theorem of existence and local uniqueness and a global comparison theorem for level-set solutions, a theorem established independently and Ohnuma and Sato [OSa].

Because of the lack of continuity of G as well as the degeneracy of (17) when $G=0$, [GSS] discuss this equation within the weak framework of viscosity solutions. This approach to geometric equations, initiated by Evans and Spruck [ES1] and Chen, Giga, and Goto [CGG], and given an intrinsic form

by Soner [So] and Barles, Soner, and Souganidis [BSS], is based on the use of level sets to characterize evolving curves, an idea due to Ohta, Jasnow, and Kawasaki [OJK], Sethian [Se], Osher and Sethian [OS], and Barles [Ba]. The difficulties concerning (17) result from the *discontinuous* nature of G; the degeneracy of the equation at angles θ with $G(\theta)=0$ causes no great difficulty; were G continuous, most of the results would follow from those in [CGG].

[GSS] establishes the following results of physical interest:

(1) Viscosity solutions of (17) not only satisfy (2) away from corners, but, what is most interesting, such solutions automatically satisfy the force balance (11) across corners.

(2) If (θ_1,θ_2) is a globally unstable angle-interval, then, as shown by [AG1], a wedge whose sides have normal angles θ_1 and θ_2 and evolve according to $b(\theta_1)V=-U$ and $b(\theta_2)V=-U$, respectively, is a solution of the basic equations (2) and (9). [GSS] shows that the foregoing choice of the effective moduli G and B is the only possible choice if all such wedges are to be viscosity solutions of (17).

(3) For $U<0$ and for the initially enclosed region Ω_0 large enough, $t^{-1}\Omega(t)$ converges to a dilation of the Wulff region for $1/B(\theta)$, a result conjectured in [AG1] and proved by Soner [So] for $G>0$ and B with a convex polar diagram, and extended in [AG2] to general $B>0$.

4. FOURTH-ORDER THEORIES. REGULARIZED EVOLUTION EQUATION

Another method of analyzing behavior within the unstable range of angles is to regularize the evolution equation (2). Such a regularization, proposed in [AG1], was developed by DiCarlo, Podio-Guidugli, and Gurtin [DPG] and yields the equation

$$b(\theta)V = g(\theta)K - U - \varepsilon(K_{ss} + \tfrac{1}{2}K^3), \tag{18}$$

where s denotes arc length and $\varepsilon>0$ is a small material parameter. The chief ingredient in the derivation of (18) is a *constitutive* dependence of interfacial energy on curvature, an idea that traces back to Gibbs [Gi] and Herring [He].

The equation (18) is very much like the Cahn-Hilliard equation (cf., [CHi]), with the angle-intervals on which $g(\theta) < 0$ playing the role of spinodals. When linearized about a flat interface at angle $\theta = \pi/2$, (18) has the form

$$u_t = \alpha u_{xx} - \delta u_{xxxx} \tag{19}$$

with $\delta > 0$, but with $\alpha < 0$ when $\theta = \pi/2$ lies in a spinodal. The linear equation (19) is exactly the equation used by Cahn [Ca] in his treatment of spinodal decomposition.

A somewhat similar model (Davi and Gurtin [DG]), based on ideas of Mullins [M2], allows for heat conduction within the interface with heat flow driven by changes in curvature; granted isotropy, it leads to the fourth-order parabolic equation

$$\beta V = -\alpha K_{ss}, \tag{20}$$

with $\alpha, \beta > 0$ material constants. This equation has been used by Mullins [M2] with great success to model the formation of grooves at intersecting grains on exposed surfaces.

There are almost no analytical or numerical results for the evolution equations (18) and (20). In particular, it would be of great interest to use (18) to study the behavior of the interface within an angle interval that defines a corner of the unregularized equation (2).

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