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Motion by Curvature in Generalized Cahn–Allen Models

Paul C. Fife[1] **and Andrew A. Lacey**[2]

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The Cahn–Allen model for the motion of phase–antiphase boundaries is generalized to account for nonlinearities in the kinetic coefficient (relaxation velocity) and the coefficient of the gradient free energy. The resulting equation is

$$\varepsilon^2 u_t = \alpha(u)(\varepsilon^2[\kappa(u)]^{1/2}\nabla\cdot\{[\kappa(u)]^{1/2}\nabla u\} - f(u))$$

where f is bistable. Here u is an order parameter and κ and α are physical quantities associated with the system's free energy and relaxation speed, respectively. Grain boundaries, away from triple junctions, are modeled by solutions with internal layers when $\varepsilon \ll 1$. The classical motion-by-curvature law for solution layers, well known when κ and α are constant, is shown by formal asymptotic analysis to be unchanged in form under this generalization, the only difference being in the value of the coefficient entering into the relation. The analysis is extended to the case when the relaxation time for the process vanishes for a set of values of u. Then α is infinite for those values.

KEY WORDS: Grain boundary; internal layers; motion by curvature; Cahn–Allen model; Allen–Cahn model; Ginzburg–Landau functional.

1. INTRODUCTION

The well-known bistable nonlinear diffusion equation (Cahn–Allen equation)

$$u_t = \bar{\alpha}(\bar{\kappa}\nabla^2 u - f(u))$$

was proposed in refs. 1 and 3 as a model for the dynamics of a phase–antiphase boundary between two grains in a solid material. The function u

Dedicated to Oliver Penrose on the occasion of his 65th birthday.

[1] Mathematics Department, University of Utah, Salt Lake City, Utah.
[2] Mathematics Department, Heriot-Watt University, Edinburgh, Scotland.

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is an order parameter attaining its extreme values ± 1 in the crystalline states: $+1$ for one grain and -1 for the other. Thus the quantity u^2 is a measure of the order of the material, and the maximum disorder occurs where $u = 0$. The Cahn–Allen equation represents a gradient flow for the free energy functional

$$\mathscr{E}[u] = \int_\Omega (\tfrac{1}{2}\bar{\kappa} |\nabla u|^2 + F(u))\, dx \tag{1}$$

where $F'(u) = f(u)$ and Ω is the spatial domain occupied by the material under consideration. Therefore in a sense which can be made more precise,[9] this evolution is in the particular "direction" in the function space $\mathscr{L}^2(\Omega)$ which will cause $\mathscr{E}$ to decrease in the most "efficient" manner. The coefficient $\frac{1}{2}\bar{\kappa}$ is of course a measure of the amount by which the system penalizes gradients in u. The other constant, $\bar{\alpha}$, is a relaxation parameter related to the speed at which the system is driven toward an equilibrium configuration. Those configurations minimize $\mathscr{E}$.

The most important property of the Cahn–Allen equation is the motion-by-curvature law.[1,3] When $\bar{\kappa}$ is very small and $\bar{\alpha}$ very large with $\bar{\alpha}\bar{\kappa} = O(1)$, there exist solutions with internal layers of thickness $O(\bar{\kappa}^{1/2})$. Considered as a surface in 3-space, such a layer represents a grain boundary. It moves with normal velocity v given approximately by

$$v = -\bar{\alpha}\bar{\kappa}K \tag{2}$$

where K is the mean curvature of the layer. The existence of such solutions was proved in refs. 11, 12, and 6. Connections between the Cahn–Allen equation and global generalized solutions (2) were established in refs. 7 and 14.

Consideration has until now been restricted to parameters $\bar{\alpha}$ and $\bar{\kappa}$ which are constant. It is expected, however, that they can depend significantly on the order parameter. In particular, the free energy penalty $\bar{\kappa}(u)$ for gradients should be least, and the relaxation parameter $\bar{\alpha}(u)$ greatest, where the atoms are freest to move. This occurs where the material is ordered least, i.e., when $u = 0$. There is some interest, therefore, in looking at the Cahn–Allen model corrected to take these nonlinearities into account. Interfacial theories of a different but related type based on increased mobility within the interface are reviewed in ref. 5.

To incorporate the required order of magnitude properties for $\bar{\alpha}(u)$ and $\bar{\kappa}(u)$, we represent

$$\bar{\kappa}(u) = \varepsilon^2 \kappa(u), \qquad \operatorname{Max}_u \kappa(u) = 1, \qquad 0 < \varepsilon \ll 1$$

$$\bar{\alpha}(u) = \varepsilon^{-2}\alpha(u)$$

and rescale the time variable t so that

$$\mathrm{Min}_u\, \alpha(u) = 1$$

The corresponding gradient flow for the functional $\mathscr{E}$ given by (1) with these notational changes and κ and α allowed to depend on u is

$$\varepsilon^2 u_t = -\alpha(u)\frac{\delta \mathscr{E}}{\delta u}$$

where $\delta\mathscr{E}/\delta u$ is the $\mathscr{L}^2$ functional derivative of $\mathscr{E}$. A straightforward calculation results in the evolution equation

$$\varepsilon^2 u_t = \alpha(u)[\varepsilon^2(\nabla \cdot \kappa(u)\,\nabla u - \tfrac{1}{2}\kappa'(u)\,|\nabla u|^2) - f(u)]$$

which we shall write in the form

$$\varepsilon^2 u_t = \alpha(u)(\varepsilon^2[\kappa(u)]^{1/2}\,\nabla \cdot \{[\kappa(u)]^{1/2}\,\nabla u\} - f(u)) \tag{3}$$

Our object here is to investigate the effect of the u dependence of α and κ on the motion-by-curvature law.

In case α and κ are constant, we may of course replace the product $\bar{\alpha}\bar{\kappa}$ in (2) by $\alpha\kappa$. In this case, the law (2) does not depend on the function f. We find that the effect of u-dependent coefficients is seen *only* through modification of that coefficient. In fact, it is to be replaced by a certain weighted harmonic average of the product $\alpha(u)\,\kappa(u)$. The weight function is $[F(u)]^{1/2}$, and so we gain dependence of (2) on the function f.

Along with the law of motion, formal analysis supplies the micro-profile of the interface, i.e., the shape of the function u in the layer where it changes rapidly from -1 on one side to 1 on the other.

Problems featuring enhanced mobility or conductivity within an interface have been studied in ref. 4 (for the Cahn–Hilliard equation) and ref. 10 (for phase field models), as well as in ref. 5. Those results are quite different from ours.

2. THE MODIFIED MOTION-BY-CURVATURE LAW: THE CASE $\alpha(u)$ AND $\kappa(u)$ BOUNDED AWAY FROM 0

We consider the modified Cahn–Allen equation (3) for an "order parameter" $u(x, t)$, $x \in \mathbf{R}^3$. The function $f(u)$ is of bistable type (see Fig. 1)

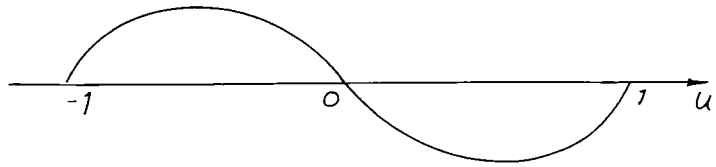

Fig. 1. A typical function $f(u)$.

with two "stable" zeros at $u = \pm 1$ and an "unstable" zero which for simplicity will be taken to be $u = 0$. The functions $\alpha(u)$ and $\kappa(u)$ are positive. The function f satisfies

$$\int_{-1}^{1} f(u)\, du = 0 \tag{4}$$

For ε small (and positive) we construct layered solutions of (3) with a thin layer of thickness $O(\varepsilon)$ separating, at each instant of time t, all the remainder of space into two regions $\mathscr{D}_{\pm}$, where u remains in a small neighborhood of ± 1, respectively.

For convenience in the asymptotic analysis, we shall use the alternate variable

$$w = g(u) \equiv \int_0^u [\kappa(s)]^{1/2}\, ds \tag{5}$$

In this section, it is assumed that the functions α and κ are positive, bounded, bounded away from 0, and smooth. Thus g is invertible. Moreover, (3) becomes

$$\varepsilon^2 \tau(w)\, w_t = \varepsilon^2 \nabla^2 w - h(w) \tag{6}$$

where

$$h(w) \equiv f(g^{-1}(w))/[\kappa(g^{-1}(w))]^{1/2} \tag{7}$$

$$\tau(w) \equiv \frac{1}{\alpha(g^{-1}(w))\, \kappa(g^{-1}(w))} \tag{8}$$

Notice that the two stable zeros of h are now

$$w = w_{\pm} \equiv g(\pm 1) \tag{9}$$

A standard asymptotic interface analysis[2,13,8,10] can now be carried out for layered families of solutions $w(x, t; \varepsilon)$ of (6).

We summarize that procedure. Let $\Gamma(t;\varepsilon)=\{x: w(x,t;\varepsilon)=0\}$; this curve is defined to be the location of the interface. A coordinate system $r(x,t;\varepsilon)$, $s(x,t;\varepsilon)$ is erected in a neighborhood of $\Gamma(t;\varepsilon)$ such that r represents the signed distance from x to Γ ($r>0$ in $\mathscr{D}_+$) and when $x\in\Gamma$, s is an arc-length parameter along Γ. Let z be the stretched normal coordinate

$$z=\frac{r}{\varepsilon} \tag{10}$$

Then if we define the inner variable $W(z,s,t;\varepsilon)\equiv w(x,t;\varepsilon)$ and (for $r=0$) the normal velocity $v(s,t;\varepsilon)=-r_t(x,t;\varepsilon)$ in the direction on $\mathscr{D}_+$ and assume that W depends in a regular manner on ε, we obtain the order relation

$$W_{zz}-h(W)+\varepsilon v\tau(W)\,W_z+\varepsilon KW_z=O(\varepsilon^2) \tag{11}$$

$$W(0,s,t;\varepsilon)=0 \tag{12}$$

where $K(s,t;\varepsilon)$ is the mean curvature of $\Gamma(t;\varepsilon)$. The curvature term in (11) results from the fact that for $x\in\Gamma$, $\nabla^2 r(x,t;0)=K(s(x),t;0)$; the sign is determined by r being positive in $\mathscr{D}_+$.

The formal inner approximation consists in representing

$$W(z,s,t;\varepsilon)=W_0(z,s,t)+\varepsilon W_1(z,s,t)+\varepsilon^2 W_2+\cdots \tag{13}$$

where the W_i are bounded.

There is also a corresponding formal outer expansion, but it trivializes to $w_0\equiv\pm 1$ in $\mathscr{D}_\pm$, with $w_k\equiv 0$ for all $k>0$.

Substituting (13) into (11) and (12) and applying a requirement that W match with the outer solution, we obtain

$$W_{0zz}-h(W_0)=0 \tag{14a}$$

$$W_0(\pm\infty,s,t)=w_\pm, \qquad W_0(0,s,t)=0 \tag{14b}$$

$$LW_1+v\tau(W_0)\,W_{0z}+KW_{0z}=0 \tag{15}$$

where L is the self-adjoint linear operator given by

$$LW\equiv W''-h'(W_0(z))\,W \tag{16}$$

(Here we have anticipated that W_0 will be independent of s and t.)

It is well known that (14) has a solution, which we will denote by $W_0(z)=\psi(z)$, if and only if

$$\int_{w_-}^{w_+} h(w)\,dw=0$$

But by changing the variable of integration to $u = g^{-1}(w)$, it is readily seen that this condition is guaranteed by (4). The solution $\psi(z)$ is unique, so does not depend on s or t. It is also known to be monotone.

Setting $W_0 = \psi$ in (15), multiplying it by $\psi'(z)$, integrating with respect to z from $-\infty$ to ∞, and using the fact that

$$L\psi' = 0$$

we obtain the solvability condition for (15):

$$v\int_{-\infty}^{\infty} \tau(\psi(z))(\psi'(z))^2\,dz + K\int_{-\infty}^{\infty} (\psi'(z))^2\,dz = 0 \tag{17}$$

From the equation

$$\psi'' - h(\psi) = 0 \tag{18}$$

we know that

$$\psi'(z) = [2H(\psi)]^{1/2} \tag{19}$$

where

$$H(\psi) \equiv \int_{w_-}^{\psi} h(s)\,ds$$

[Note that the bistability of f and (4) imply that $H(\psi) > 0$, $\psi \in (w_-, w_+)$; $H(w_+) = 0$.]

Changing the variable of integration in (17) from z to $s = \psi(z)$, we obtain from (19)

$$v = -\sigma K \tag{20}$$

where

$$\sigma = \frac{\int_{w_-}^{w_+} [H(s)]^{1/2}\,ds}{\int_{w_-}^{w_+} \tau(s)[H(s)]^{1/2}\,ds}$$

But we may again change variables to simplify this expression for σ. Set $s = g(\xi)$ and recall

$$F(\xi) = \int_{-1}^{\xi} f(u)\,du$$

Then

$$H(s) = \int_{w_-}^{s} \frac{f(g^{-1}(w))}{[\kappa(g^{-1}(w))]^{1/2}}\,dw = F(g^{-1}(s)) = F(\xi)$$

and

$$\sigma = \frac{\int_{-1}^{1} [F(\xi)]^{1/2}\, d\xi}{\int_{-1}^{1} [1/\alpha(\xi)\,\kappa(\xi)][F(\xi)]^{1/2}\, d\xi} \tag{21}$$

which is a harmonic weighted average of $\alpha\kappa$.

This parameter σ incorporates the effect on the motion-by-curvature law of the functions α and κ. It should be borne in mind that (20) is only the dominant-order law of motion; it is formally correct up to terms of order ε.

The case normally considered is that when α and κ are constant; then clearly $\sigma = \alpha\kappa$, and (20) becomes

$$v = -\alpha\kappa K$$

It is noteworthy that the motion-by-curvature law in this case does not depend on the function $f(u)$. This important observation was made in refs. 1 and 3.

In general, (21) shows σ to be a harmonic weighted average of $\alpha(u)\,\kappa(u)$, the weight function being proportional to $[F(u)]^{1/2}$, hence depending on the function f, but on nothing else. As a consequence, we conclude that

$$\text{Min}(\alpha(u)\,\kappa(u)) \leqslant \sigma \leqslant \text{Max}(\alpha(u)\,\kappa(u))$$

As we have seen, the lowest-order interfacial profile is given by

$$W_0(z) = \psi(z)$$

Reverting to the original order parameter u and denoting the interfacial profile in that variable by $U(z)$, we then obtain

$$U_0(z) = g^{-1}(W_0(z)) = g^{-1}(\psi(z)) \tag{22}$$

This, again, is a monotone profile leading from $-1 = U_0(-\infty)$ to $1 = U_0(\infty)$.

3. MECHANISMS FOR SLOWING INTERFACES

Several conclusions can be drawn from (21). Suppose, for example, that in some u subinterval $I \subset (-1, 1)$, we have

$$\alpha(u)\,\kappa(u) < \eta$$

for some small number η. Then from (21), we have

$$\sigma < \eta \frac{\int_{-1}^{1} [F(\xi)]^{1/2}\, d\xi}{\int_{I} [F(\xi)]^{1/2}\, d\xi} = \eta c$$

with c depending only on F and I. It follows that *the velocity coefficient in the motion-by-curvature law can be made as small as desired by fixing α and taking κ to be small enough in any fixed subinterval I.*

The interpretation is that making the penalty for gradients small in some u interval, for example, near the value $u = 0$, has the effect of slowing the interfacial motion. This is because the propagation mechanism relies in part on the gradient penalty, which forces an interaction between neighboring points in space.

Similarly, if we relax the requirement that $\mathrm{Min}_u\, \alpha(u) = 1$ and allow α to be very small on some interval J, slowing down occurs for quite a different reason. Propagation, in fact, also depends on the force driving u toward the states ± 1, and this force, being proportional to α, is small on J. In both examples, the smallness of κ or α is not assumed for all u, but only on a subinterval.

4. INFINITE RELAXATION SPEED

It is easy to extend the foregoing analysis to cases when the relaxation speed is infinite for some values of u. Suppose, for example, that this is so for u in a closed set I. In some applications, it may indeed be useful to assume this for an interval containing the value $u = 0$. For u in I, then, (3) becomes an elliptic equation

$$\varepsilon^2 \sqrt{\kappa}\, \nabla \cdot (\sqrt{\kappa}\, \nabla u) - f(u) = 0$$

whose solutions must extend continuously to those of the parabolic equation (3), valid outside I. A layered solution of this elliptic–parabolic equation can still be constructed by formal analysis, and again the velocity of its layer follows the usual motion-by-curvature law.

We define the relaxation time $\beta(u) = 1/\alpha(u)$, so that $\beta = 0$ exactly on I. Then (6) holds with

$$\tau(w) = \frac{\beta(g^{-1}(w))}{\kappa(g^{-1}(w))}$$

which also vanishes on I.

The asymptotics in Section 2 remains valid. In fact, the function $\psi(z)$ is the same as before, and (20) holds with

$$\sigma = \frac{\int_{-1}^{1} [F(\xi)]^{1/2}\, d\xi}{\int_{I'} [\beta(\xi)/\kappa(\xi)][F(\xi)]^{1/2}\, d\xi} > 0$$

where I' is the complement of I.

Although we have seen in the last section that the velocity can be made arbitrarily small by making α small on a fixed proper subinterval of $(-1, 1)$, it cannot be made arbitrarily large by making α large on such an interval I. However, it can by increasing the size of I.

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