A free boundary model for diffusion induced grain boundary motion *

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Abstract

On the basis of a phase-field model previously proposed in [4] to describe the phenomenon of diffusion-induced grain boundary motion (DIGM), we present a formal asymptotic reduction to a moving free boundary problem. This problem is one of enhanced motion by curvature. The enhancement depends on the local concentration jump across the grain boundary of a solute species that is diffusing along the boundary.

A rigorous theory is given for two-dimensional solutions of the equations when there is steady motion of the grain boundary spanning a plate from face to face, solute being supplied at the faces of the plate. The motion is in the directional parallel to the face. This situation represents well known experiments designed to illustrate DIGM. The corresponding theory is also given for grain boundaries which do not span the plate, but rather trail behind the moving intersection with one of the faces, never reaching the other one.

1 Introduction

$\boxed{\text{intro}}$

A common experimental observation in materials science is that boundaries between crystalline grains (grain boundaries) in a metallic alloy support enhanced diffusion of atoms of the alloy species,

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and the presence of concentration gradients in these boundaries may induce the migration of the boundary itself. This effect, which has been thoroughly studied, is called diffusion induced grain boundary motion (DIGM) (see the review [11] and the other references in [4]).

Various theoretical explanations have been given. In particular, some of the present authors developed a phase-field model in [4] based on a gradient flow with respect to a proposed free energy functional that depends on the concentration distribution u of a solute species in the grain boundary, an order parameter ϕ relevant to the local crystallinity, and spatial gradients of the latter. We showed that there was no motion unless free energy interaction terms between u and ϕ were introduced. These are terms in the free energy which depend on both u and ϕ.

The lowest order interaction term that was found to support DIGM represented an elastic effect, and it led to a forcing term for the motion. Experiments have shown that the elastic energy due to composition inhomogeneities in the crystals gives rise to the principal driving force for DIGM [16, 17].

Our analysis was limited to a simple thin plate geometry, in which the grain boundary remained planar at all times, and for which the gradients in composition along the boundary were small. This is a reasonable assumption consistent with experiments on thin plates. Experiments have shown, however, that for thicker plates the grain boundary becomes curved and there are important composition gradients along it.

In this paper the assumption that the boundary is planar will be avoided. The mathematics will be made tractable by means of a sharp interface approximation based on the phase-field model of DIGM given in [4], with the assumption that the driving force is the elastic interaction. The detailed derivation of this approximation is given in Sec. 2.

The model we obtain is a free boundary problem in the plane for a mobile curve or interface representing the moving grain boundary. It takes the form of a forced motion by curvature problem, the force depending on the local concentration of a solute species in the grain boundary. In addition, the solute diffuses along the moving interface from a source (or sink) on the faces of the plate and is absorbed into the growing grain (or depleted from the shrinking grain) by the motion of the grain boundary.

Formal asymptotics with respect to a small parameter ϵ representing a nondimensional DIGM forcing is used in this reduction. Three versions of the free boundary problem are derived in Secs. 2.4 (to give equations (2.57)and (2.58)), 2.6, and 2.7. The second version is a higher order (in ϵ) version of the first, and results in replacing equation (2.58) with (2.68). In simple cases the third version constitutes an equation for the quick redistribution of an arbitrary initial solute distribution to become compatible with the version in Sec. 2.4; then equation (2.68) is replaced with (2.69).

These are models incorporating full dynamics. But there is a special class of steady problems which is of great interest. These problems have to do with experimental setups involving metallic plates with grain boundaries intersecting the plate faces, where a source or sink of solute atoms is located. That class of problems can be formulated as an overdetermined system of ordinary differential equations for the determination of the velocity, distribution of solute, and shape of the boundary. There are only two (dimensionless) parameters in these equations: the thickness of the plate and a parameter ρ representing a different nondimensionalization of the elastic interaction strength mentioned before. These steady problems are investigated rigorously in Sec. 3. Conditions for the existence of solutions are given, and the case when $\rho \ll 1$ is explored.

A discussion of the results of the paper, including a review of order of magnitude assumptions, is given in Sec. 4.

We note that travelling wave solutions for forced mean curvature flow with prescribed forcing have previously been studied in various settings, cf [5, 6]. Numerical calculations based on both phase field and sharp interface models support the formal asymptotics of this paper and yield for both models travelling wave solutions in appropriate parameter regimes as the long time limit of intial value problems, [13, 8].

In [3] further results on the model derived here are given. In addition, the effects of various boundary conditions imposed by the physics at the junctions of the grain boundary with the plate surfaces are examined. One of these, which considers grooving at this moving junction by surface diffusion, has a profound effect on the solutions.

2 The sharp-interface model

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2.1 Formulation and scaling

form

The phase field model described in [4] uses two field variables: $\hat{u}$, representing the concentration of solute atoms in the metal plate, and an order parameter ϕ which takes the value $+1$ in one of the crystal grains, -1 in the other, and intermediate values in the grain boundary. We use the symbol $\hat{x}$ for (two-dimensional) space and $\hat{t}$ for dimensional time. The field variables obey the kinetic equations

$$\begin{aligned}
\tau\partial\phi/\partial\hat{t} &= \phi+\delta^2\hat{\nabla}^2\phi-\hat{\epsilon}\partial\hat{p}(\hat{\phi},\hat{u})/\partial\phi \;\text{ if }\; -1<\phi<1, \;\text{ else }\; \partial\phi/\partial\hat{t}=0, \qquad \boxed{\text{eq1a}} \quad (2.1)\\
&\quad \phi \text{ continuously differentiable,}\\
\partial\hat{u}/\partial\hat{t} &= \hat{\nabla}\cdot[\hat{D}(\phi)\hat{\nabla}\hat{w}], \qquad \boxed{\text{eq1b}} \quad (2.2)\\
\hat{w} &= \hat{u}+\hat{\epsilon}\partial\hat{p}(\hat{\phi},\hat{u})/\partial\hat{u}, \qquad \boxed{\text{eq1c}} \quad (2.3)
\end{aligned}$$

where gradients are with respect to $\hat{x}$, τ is a constant which can be thought of as a relaxation time for the crystallization process, δ is a constant length associated with gradient contributions to the free energy density of the system, $D(\phi)$ is the diffusivity, which is taken to be zero outside the grain boundary, i.e. where $\phi=\pm1$, and $\hat{\epsilon}$ is a scaled dimensionless stress that results from a unit composition change. It will turn out that δ is also comparable with the thickness of the grain boundary. No traveling wave solution results if $\hat{\epsilon}=0$, from which we concluded that an interaction is necessary to produce grain boundary movement.

The elastic interaction will be modeled as in [4] by taking

$$\hat{p}(\phi,\hat{u}) \approx \frac{\pi}{8}(1+\phi)^2(\hat{u}-\hat{u}_0)^2, \qquad \boxed{\text{papprox}} \quad (2.4)$$

The conditions in the undisturbed part of the metal, just in front of the moving grain boundary, are taken to be $\hat{u}=\hat{u}_0$, $\phi=1$. Just behind it, we have $\phi=-1$. In this paper we shall assume that $\hat{u}_0=0$. If this is not the case, then easy adjustments to the analysis can be made. The interaction term $\hat{p}$ in (2.4) differs slightly in appearance ($(1+\phi)$ vs $(1-\phi)$) from that in [4], because in that paper the leading edge of the grain boundary was taken to be where $\phi=-1$. In the present paper we use a different convention, characterizing the leading edge by $\phi=1$ and the trailing edge by $\phi=-1$.

We now nondimensionalize the equations (2.1)-(2.3).

Let $u^* < 1$ be the maximal value of $\hat{u}$ attained in the process and D_m be a certain average value of the function $\hat{D}(\phi)$, to be given later (2.56). We set

$$\hat{u} = u^* u, \quad \epsilon = \hat{\epsilon}(u^*)^2, \quad \hat{D}(\phi) = D_m D(\phi), \quad \hat{p} = (u^*)^2 p. \qquad \boxed{\text{scales2}} \tag{2.5}$$

We use the dimensionless combinations

$$A = \frac{\delta^2}{D_m \tau}, \qquad \rho = \frac{\epsilon}{A}, \qquad \boxed{\text{dcom}} \tag{2.6}$$

and characteristic length and time

$$L = \frac{\delta}{\epsilon}, \qquad T = \frac{\tau}{\rho\epsilon^2} = \frac{\delta^2}{\epsilon^3 D_m}. \qquad \boxed{\text{LT}} \tag{2.7}$$

It will turn out that in typical cases, the variation of u along the grain boundary, as well as the variation of the shape of the grain boundary itself, will occur with characteristic length L, and its motion with characteristic velocity L/T. We set

$$\hat{x} = Lx, \quad \hat{t} = Tt. \qquad \boxed{\text{scales}} \tag{2.8}$$

Making these substitutions, we arrive at the equations

$$\rho\epsilon^2 \phi_t = \phi + \epsilon^2 \nabla^2 \phi - \epsilon p_\phi, \qquad \boxed{\text{dl1}} \tag{2.9}$$

$$\nabla \cdot D \nabla w = \epsilon u_t, \qquad \boxed{\text{dl2}} \tag{2.10}$$

$$w = u + \frac{\epsilon}{u^*} p_u. \qquad \boxed{\text{dl3}} \tag{2.11}$$

Our asymptotics will be based on the assumptions

$$\frac{\epsilon}{u^*} = \hat{\epsilon} u^* \ll 1, \qquad \rho \leq O(1). \qquad \boxed{\text{ass}} \tag{2.12}$$

Thus $\epsilon \ll 1$ and $A \geq O(\epsilon)$. Generally the analysis will operate under the assumption that all derivatives appearing in (2.9)–(2.11) are bounded independently of ϵ and ρ; however in some cases we relax this to allow the time derivatives to be large, still requiring $\rho\phi_t$ and ϵu_t to be so bounded.

We restrict attention to two-dimensional problems, the grain boundary being represented by a mobile curved strip $G(t)$ in the (x, y)-plane bounded on two sides by curves $\Gamma_\pm(t)$. (The picture in 3–space will have the grain boundary extending with no change infinitely far in the positive and negative z–directions.) The two grains lie on either side of this strip; we represent them by the two domains Ω_+ and Ω_-. The curve $\Gamma_\pm$ is the common boundary between G and $\Omega_\pm$.

By definition, G is tied to the phase function by the relation

$$G(t) = \{x : -1 < \phi(x, t) < 1\}, \qquad \boxed{\text{G}} \tag{2.13}$$

with

$$\phi(x, t) = \pm 1, \ \nabla\phi(x, t) = 0 \ \text{ for } x \in \Gamma_\pm(t). \qquad \boxed{\text{Gbc}} \tag{2.14}$$

Recall that the function ϕ is extended continuously outside G with $\phi(x, t) = \pm 1$ for $x \in \Gamma_\pm(t) \cup \Omega_\pm(t)$.

For the time being, we disregard the possible intersections of G with the boundary of the domain occupied by the metal specimen. Those intersections will generate additional pieces of the boundary of G. They will be dealt with in Secs. 2.5 and 3.

We consider only motions such that G moves into $\Omega_+(t)$, i.e. Γ_+ is the leading edge and Γ_- the trailing edge. As mentioned above, we have $u(x, t) = 0$ in Ω_+, and since $D = 0$ in $\Omega_\pm$, we have from $(2.2)_3$ that u is independent of t in Ω_-. It may of course depend on x. In fact for $x \in \Omega_-(t)$, $u(x, t) = u(x, T(x))$, where $T(x)$ is the time at which $x \in \Gamma_-(T)$.

2.2 Coordinates tied to G

coords

For notational convenience we replace the symbol Γ_- by Γ. Fix a specific time, say $t = 0$. We shall derive equations for the motion of $\Gamma(t)$ and evolution of u which are valid at $t = 0$. But since that fixed time was arbitrary, those equations will in fact be valid at any other time as well.

Let s_0 denote signed arclength on $\Gamma(0) = \Gamma_-(0)$, measured from some definite point on that curve. For $x \in G(0)$, let $r_0(x)$ be the distance from x to $\Gamma(0)$. We assume that G is so narrow that $r_0(x)$ is well-defined and the transformation $x \to (s_0, r_0)$ is smooth and invertible for $x \in G(0)$.

As t changes, remaining small, we let this coordinate system evolve in the following way. At each point $(s_0, 0)$ on $\Gamma(0)$, let N_{s_0} be a curve through $(s_0, 0)$, parameterized by t. For each (small) t, N_{s_0} is required to be perpendicular to $\Gamma(t)$ where the two intersect. Now $G(t)$ is coordinatized by setting $s^{(t)} = s_0$ at each such intersection point (so that $s^{(t)}$ for each fixed t is a parameter for $\Gamma(t)$ but is no longer necessarily arclength), and again for $x \in G(t)$, $r^{(t)}(x, t)$ is distance from x to $\Gamma(t)$.

Let $v(s^{(t)}, t)$ be the normal velocity of $\Gamma(t)$ at the point $(s^{(t)}, t)$, counted positive if the direction of motion is into Ω_+. Since we assume this is always the case, we have $v > 0$. Then

$$v(s^{(t)}, t) = -\partial_t r^{(t)}(x) \qquad \text{when } x \text{ lies on } \Gamma(t) \text{ at the point } s^{(t)}. \qquad \boxed{\text{vel}} \tag{2.15}$$

In accordance with our comments following (2.12), we shall consider solutions such that

$$\rho v \leq O(1), \qquad \boxed{\text{rhov}} \tag{2.16}$$

thus allowing large velocities when ρ is small. This does not conflict with the asymptotics below.

We now rewrite the basic equations (2.9), (2.10) in terms of the coordinates (r, s), having dropped the superscript "(t)". In the following, the functions ϕ, u, w are therefore considered to be functions of (r, s, t), and subscripts denote partial derivatives.

The dimensionless curvature of $\Gamma(t)$ is denoted by $\kappa(s, t)$, considered to be positive if the center of curvature lies on the negative (toward Ω_-) side of Γ.

We have

$$\rho\epsilon^2(\phi_t - v\phi_r) = \phi + \epsilon^2 \left[\partial_r^2\phi - \frac{\kappa}{1 - r\kappa}\partial_r\phi + \frac{1}{1 - r\kappa}\partial_s\left(\frac{1}{1 - r\kappa}\partial_s\phi\right)\right] - \epsilon p_\phi, \qquad \boxed{\text{eqrs1}} \tag{2.17}$$

$$\epsilon(u_t - vu_r) = \partial_r(D\partial_r w) - \frac{\kappa}{1 - r\kappa}D\partial_r w + \frac{1}{1 - r\kappa}\partial_s\left(\frac{D}{1 - r\kappa}\partial_s w\right). \qquad \boxed{\text{eqrs2}} \tag{2.18}$$

These equations hold in $G(t)$. We must add to them boundary conditions on the boundaries of $G(t)$. For ϕ, we have (2.14):

$$\phi = \pm 1, \quad \nabla\phi = 0 \quad \text{on } \Gamma_\pm(t). \qquad \boxed{\text{bcphi}} \tag{2.19}$$

Consider now the proper boundary conditions for u on the trailing edge $\Gamma(t)$ of G. It was argued in Appendix A of [4] that the normal component $D\partial_n w$ of the flux and the concentration u are continuous on that trailing edge. This flux vanishes in $\Omega_-(t)$ and therefore its continuity will be guaranteed if the normal derivative of u, hence that of w, vanishes as Γ_- is approached from within G, i.e.

$$\left.\frac{\partial u}{\partial n}\right|_{\Gamma_-}^{+} = 0. \qquad \boxed{\text{bcw}} \tag{2.20}$$

In fact the solutions constructed in [4] have that property. We shall require it.

On the leading edge $\Gamma_+(t)$, the normal component of the flux relative to the moving curve $\Gamma_+(t)$ vanishes, because there exists no net transport of solute material through that curve. However, according to a more accurate model in which the diffusivity in the two crystalline grains is very small but nonzero, there will generally be an abrupt change in the concentration and the flux in a narrow region adjacent to Γ_+. An argument leading to this conclusion was given in Appendix A of [4].

The initial value problem for (2.17), (2.18) would require conditions at $t = 0$ to be imposed as well. However, we do not consider the general initial value problem; rather we use internal layer asymptotics to construct solutions for which ϕ makes a transition from -1 to 1 within the narrow boundary region. Viewed on a macroscopic scale, the boundary regions will reduce to a curve and the solutions will be discontinuous there.

2.3 Structure of the solution inside $G(t)$

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2.3.1 The phase function

strpf

We use stretched coordinates (z, s, t) where $z = \frac{r}{\epsilon}$. Recall that r and $z > 0$ in G. We seek solutions which are regular in these variables and in ϵ at $\epsilon = 0$. We also assume that the shape of G and Γ varies smoothly in (s, t); in particular the curvature with respect to the variable s is bounded independently of ϵ. We express functions of the stretched variable by capital letters:

$$\phi(r, s, t; \epsilon) = \Phi(z, s, t; \epsilon)$$

and similarly for U and W. (Here we have symbolized explicitly the fact that our solutions depend on ϵ; usually we shall not do that.) In view of the comments following (2.20), we cannot expect $U(z, s, t; \epsilon)$ and $W(z, s, t; \epsilon)$ to be regular in ϵ uniformly up to Γ_+; there will generally be a thin region near Γ_+ across which u and the material flux change quickly. We shall have no need to analyze that region; we simply assume that U and W are regular in ϵ for all z outside a negligible interval near Γ_+.

In terms of the stretched variables defined above, (2.17) takes the form

$$\Phi_{zz} + \Phi = \epsilon\left[-\rho v \Phi_z + \kappa \Phi_z + p_\phi\right] + O(\epsilon^2). \quad \boxed{\text{eqzs1}} \tag{2.21}$$

This equation is to hold in the region G defined by (2.13), i.e. $-1 < \Phi < 1$, on the boundary of which, by (2.19),

$$\Phi = \pm 1 \quad \text{and} \quad \Phi_z = 0. \quad \boxed{\text{bcPhi}} \tag{2.22}$$

This problem has the unusual feature that the domain of the unknown function Φ depends on Φ itself; that feature results from the double-obstacle nature of the equation (2.1-(2.3) for ϕ. In effect, we have a free boundary problem for the determination of the boundaries of G with reference to the stretched coordinates (our eventual aim is to derive a quite different free boundary problem, namely one for the determination of $\Gamma(t)$ with reference to the original coordinates (x, t)).

A simple expansion in powers of ϵ is therefore inappropriate as an approximation scheme. Instead, we shall employ a ϵ-dependent change of variable (to be determined)

$$\zeta = (1 + \alpha\epsilon) z \quad \boxed{\text{zeta}} \tag{2.23}$$

and find a solution of (2.21) in the form

$$\Phi(z,s,t) = \Phi^0(\zeta,s,t) + \epsilon\Phi^1(\zeta,s,t). \qquad \boxed{\text{unus}} \tag{2.24}$$

The task will be to find Φ^0, Φ^1 and the constant α.

Substituting (2.24) into (2.21), we find

$$(1+\alpha\epsilon)^2(\Phi^0_{\zeta\zeta} + \epsilon\Phi^1_{\zeta\zeta}) + \Phi^0 + \epsilon\Phi^1 = \epsilon\left[(-\rho v + \kappa)\Phi^0_\zeta + p_\phi\right] + O(\epsilon^2). \qquad \boxed{\text{aa1}} \tag{2.25}$$

Expanding in ϵ, we obtain

$$\Phi^0_{\zeta\zeta} + \Phi^0 = 0. \qquad \boxed{\text{aa2}} \tag{2.26}$$

The only monotone solution of this equation satisfying the boundary requirements (2.22) is

$$\Phi^0(\zeta,s,t) = -\cos\zeta, \quad 0 < \zeta < \pi. \qquad \boxed{\text{aa3}} \tag{2.27}$$

(It is natural to select the monotone solution; this simply reflects a gradual change in the structure of the material from that associated with one grain to that of the other.)

From this, we conclude that the trailing and leading edges are characterized by $\zeta = 0, \pi$, respectively. In terms of the original variable r, we obtain that the nondimensional thickness of the grain boundary is $\pi\epsilon$ to leading order. From (2.8) we therefore see that the dimensional grain boundary thickness is $\pi\delta$, corroborating the claim made earlier that δ is a constant comparable to that thickness. An $O(\epsilon)$ approximation to the thickness which follows from (2.23) is $\pi\epsilon(1+\alpha\epsilon)$, where α will be obtained shortly.

The $O(\epsilon)$ part of (2.25) is

$$\Phi^1_{\zeta\zeta} + \Phi^1 = [-(\rho v - \kappa)\sin\zeta + p_\phi] - 2\alpha\cos\zeta. \qquad \boxed{\text{aa4}} \tag{2.28}$$

Since the boundary of the domain of Φ is now set at $\zeta = 0, \pi$, we must impose the following boundary conditions on the solution of (2.28), which follow from (2.19):

$$\Phi^1 = 0 \quad \text{at} \quad \zeta = 0, \pi, \qquad \boxed{\text{aa5}} \tag{2.29}$$

$$\Phi^1_\zeta = 0 \quad \text{at} \quad \zeta = 0, \pi. \qquad \boxed{\text{aa5a}} \tag{2.30}$$

This constitutes four conditions, although (2.28) is only a second order equation. The extra two conditions can be fulfilled by (1) choosing α appropriately, and (2) noting that any solution of (2.28) and (2.29) may be supplemented by a term $\gamma\sin\zeta$, for arbitrary γ, thus affecting the boundary values of Φ^1_ζ. One then chooses γ appropriately.

Consider first the boundary value problem (2.28) under only the Dirichlet conditions, i.e. (2.29). The operator on the left is singular, having $\sin\zeta$ as nullfunction. Therefore for solvability, the right side must be L^2–orthogonal to $\sin\zeta$. From (2.4) we have

$$p_\phi = \frac{\pi}{4}(1+\Phi^0)(U^0)^2 + O(\epsilon). \qquad \boxed{\text{papp2}} \tag{2.31}$$

From this and (2.27), the orthogonality condition assumes the form

$$\rho v(s,t) = \kappa(s,t) + \frac{1}{2}\int_0^\pi U^0(z,s,t)^2 \sin\zeta(1-\cos\zeta)\,d\zeta, \qquad \boxed{\text{oc1}} \tag{2.32}$$

since the last term in (2.28) is already orthogonal to $\sin\zeta$. This provides an enhanced motion by curvature law in leading order. It will appear later in the simpler form (2.57).

Once the condition (2.32) is satisfied, the Dirichlet problem (2.28), (2.29) can be solved in the form

$$\Phi^1 = \Phi^\dagger + \alpha\Phi^* + \gamma \sin\zeta, \qquad \boxed{\text{aa6}} \tag{2.33}$$

where $\Phi^\dagger$ is a particular solution of (2.28), (2.29) with $\alpha = 0$, Φ^* is such a particular solution with right side of (2.28) replaced by $-2\cos\zeta$, and γ is an arbitrary (for the moment) constant reflecting the fact that any solution of the Dirichlet problem may be supplemented by a nullfunction. One immediately determines $\Phi^* = \zeta \sin\zeta$.

Our last task is to choose the remaining unknown constants γ and α so that (2.30) is satisfied. The vanishing of the ζ-derivative at the two points $\zeta = 0$, π results in the two equations

$$\Phi^\dagger_\zeta(0) + \gamma = 0,$$

$$\Phi^\dagger_\zeta(\pi) - \alpha\pi - \gamma = 0.$$

These two equations have a unique solution (α, γ). This completes our construction of the solution (2.24) of (2.21).

2.3.2 The concentration

$\boxed{\text{conc}}$

Again in our stretched coordinates, (2.18) assumes the form

$$\partial_z(D\partial_z W) = -\epsilon\kappa D\partial_z W + \epsilon^2\left[-\kappa^2 z D\partial_z W - \partial_s(D\partial_s W) + vU_z\right] + O(\epsilon^3), \qquad \boxed{\text{Ueq}} \tag{2.34}$$

where from (2.11), (2.4) and (2.27) we have

$$W = U + \frac{\pi\epsilon}{4u^*}(1-\cos\zeta)^2 U + O(\epsilon^2). \qquad \boxed{\text{aa14}} \tag{2.35}$$

On $\Gamma = \Gamma_-$, which is at $z = 0$, we have (2.20). The normal vector n is the vector in the direction of decreasing z. Therefore at that boundary,

$$\partial_z W = \epsilon\partial_r w = O(\epsilon^2). \qquad \boxed{\text{Wbc}} \tag{2.36}$$

We expand $W = W^0 + \epsilon W^1 + \ldots$ and obtain from (2.34) and (2.36)

$$\partial_z(D\partial_z W^0) = 0, \quad \partial_z W^0 = 0 \ \text{ at } z = 0. \qquad \boxed{\text{W0}} \tag{2.37}$$

This implies that $D\partial_z W^0 = 0$, and since $D > 0$ inside, we have that W^0 is constant in z, i.e.

$$W^0 = W^0(s,t). \qquad \boxed{\text{W0a}} \tag{2.38}$$

From (2.35) we also have

$$U^0 = U^0(s,t). \qquad \boxed{\text{aa20}} \tag{2.39}$$

In a similar manner, we obtain that W^1 is also independent of z, so that except for a correction of the order ϵ^2, W is independent of z. Let $\overline{W}$ and $\overline{U}$ denote the averages, with respect to z in G, of the functions W and U. They will be functions of (s,t). From the above, we obtain

$$W(z,s,t) = \overline{W}(s,t) + O(\epsilon^2). \qquad \boxed{\text{ave-1}} \tag{2.40}$$

From (2.35), we get

$$U = \overline{W} - \frac{\pi\epsilon}{4u^*}(1-\cos\zeta)^2 U + O(\epsilon^2), \qquad \boxed{\text{ave0}} \tag{2.41}$$

hence taking averages over z,

$$(1 + a_1\epsilon)\overline{U} = \overline{W} + O(\epsilon^2), \qquad \boxed{\text{ave1}} \tag{2.42}$$

where a_1 is some easily calculated constant independent of (z, s, t). Moreover, combining (2.41) (with $\zeta = 0$) and (2.42), we have

$$U(0, s, t) = \overline{U}\,(1 + a_1\epsilon) + O(\epsilon^2). \qquad \boxed{\text{ave2}} \tag{2.43}$$

2.4 The motion of G: the developed case to lowest order

$\boxed{\text{mot}}$

By "developed" we mean that transients operating on a faster time scale, as explained below, have disappeared.

Fix $s_1 < s_2$. We consider only the portion of G given by

$$G_0(t) = G(t) \cap \{s_1 < s < s_2\}. \qquad \boxed{\text{bb1}} \tag{2.44}$$

Set

$$M(t) = \int_{G_0(t)} u(x, t)\, dx. \qquad \boxed{\text{M}} \tag{2.45}$$

This is the total mass of solute contained in G_0. In this section we assume that in the coordinate system attached to the moving strip $G(t)$, the time rate of change of u is at most an $O(1)$ quantity. We interpret this as saying that any fast transients have disappeared. Since the size of G_0 is $O(\epsilon)$, we have

$$M,\ \frac{dM}{dt} = O(\epsilon) \quad \text{if} \quad \left.\frac{\partial u}{\partial t}\right|_{(r,s)} = O(1). \qquad \boxed{\text{M0}} \tag{2.46}$$

We now write an equation for the conservation of mass $M(t)$ in G_0. It changes only due to the flux of solute through the boundary of G_0, which consists of four parts: Γ, Γ_+, and the two ends where $s = s_1$ and $s = s_2$. We consider them separately.

As was brought out before (following (2.20)), there is no such flux through Γ_+. Consider the trailing edge Γ. Because of (2.20) there is no diffusive flux through it, and the convective flux is

$$\sigma_1(0) = -\int_{s_1}^{s_2} v(s, 0) U(0, s, 0)\, ds < 0. \qquad \boxed{\text{bb4}} \tag{2.47}$$

This represents flux of material out of G_0 being deposited in the growing grain.

From (2.43) we have

$$\sigma_1(0) = -\int_{s_1}^{s_2} v(s, 0)\overline{u}(s, 0)\, ds + O(\epsilon), \qquad \boxed{\text{bb10}} \tag{2.48}$$

$\overline{u}$ being the average over r in G for fixed (s, t).

Next, we consider the flux through the ends $\{s = s_1,\, s_2\}$ of G_0. It is given in terms of the internal material flux vector $\boldsymbol{J}(r, s, t)$ as

$$\sigma_2 = \left[\int_{\{s=s_1\}} - \int_{\{s=s_2\}}\right] \boldsymbol{J}(r, s, 0)\cdot\boldsymbol{\tau}(r, s, 0) dr, \qquad \boxed{\text{bb5}} \tag{2.49}$$

where $\boldsymbol{\tau}$ is the unit vector normal to the boundary of G_0 at the ends pointing in the direction of increasing s. By the orthogonality of the coordinate system, $\boldsymbol{\tau}\cdot\nabla w = \frac{\partial w}{\partial s}$.

From (2.10) we know that

$$\boldsymbol{J} = -\epsilon^{-1} D(\phi)\nabla w. \qquad \boxed{\text{J}} \tag{2.50}$$

From (2.49), (2.50) and the fact that the thickness of G is $\pi\epsilon$ to lowest order, we obtain

$$\sigma_2 = \pi\overline{Dw_s}\Big|_{s_2} - \pi\overline{Dw_s}\Big|_{s_1} + O(\epsilon) = \pi\int_{s_1}^{s_2} \frac{\partial}{\partial s}\overline{D\frac{\partial w}{\partial s}}ds + O(\epsilon). \qquad \boxed{\text{bb6}} \tag{2.51}$$

On the basis of (2.40) and (2.42), we have

$$\overline{Dw_s} = \overline{D}\overline{w}_s + O(\epsilon) = D_0\overline{u}_s + O(\epsilon), \qquad \boxed{\text{bb18}} \tag{2.52}$$

where $D_0 = \overline{D(-\cos\zeta)} = \frac{1}{\pi}\int_0^\pi D(-\cos\zeta)\,d\zeta$, since $\phi = -\cos\zeta + O(\epsilon)$. We obtain

$$\sigma_2 = \pi D_0\int_{s_1}^{s_2} \overline{u}_{ss}ds + O(\epsilon). \qquad \boxed{\text{bb9}} \tag{2.53}$$

Our conservation equation is

$$\frac{d}{dt}M(0) = \sigma_1 + \sigma_2. \qquad \boxed{\text{bb7}} \tag{2.54}$$

From (2.46), (2.48), (2.53) and the arbitrariness of s_i, this implies

$$\pi D_0\overline{u}_{ss} - v\overline{u} = O(\epsilon). \qquad \boxed{\text{bb13}} \tag{2.55}$$

At this point we specify the constant D_m in (2.5) so that $\pi D_0 = 1$. This means that in terms of the original dimensional diffusivity $D(\phi)$,

$$D_m = \int_0^\pi D(-\cos\zeta)d\zeta. \qquad \boxed{\text{Dm}} \tag{2.56}$$

A limiting evolution problem can be obtained by setting $\pi D_0 = 1$, $\epsilon = 0$ in (2.55), and using (from (2.39)) $U^0 = \overline{u}$ in (2.32). We drop the bars on the variable $\overline{u}(s,t)$, thus obtaining

$$\rho v = \kappa + u^2, \qquad \boxed{\text{cc1}} \tag{2.57}$$

$$u_{ss} - vu = 0. \qquad \boxed{\text{cc2}} \tag{2.58}$$

Although typically $\rho \ll 1$, v is often large so that the term on the left of (2.57) cannot be neglected. However, we always have $\rho v \leq O(1)$.

The importance of the curvature κ in grain boundary motion was first shown by Allen and Cahn [1] in a different connection. Rigorous asymptotics for the double obstacle phase field equation in the form (2.1) with u being prescribed were carried out in [9]; see [7] for a review.

With $\rho > 0$, these equations, together with the prescription of initial data for u and Γ, make a reasonable problem for the evolution of $\Gamma(t)$ and $u(s,t)$, except that there is apparently a severe compatibility constraint which the initial data $(u(s,0),\Gamma(0))$ must satisfy. Namely, $u(s,0)$ and $\kappa(s,0)$ should be such that there exists a function $v(s,0)$ so that (2.57), (2.58) are satisfied at $t = 0$. In other words, at $t = 0$, $u_{ss} - \frac{1}{\rho}(\kappa + u^2)u = 0$.

Instead of the initial value problem, one may instead wish to consider solutions for which $\Gamma(t)$ represents a curve moving with constant speed without changing its shape and $u(s,t)$ is independent of t. Such a steady problem will be the subject of the next section of this paper.

If ρ is very small, which is the typical case, one is tempted to approximate the problem by setting $\rho = 0$ in (2.57). However, it is not likely that the resulting equations specify a well-posed evolution problem. On the other hand, the steady Problem II considered in the next section does make sense.

2.5 Plate problems

film

In all this, we have supposed that G does not meet the boundary of the domain Ω. However in experiments involving metal plates, the grain boundary will typically meet at least one of the plate's faces and terminate there. The point of intersection will itself move along the face. If there is no grooving, the appropriate boundary condition at the intersection, in our phase-field model, will be $\frac{\partial \phi}{\partial n} = 0$, where n is normal to the face, and since ϕ is a function of r alone to lowest order, this translates in the sharp interface limit into the condition that $\Gamma(t)$ must, for each value of t, meet the face orthogonally.

The concentration will also be subject to a boundary condition at the face. If the plate is immersed in a reservoir which acts as a source for solute material, the concentration in that reservoir can (and will) be taken as the characteristic value u^*, and the boundary condition there for the nondimensional concentration will be $u = 1$.

For example, suppose the plate is given as the slab $\{-2H \le x_2 \le 0\}$ in the x_1, x_2 plane, $\Gamma(t)$ connects the faces $\{x_2 = 0\}$ and $\{x_2 = -2H\}$, and there is such a reservoir outside the plate. Then the conditions

$$\Gamma(t) \text{ has a tangent perpendicular to the face at } x_2 = 0,\ -2H, \qquad \boxed{\text{bc22}} \tag{2.59}$$

$$u = 1 \text{ at } x_2 = 0,\ -2H, \qquad \boxed{\text{bc23}} \tag{2.60}$$

must be added to the equations (2.57), (2.58).

In the variations discussed below, similar comments can be made about boundary conditions.

2.6 The full problem, accurate to $O(\epsilon)$

full

A more accurate evolution problem which obviates the stated constraint on the initial conditions is obtained by keeping the $O(\epsilon)$ terms in the above analysis. We give the details in the case that $D = D_0$ is a constant in the grain boundary, so that it is discontinuous at $\Gamma_\pm(t)$.

First we develop an expression for $\frac{d}{dt}M(0)$.

In terms of our local coordinate system, we have

$$M(t) = \int_{s_1}^{s_2} \int_0^{\epsilon\pi} u(r, \hat{s}^{(t)}, t) \frac{d\hat{s}^{(t)}}{ds_0} dr\, ds_0 (1 + O(\epsilon)), \qquad \boxed{\text{M1}} \tag{2.61}$$

where $\hat{s}^{(t)}$ is arclength on $\Gamma(t)$, and (recall) s_0 is arclength on the curve $\Gamma(0)$ at $t = 0$ as well as our original non-arclength parameter on $\Gamma(t)$ for $t \neq 0$. The ratio $\frac{d\hat{s}^{(t)}}{ds_0}$ represents the stretching or contracting of the curve $\Gamma(t)$ as it evolves in time. It can be calculated as follows. The change in the length $L(\Gamma(t))$ of any mobile curve $\Gamma(t)$ is given by the formula $\frac{d}{dt}L(\Gamma(t))\Big|_{t=0} = -\int_\Gamma v(s_0)\kappa(s_0)\, ds_0$, where s_0 is arclength. It follows that

$$\frac{d\hat{s}^{(t)}}{ds_0} = 1 + tv\kappa + O(t^2) \qquad (t \to 0). \qquad \boxed{\text{bb2}} \tag{2.62}$$

Hence

$$M(t) = \epsilon \int_{s_1}^{s_2} \overline{u}(s_0, t)(1 + tv(s_0, t)\kappa(s_0, t) + O(t^2))ds_0 + O(\epsilon^2), \qquad \boxed{\text{bb3}}) \tag{2.63}$$

where recall $\overline{u} = \overline{U}$ is the average of u over the variable r or z at fixed (s_0, t). It follows that

$$\frac{d}{dt}M(0) = \epsilon \int_{s_1}^{s_2} (\overline{u}_t + \overline{u} v \kappa)\, ds_0 + O(\epsilon^2). \qquad \boxed{\text{bb8}} \tag{2.64}$$

Next, with a more careful analysis than before, we find the following expressions for the fluxes, accurate to $O(\epsilon)$:

$$\sigma_1(s,t) = -(1 + a_1\epsilon) \int_{s_1}^{s_2} v(s,t)\overline{u}(s,t)\, ds + O(\epsilon^2), \qquad \boxed{\text{bb10a}} \tag{2.65}$$

where a_1 is the constant in (2.42), and

$$\sigma_2 = \pi D(1 + a_1\epsilon) \int_{s_1}^{s_2} \overline{u}_{ss} ds + O(\epsilon^2). \qquad \boxed{\text{bb9a}} \tag{2.66}$$

In place of (2.55) we now have

$$\epsilon\,(\overline{u}_t + \overline{u} v \kappa) = -(1 + a_1\epsilon) v(s,t)\overline{u}(s,t) + (1 + a_1\epsilon)\overline{u}_{ss} + O(\epsilon^2). \qquad \boxed{\text{bb11a}} \tag{2.67}$$

Again, we drop the bars over u and omit the final error term to obtain

$$u_t = \frac{1}{\epsilon^*} u_{ss} - \frac{1}{\epsilon^*} v(s,t)u(s,t) - uv\kappa, \qquad \boxed{\text{bb11}} \tag{2.68}$$

where $\epsilon^* = \frac{\epsilon}{1+a_1\epsilon}$.

The pair of equations (2.68), (2.57), together with the arbitrary initial prescription of $\Gamma(0)$ and $u(s,0)$, constitute a reasonable initial value problem. The short time existence of a solution of this initial-value problem was proved by Mayer and Simonett [14], [15].

The significance of the terms on the right side of (2.68) is as follows. The first represents the change in concentration due to diffusion along the grain boundary, the second is the change due to loss of solute atoms to the crystal during the motion of the grain boundary, and the last is the change due to the stretching of the boundary during its motion.

2.7 The quick transient problem

$\boxed{\text{tran}}$

When the prescribed initial data $(u(s,0), \Gamma(0))$ for (2.68), (2.57) does not satisfy the compatibility constraint given for (2.57), (2.58), there may be an initial rapid process wherein u is adjusted to satisfy the constraint. We give here an approximate description of that process in some cases.

The quick transient operates on a faster time scale $\bar{t} = t/\epsilon$. Making this change of variable, we see that to lowest order (2.68) becomes

$$u_{\bar{t}} = u_{ss} - vu. \qquad \boxed{\text{cc3}} \tag{2.69}$$

Equation (2.57) remains the same.

If $\rho \ll 1$, $\kappa(s,0) > 0$, and there exists no source such as occurs for the plate problem described in Sec. 2.5, then initially $v = O\left(\frac{1}{\rho}\right) \gg 1$ from (2.57), and hence from (2.69), u will decay rapidly to 0. At the same time, $\Gamma(t)$ moves rapidly by a dynamic forced motion by curvature law according to (2.57). In this transient process, there is still a difficult coupling between the dynamics of u and Γ.

In the case of the plate problem described in Sec. 2.5 and studied in steady state in Sec. 3, again when $\rho \ll 1$, we expect that a rapid transient will bring a wide range of initial states to one of the steady solutions of Prob. I or II in Sec. 3.1. The general mechanism of this process, however, is still unknown.

An easier case is when $\rho = O(1)$. Then the speed remains $O(1)$, so that the curve Γ moves only a small distance from its initial position $\Gamma(0)$ during the short time evolution governed by the time scale of $\bar{t}$. Therefore the term κ in (2.57) may be considered fixed and known, and the value of v obtained therefore substituted into (2.69) to yield a single equation

$$u_{\bar{t}} = u_{ss} - \frac{1}{\rho}(\kappa + u^2)u, \qquad \boxed{\text{cc4}} \tag{2.70}$$

a semilinear heat equation to be solved with initial data $u(s,0)$ given. If $\kappa > 0$, the solution can be expected to approach a unique $\bar{t}$-independent solution of (2.70) as $\bar{t} \to \infty$. In fact, this can be proved for all physically interesting boundary conditions on $\Gamma(t)$, since the nonlinearity in (2.70) is monotone decreasing in u.

This $\bar{t}$-limiting state can then be used as initial condition for the evolution (2.57), (2.58) under the slower time scale t.

If $\kappa < 0$ or κ changes sign, then sub- and super-solutions can be used to prove the existence of stable stationary solutions of (2.70), not necessarily unique, which are limits as $\bar{t} \to \infty$ of wide classes of solutions. Again, the evolution now proceeds under the slower time scale.

3 Steady motion of a grain boundary with source at one or two ends

$\boxed{\text{SS}}$

In this section we look for special solutions of (2.57), (2.58) corresponding to experiments involving a metal plate immersed in a solute vapor.

Problem I below represents a plate of dimensionless width H with a single grain boundary connecting the two faces. At the faces there is a vapor with given concentration. Solute is supplied equally at the two plate faces and after diffusing, is deposited in the growing grain. As before, the geometry is 2D. The motion has reached a steady state, so that $\Gamma(t)$ moves without changing shape to the left with speed c in a direction along the surface of the plate.

More general solutions of (2.57), (2.58) with appropriate boundary conditions presumably converge to those of the equations below, which are for steady traveling waves.

Symmetry with respect to the midline is assumed. The problem when vapor is present at only one of the two faces can be handled as easily; only obvious changes need be made.

Problem II corresponds to a plate so thick that no steady configuration can exist with the grain boundary passing completely through the plate.

The theorems give basic existence of traveling waves for the two problems, together with finiteness of the penetration distance into the metal plate, in the case of the second problem. We have not as yet been able to prove uniqueness of the solutions of this steady-state model.

For H near a critical value beyond which no solution of Prob. I exists, we argue in Sec. 3.3 that the grain boundary bulges out in the region in the middle of the plate and moves approximately by curvature alone. In that section we approximate the solution in the bulge region and find its width as a function of c. This gives rise to the conjecture given there about the relation between the critical value of H and the penetration distance H_∞ associated with Prob. II.

Note: The forcing relation does not have to be u^2 for most of the following to work. The term $-u^2$ in (3.2) can be replaced by $-f(u)$, where f is any differentiable strictly increasing function with $f(0) = 0$, and many analogous results continue to hold.

3.1 Problems and results

prres

In Prob. I, H is the half-thickness of the plate. The top face is at $x_2 = 0$ in the (x_1, x_2) plane, so the plate occupies the strip $\{-2H \le x_2 \le 0\}$. The migrating grain boundary can be represented in the form $x_1 = X(x_2) - ct$.

We generally formulate the problems in terms of its angle of inclination $\theta = \arctan X'(x_2)$, and consider only the top half $\{-H \le x_2 \le 0\}$ of the plate; the bottom half is then obtained by symmetry. The steady migration is to the left, and the top half of the grain boundary lags further behind as one goes deeper into the plate, so that $\theta \in (-\frac{\pi}{2}, 0]$.

Let s denote arclength along the grain boundary measured from the top ($x_2 = s = 0$), and in Prob. I let S be the unknown arclength to the midpoint ($x_2 = -H$), where $\theta(S) = 0$. Then we may consider the variables θ and u each to be a function only of s. The relation between the function $\theta(s)$ and the Cartesian coordinates of points on Γ is given by

$$x_2 = -\int_0^s \cos\theta(\sigma)d\sigma, \quad x_1 = -\int_0^s \sin\theta(\sigma)d\sigma - ct. \qquad \boxed{\text{yrep}} \tag{3.1}$$

We have

$$\kappa = \theta'(s), \quad v = c\cos\theta(s).$$

Our solutions satisfy $\kappa < 0$ near the edge $\{s = 0\}$ and $v > 0$ everywhere.

In terms of these variables, the equations (2.57), (2.58) become (3.2) and (3.3) below.

Problem I: Given numbers $0 < \rho \le 1$ and $H > 0$, find numbers c, S and functions $\theta(s)$, $u(s)$ defined on $[0, S]$ such that

$$\theta'(s) = \rho c \cos\theta(s) - u^2(s), \qquad \boxed{\text{th-eq}} \tag{3.2}$$

$$u''(s) - c\cos\theta(s)u(s) = 0, \qquad \boxed{\text{u-eq}} \tag{3.3}$$

$$\theta(s) \in (-\pi/2, 0], \quad \theta(0) = 0, \quad \theta(S) = 0, \qquad \boxed{\text{th-bc}} \tag{3.4}$$

$$u(s) \in (0, 1], \quad u(0) = 1, \quad u'(S) = 0, \qquad \boxed{\text{u-bc}} \tag{3.5}$$

$$\int_0^S \cos\theta(s)ds = H. \qquad \boxed{\text{H}} \tag{3.6}$$

Problem II: Given a number $0 \le \rho \le 1$, find a number c and functions $\theta(s)$, $u(s)$ defined on $[0, \infty)$ such that (3.2) and (3.3) hold, as well as

$$\theta(s) \in (-\pi/2, 0], \quad \theta(0) = 0, \qquad \boxed{\text{th-bc2}} \tag{3.7}$$

$$u(s) \in (0, 1], \quad u(0) = 1. \qquad \boxed{\text{u-bc2}} \tag{3.8}$$

Theorem 1 *(a) Problem II has a solution. It satisfies*

$$u(\infty) = 0, \quad \theta(\infty) = -\pi/2. \qquad \boxed{\textit{inf}} \tag{3.9}$$

(b) If $H < \sqrt{\rho}$, there exists a solution of Prob. I.

We have not yet been able to prove the solutions are unique, although we conjecture that they are. In any case, there are certain properties which all solutions share.

Theorem 2 *There exist functions $H^*(\rho) > 0$ and $c_*(\rho) > 0$, depending only on ρ, such that*
(a) The condition

$$H < H^* \qquad \boxed{\textit{finH}} \tag{3.10}$$

is necessary for the existence of a solution of Prob. I.
(b) Every solution of Prob. I or II satisfies

$$c \geq c_*. \qquad \boxed{\textit{cstar}} \tag{3.11}$$

(c) For each solution of Prob. II, there exists a finite number H_∞ satisfying

$$H_\infty \doteq 2\int_0^\infty \cos\theta(s)ds = 2c^{-1}\left[\int_0^\infty u^2(s)ds - \frac{\pi}{2}\right] < \infty. \qquad \boxed{\textit{H0}} \tag{3.12}$$

Moreover,

$$u(s) \leq O(s^{-1}), \quad \theta(s) + \frac{\pi}{2} \leq O(s^{-2}) \qquad \boxed{\textit{as}} \tag{3.13}$$

as $s \to \infty$.

Part (a) of this theorem means that when the plate's thickness surpasses some critical amount, depending on ρ, there is no steady solution representing a grain boundary which extends clear through the plate. Part (c) implies that when the plate is infinitely thick, the steady solution (Prob. II) penetrates only a finite distance H_∞ into the material.

3.2 Proofs

$\boxed{\text{prs}}$ We shall need the following lemmas.

Lemma 1 $\boxed{\textit{lm1}}$ *Let (θ, u, c) satisfy (3.2) and (3.7) for $s \in [0, S]$ for some $0 < S \leq \infty$, $0 \leq \rho \leq 1$, with $\theta(S) = 0$ if $S < \infty$ and $S = \infty$ if $\rho = 0$. Assume $u(s) > 0$ is differentiable, decreasing, and strictly decreasing for small positive s. Then*
(a) If $\theta'(s_1) \geq 0$ and $s > s_1$, then $\theta'(s) \geq \theta'(s_1)$.
(b) If $S = \infty$, then θ is a nonincreasing function.
(c) If $S < \infty$, then $\theta'(S) > 0$.
(d) $\rho c < 1$.

Lemma 2 $\boxed{\textit{lm2}}$
Let (θ, u, c) satisfy (3.3) for $s \in [0, S]$ for some $0 < S \leq \infty$. Assume $c\cos\theta(s) > 0$, $u(0) = 1$, $u'(S) = 0$ if $S < \infty$, and u bounded in any case. Then
(a) $u(s) > 0$.
(b) $u'(s) < 0$.

Proof of Lemma 1.

(a) The case $\rho = 0$ is trivial, since $\theta' = -u^2 < 0$. Assume $\rho > 0$. Note that

$$\theta''(s) = -\rho c(\sin\theta)\theta' - (u^2)'. \qquad \boxed{\text{th-eq3}} \tag{3.14}$$

Let $a > 0$, and $e(s) = \exp\left[\rho c \int_a^s \sin\theta(s) ds\right]$, so that (since $\sin\theta \leq 0$ and $c > 0$ by (d)) e is nonincreasing in s. Multiplying the above equation by $e(s)$, we get

$$(e(s)\theta'(s))' = -e(s)(u^2)' \geq 0,$$

so that for $s > a$, $\theta'(s) \geq \theta'(a)[e(s)]^{-1} \geq \theta'(a)$ if $\theta'(a) \geq 0$.

(b) and (c) follow from (a).

(d) Again the case $\rho = 0$ is trivial, so assume $\rho > 0$. From (3.2), (3.7), (3.8) we have $\theta'(0) = \rho c - 1$. Since $\theta(s) \leq 0$ for $s \in (0, S)$, we must have $\theta'(0) \leq 0$, i.e. $\rho c \leq 1$. We can exclude equality here, since in that case $\theta(s)$ would be > 0 for small $s > 0$ due to the fact that u is strictly decreasing. $\diamond$

Proof of Lemma 2.

(a) Since $c\cos\theta(s) > 0$, the equation (3.3) for u obeys a maximum principle, whether its domain $[0, S]$ be finite or infinite. The function $\underline{u} \equiv 0$ is a subsolution, so if u is bounded, $u > 0$.

(b) From part (a) and (3.3), we have $u'' > 0$. If $u' \geq 0$ somewhere, u could not be bounded if $S = \infty$, nor satisfy $u'(S) = 0$ if $S < \infty$. So $u'(s) < 0$. $\diamond$

Lemma 3 $\boxed{\textit{lm3}}$
Let $S \in (0, \infty)$, $\rho > 0$, and let $u(s) > 0$ be a continuous decreasing function defined on $[0, S]$, satisfying $u(0) = 1$, $u'(s) < 0$ for $0 < s < S_0$ for some $S_0 \in (0, S)$.
(a) There exists a unique solution (θ, c) of (3.2), (3.4).
(b) Both $\theta(s)$ and c are strictly decreasing functions of S for $s > 0$.
(c) If $u \geq e^{-s/\sqrt{\rho}}$, then

$$\rho c \geq \frac{\sqrt{\rho}}{2S}\left(1 - e^{-2S/\sqrt{\rho}}\right) \equiv c_0 > 0. \qquad \boxed{\textit{cbd}} \tag{3.15}$$

Proof.
(a) Consider the initial value problem for (3.2) with $\theta(S) = 0$ and c in the interval $u^2(S) < \rho c \leq 1$. Since $\theta'(S) = \rho c - u^2(S) > 0$, the solution $\theta(s)$ is near and less than 0 for s near and less than S. Also $\theta(s) > -\frac{\pi}{2}$ for $0 \leq s \leq S$, since $\theta'(s)$ would have to be nonnegative at the last place where $\theta = -\frac{\pi}{2}$, contradicting (3.2).
Let M be the set of values of c such that $u^2(S) < \rho c \leq 1$ and the solution of the initial value problem satisfies

$$\theta(0) \leq 0. \qquad \boxed{\text{cond7}} \tag{3.16}$$

First, we show that $\frac{1}{\rho} \in M$. Setting $c = \frac{1}{\rho}$ implies that $-\frac{\pi}{2} < \theta(s) < 0$ for $s \in (0, S)$; in fact if $\theta(s^*) = 0$ for s^* in that interval (let it be the last one), then $\theta'(s^*) \leq 0$, which contradicts (3.2) and the decreasing nature of u.

Now let $c^* = \inf M$. Integrating (3.2) with $c = c^*$ after dividing by $\cos\theta$, we find

$$S\rho c^* = \int_{\theta(0)}^{0} \sec\theta d\theta + \int_0^S u^2(s) \sec\theta(s) ds > \int_0^S u^2(s)\, ds > Su^2(S),$$

so that c^* lies in the interior of the allowed c-interval. But the continuity of the solution with respect to c implies that if $\theta(0) < 0$, c^* could not be the infimum. Therefore the solution $\theta(s)$ associated with c^* must satisfy $\theta(0) = 0$.

This provides existence. The uniqueness follows from the monotonicity in c to be proved next (which shows that two solutions must have the same c), together with the uniqueness of solutions of the initial value problem.

(b) For any number $c \in \left(0, \frac{1}{\rho}\right)$, Let $\theta_c(s)$ be the solution of (3.2) with $\theta_c(0) = 0$. Let $\phi(s) = \frac{\partial}{\partial c}\theta_c(s)$, so that as long as $\cos\theta_c \in (-\frac{\pi}{2}, 0]$,

$$\phi' + \rho c \sin(\theta_c(s))\phi = \rho\cos\theta_c(s) > 0, \quad s \in (0, S].$$

This, together with $\phi(0) = 0$, implies $\phi(s) > 0$. We conclude that θ_c is strictly increasing and continuous in c as long as $\cos\theta_c \in (-\frac{\pi}{2}, 0]$.

Now consider a number $S_0 > 0$ and the solution (θ_0, c_0) considered in the proof of (a) corresponding to this value of S. Let $S_1 > S_0$ and let (θ_1, c_1) be its corresponding solution. Then $c_1 < c_0$ because if $c_1 \geq c_0$, the monotonicity with respect to c shown above would imply $\theta_1(S_0) \geq \theta_0(S_0) = 0$, which is a contradiction. Therefore c is a strictly decreasing function of S.

The other part of (b) follows from this since θ_c is increasing in c.

(c) An upper bound for the solution of (3.2), (3.4) is provided as follows. $\theta' \leq \rho c - u^2$, hence $\theta(s) \leq \rho cs - \int_0^s u^2(t)dt$. Therefore $\theta(s) < 0$ for $s \in (0, \hat{S})$ if

$$\rho c < \inf_{s \in (0,\hat{S}]} \left[s^{-1} \int_0^s u^2(t)dt \right] \doteq \tilde{c}[u, \hat{S}] > 0.$$

Thus when $\rho c < \tilde{c}[u, \hat{S}]$, $S > \hat{S}$.

Set $\underline{u} = e^{-s/\sqrt{\rho}}$ and $c_0(\rho, S) = \tilde{c}[\underline{u}, S] > 0$. If $\rho c < c_0$, then also $\rho c < \tilde{c}(\underline{u}, S)$ if $u \geq \underline{u}$. This would yield the contradiction $S > S$. For our solution we must therefore have $\rho c \geq c_0$. A calculation yields that this number c_0 is given by (3.15). $\diamond$

Lemma 4 $\boxed{lm4}$

Given $S \in (0, \infty)$ and a continuous function $c\cos\theta(s)$ such that $0 \leq c\cos\theta(s) \leq \frac{1}{\rho}$ for $0 \leq s \leq S$, there exists a unique solution of (3.3), (3.5), on $[0, S]$. Moreover,

$$e^{-s/\sqrt{\rho}} \leq u(s) \leq 1.$$

Proof. The functions $\bar{u} \equiv 1$ and $\underline{u} \equiv e^{-s/\sqrt{\rho}}$ are super- and sub-solutions of (3.3), (3.5). To check the latter, note that

$$\underline{u}'' - c\cos\theta\underline{u} = (\frac{1}{\rho} - c\cos\theta)\underline{u} \geq 0, \;\; \underline{u}(0) = 1, \;\; \underline{u}'(S) \leq 0.$$

Thus there exists an exact solution between them. It is unique, by the maximum principle. $\diamond$

Proof of Thm 1(a) in the case $\rho > 0$. First, for any given finite $S > 0$, we prove the existence of a solution of (3.2)–(3.5). (This is Problem I with the last condition (3.6) deleted and S prescribed.)

Given $S > 0$, let $K_S = \{(\theta, c) :\ \theta$ a continuous function on $[0, S]$, $-\pi/2 \le \theta(s) \le 0$, $\theta(0) = \theta(S) = 0$, and $c_0(\rho, S) \le \rho c \le 1\}$, where c_0 is given by (3.15). We think of K_S as a closed convex set in the Banach space of pairs (θ, c), where θ is given the uniform norm.

We define a mapping F from K_S into itself. This is done in two steps. We start with a given $(\tilde\theta, \tilde c) \in K_S$.

(i) Solve the following for a function $u(s) > 0$:

$$u''(s) - \tilde c \cos\tilde\theta(s) u(s) = 0, \qquad \boxed{\text{u-eq3}} \tag{3.17}$$

$$u(0) = 1; \quad u'(S) = 0. \qquad \boxed{\text{u-bc3}} \tag{3.18}$$

The existence of a unique solution follows from Lemma 4. Moreover, $u \in C^2([0, S])$ with corresponding norm bounded independently of everything. From Lemma 2(b), $u'(s) < 0$.

(ii) Solve (3.2), (3.4) with the function u already found in (i) inserted into (3.2), for the pair (θ, c).

Again, the existence of a unique solution follows from Lemma 3. Moreover, because of the regularity of u mentioned above, $\theta \in C^3([0, S])$, with corresponding norm bounded in terms of only . From Lemma 4, we have bounds on u which imply, by Lemmas 3(c) and 1(d), that $c_0(\rho, S) \le \rho c < 1$.

This defines the map $(\theta, c) = F(\tilde\theta, \tilde c)$ from K_S into itself. Also F is compact, due to the estimates on the derivatives of u and θ indicated above. The existence of a fixed point follows from the Schauder theorem. This fixed point, together with the associated function u, will satisfy (3.2)–(3.5).

Next we obtain a solution of Prob. II by passing to the limit $S \to \infty$. Again, the above estimates on derivatives of u and θ show that they form an equicontinuous family, depending on the parameter S. On each s-interval $I_k = [0, k]$ (k an integer), there is therefore a subsequence $S_{n_k} \to \infty$ along which the corresponding solutions $(\theta_{n_k}, u_{n_k}, c_{n_k})$ converge to a limit. A diagonal subsequence converges everywhere to a limit (θ, u, c) which satisfies (3.2), (3.3), (3.7) and (3.8).

We finally prove (3.9). By the monotonicity of θ and u (Lemmas 1b and 2b), $\theta(\infty)$ and $u(\infty)$ exist. And by (3.2), $\rho c \cos\theta(\infty) = u^2(\infty)$. If the two sides of this equation did not vanish, then the coefficient $c\cos\theta(s)$ of u in (3.3) would be positive and bounded away from zero. Therefore by comparison with a solution of the same equation with that coefficient replaced by a positive constant, we would have that u decays to 0 as $s \to \infty$, a contradiction.

Therefore $u(\infty) = 0 = c\cos\theta(\infty)$. Thus either $\theta(\infty) = -\frac{\pi}{2}$ or $c = 0$. If $c = 0$, (3.3), (3.5), would imply $u \equiv 1$, which is impossible since $u(\infty) = 0$. Therefore $c \ne 0$ and $\theta(\infty) = -\frac{\pi}{2}$. This completes the proof.

Proof of Thm 1(a) in the case $\rho = 0$.

We start with an auxiliary problem: given $S > \pi$ and $\delta > 0$, solve

$$\theta'(s) = -u^2(s), \quad \theta(0) = 0,\ \theta(S) = -\frac{\pi}{2} + \delta, \qquad \boxed{\text{kk1}} \tag{3.19}$$

$$u''(s) = c\cos\theta(s) u(s), \quad u(0) = 1,\ u'(S) = 0. \qquad \boxed{\text{kk2}} \tag{3.20}$$

Let $g(k) = \frac{1-e^{-k}}{k}$; it is a decreasing function of $k > 0$ satisfying $g(0) = 1,\ g(\infty) = 0$. Let $c_1 < c_2$ satisfy

$$Sg(2\sqrt{c_2\alpha}S) < \frac{\pi}{2} - \delta < Sg(2\sqrt{c_1}S), \qquad \boxed{\text{c1c2}} \tag{3.21}$$

where $\alpha = \cos\left(-\frac{\pi}{2} + \delta\right) > 0$. This is possible by the properties of g.

Let K be the set of all continuous functions $\theta(s),\ 0 \le s \le S$ satisfying $\theta(0) = 0,\ \theta(S) = -\frac{\pi}{2} + \delta,\ \theta(s) \in [-\frac{\pi}{2} + \delta, 0]$. We supply θ with the uniform norm and construct a compact mapping ¿From K into itself.

Given $\tilde\theta \in K$, (i) solve for u and c:

$$u'' = c\cos\tilde\theta u, \quad u(0) = 1,\ u'(S) = 0, \quad \int_0^S u^2 ds = \frac{\pi}{2} - \delta. \qquad \boxed{\text{kk3}} \tag{3.22}$$

We show that a unique solution exists. If $c > c_2$, then $c\cos\tilde\theta > c_2\alpha$, and by an estimate like that in the proof of Lemma 4, $u < e^{-\sqrt{c_2\alpha}s}$. Hence

$$\int_0^S u^2 ds < Sg\left(2\sqrt{c_2\alpha}S\right) < \frac{\pi}{2} - \delta. \qquad \boxed{\text{kk5}} \tag{3.23}$$

On the other hand if $c < c_1$, by the analogous argument,

$$\int_0^S u^2 ds > Sg\left(2\sqrt{c_1}S\right) > \frac{\pi}{2} - \delta. \qquad \boxed{\text{kk7}} \tag{3.24}$$

Since the solution u depends continuously and monotonically on c, there is a unique value of $c \in (c_1, c_2)$ for which the integral condition is satisfied.

(ii) With this value of u, set $\theta(s) = -\int_0^s u^2(t)dt$. This function is in K.

This gives a mapping of K into itself; it is compact because a priori estimates on derivatives of the image follow from the differential equations. It therefore has a fixed point, which will generate, for given $S,\ \delta$, a solution of the problem (3.19), (3.20).

We now let $S \to \infty$ and $\delta \downarrow 0$. A standard equicontinuity argument shows the existence of a subsequence approaching a solution of the parts of (3.19), (3.20) not involving S. Moreover the limit functions will have ranges in the intervals $u(s) \in [0,1],\ \theta(s) \in (-\frac{\pi}{2}, 0)$. By the dominated convergence theorem, we have

$$\int_0^\infty u^2(s)ds = \frac{\pi}{2},$$

and since u is monotone decreasing, it satisfies $u(\infty) = 0$. Similarly, $\theta(\infty) = -\frac{\pi}{2}$. This finishes the proof of Thm. 1(a) in the case $\rho = 0$. $\diamond$

Proof of Thm. 1(b)

We shall use the notation $s = \xi S,\ u(\xi S) = v_S(\xi),\ \theta(\xi S) = \phi_S(\xi)$. We work with the functions ϕ and v on the interval $0 \le \xi \le 1$. Let M be the following closed convex set in the Banach space of triples (ϕ, c, S), where $\phi \in C^0([0,1])$ with the uniform norm, and c and S are real numbers:

$$M = \{(\phi, c, S) : \phi(0) = \phi(1) = 0,\ -\frac{\pi}{2} \le \phi(s) \le 0,\ c_0 \le \rho c \le 1,\ 0 \le S \le T\}, \qquad \boxed{\text{MM}} \tag{3.25}$$

where $c_0 > 0$ will be chosen later and T is chosen so large that

$$H < \sqrt{\rho}\left(1 - e^{-2T/\sqrt{\rho}}\right). \qquad \boxed{\text{TT}} \tag{3.26}$$

This is possible by the assumption on H.

We now define a compact mapping from M into itself, in three steps. Let $(\tilde{\phi}, \tilde{c}, \tilde{S})$ be an arbitrary element of M.

(i) Solve the following for a function $v(\xi)$, $\xi \in [0,1]$:

$$\ddot{v} - \tilde{S}^2 \tilde{c}(\cos\tilde{\phi})v = 0, \quad v(0) = 0, \ \dot{v}(1) = 0. \qquad \boxed{\text{TT1}} \qquad (3.27)$$

where dots mean $\frac{d}{d\xi}$.

The solution exists by a slightly altered Lemma 4, which provides the bounds

$$e^{-\tilde{S}\xi/\sqrt{\rho}} < v(\xi) \le 1. \qquad \boxed{\text{vb}} \qquad (3.28)$$

(ii) Let

$$u(s) = \begin{cases} v\left(\frac{s}{\tilde{S}}\right), & s \le \tilde{S}, \\ v(1), & s \ge \tilde{S}. \end{cases} \qquad \boxed{\text{uuu}} \qquad (3.29)$$

By (3.28), it satisfies

$$u(s) \ge e^{-s/\sqrt{\rho}}. \qquad \boxed{\text{ubb}} \qquad (3.30)$$

For each $S \le T$, solve for $\theta = \theta_S(s)$, $c = c_S$:

$$\theta' = \rho c \cos\theta - u^2, \quad \theta(0) = \theta(S) = 0, \quad \theta \in (-\frac{\pi}{2}, 0]. \qquad \boxed{\text{phi}} \qquad (3.31)$$

Lemma 3(a) provides a unique solution, depending continuously on S. Moreover by Lemma 3(b), c_S is a decreasing function of S and satisfies (3.15). The argument leading to (3.15) now yields the lower bound

$$\rho c_S \ge \frac{\sqrt{\rho}(1 - e^{-2S/\sqrt{\rho}})}{2S} = g(2S/\sqrt{\rho}) \ge g(2T/\sqrt{\rho}) \equiv c_0. \qquad \boxed{\text{cb}} \qquad (3.32)$$

This is the value of c_0 we use in the definition of M.

Now define $h(S) = \frac{2}{\rho c_S}\int_0^S u^2(s)ds$, a continuous function of S with $h(0) = 0$. We wish to choose $S < T$ so that

$$H = h(S). \qquad \boxed{\text{Heq}} \qquad (3.33)$$

By the decreasing nature of c_S, we see that $h(S)$ is an increasing function of S. Therefore there will be a unique solution of (3.33) with the required bound provided that $h(T) > H$.

By the lower bound (3.30), the estimate $c_S < \frac{1}{\rho}$ from Lemma 1(d) and the definition (3.26), we determine that

$$\begin{aligned} h(T) &\ge 2\int_0^T e^{-2s/\sqrt{\rho}} ds \\ &= \sqrt{\rho}\left(1 - e^{-2T/\sqrt{\rho}}\right) > H. \end{aligned}$$

The next step is therefore possible:

(iii) Select $S < T$ such that $h(S) = H$.

With this choice of S, we set $\phi(\xi) = \theta_S(S\xi)$, $c = c_S$, and the definition of our map from M into itself is complete. The mapping is compact; in fact by (3.27) and (3.29), $\ddot{u}$ has a uniform bound, and hence from (3.31), θ_S and therefore the new function ϕ has derivative bounded independently of the initial function $\tilde{\phi}$.

The map therefore has a fixed point (ϕ, c, S). The corresponding functions $\theta(s) = \phi(s/S)$, $u(s) = v(s/S)$ provide the solution of Prob. I. In fact the equations (3.2)–(3.5) are immediate, and we need only check (3.6). But that also follows from (3.33) and integrating (3.2) from 0 to S. $\diamond$

We now turn to the proof of Thm. 2, for which we need the following two lemmas.

Lemma 5 $\boxed{\textit{l-1}}$ *Let $S > 0$ and let the functions u, ψ satisfy*

$$u'' - \psi u = 0, \quad 0 < s < S, \qquad \boxed{\textit{upsi}} \tag{3.34}$$

$$u(0) = 1, \quad u'(S) = 0, \quad \psi > 0, \qquad \boxed{\textit{upsi-bc}} \tag{3.35}$$

$$au^2 + buu' < \psi \qquad \boxed{\textit{upsi-ineq}} \tag{3.36}$$

for some positive numbers a and b.

Then there exists a number m, depending on a and b but not on S, such that

$$0 < u(s) < \frac{m}{s+1}. \qquad \boxed{\textit{u-bd}} \tag{3.37}$$

The same conclusion holds if $S = \infty$ and the boundary condition at S is replaced by $u(\infty) = 0$.

Proof. Note that $u > 0,\ u' < 0$ by Lemma 2. Consider the nonlinear differential operator

$$N_S[v] \doteq v'' - (av^2 + bvv')v, \quad 0 < s < S,$$

with associated boundary conditions $v(0) = 1,\ \ v'(S) = 0$. Now u is a subfunction for N_S, because (3.36) shows that $N_S[u] > 0$.

We also construct a superfunction in the form

$$\overline{v} = \frac{A}{s+B} + \epsilon s \qquad \boxed{\text{olv}} \tag{3.38}$$

for A and B to be specified below, and $\epsilon = \frac{2A}{(S+B)^2}$ designed so that $\overline{v}'(S) > 0$. We write

$$N_S[\overline{v}] = \overline{v}'' + \overline{v}^2(-a\overline{v} + b(-\overline{v}'))$$

and use the facts that $-\overline{v}' < \frac{A}{(s+B)^2}$ and $\overline{v} > \frac{A}{s+B}$ to estimate

$$-a\overline{v} + b(-\overline{v}') < \frac{A}{s+B}\left[-a + \frac{b}{s+B}\right].$$

We now choose $B = \frac{2b}{a}$ so that the bracket on the right $\leq -\frac{a}{2} < 0$, and hence

$$N_S\overline{v} < \overline{v}'' - \overline{v}^2 \frac{aA}{2(s+B)} < \frac{A}{(s+B)^3}\left[2 - \frac{A^2 a}{2}\right].$$

We finally choose A so large that $N_S\overline{v} < 0$, and also $\overline{v}(0) > 1$. Both A and B are independent of S.

We now have a superfunction $\overline{v}$ and a subfunction u. We must show specifically that this implies $u \leq \bar{v}$, because N_S does not enjoy a general comparison principle. If it were not true, then $w = \bar{v} - u$ would have a negative minimum at some point s_0, which cannot be 0 or S, by our choice of boundary conditions on $\bar{v}$. Therefore at $s_0 \in (0, S)$, we have $w' = 0,\ w'' \geq 0,\ \bar{v} < u$. Now

$$\begin{aligned} 0 > N_S[\bar{v}] - N_S[u] &= w'' - a(\bar{v}^3 - u^3) - b(\bar{v}^2 - u^2)\bar{v}' \\ &\geq (u - \bar{v})[a(\bar{v}^2 + u^2) + b\bar{v}'(\bar{v} + u)] \\ &\geq (u - \bar{v})(u + \bar{v})(a\bar{v} + b\bar{v}'). \end{aligned}$$

If $a\bar{v}+b\bar{v}'>0$ at s_0, then we obtain a contradiction, proving that $u \le \bar{v}$. but

$$a\bar{v}+b\bar{v}' = \frac{A}{s+B}\left(a-\frac{b}{s+B}\right)+\epsilon(s+1)>0$$

by our previous choice of B. Hence

$$u(s) \le \overline{v}(s) = \frac{A}{s+B}+\epsilon s$$

for $0 \le s \le S$. Since $\epsilon s \le \frac{2As}{(S+B)^2} < \frac{2A}{s+B}$, we obtain the desired conclusion (3.37) if $S<\infty$.

The case $S=\infty$ may be handled as follows. In the above proof, replace S by any finite positive number S^*, and use, as subfunction, the restriction of u to $[0,S^*]$. The superfunction $\overline{v}$ remains the same. We thus obtain (3.37) for $s \in [0,S^*]$ with m independent of S^*. It therefore holds for all s. $\diamond$

Lemma 6 $\boxed{\text{l-2}}$ *For some $S>0$ and $c_*>0$, let θ and u satisfy (3.2), (3.4), $u>0,\ u'<0,\ u''>0,\ c\ge c_*$. Then there exist positive a and b, depending only on c_* and β, such that*

$$au^2+buu' < c\cos\theta. \qquad \boxed{\text{ineq1}} \tag{3.39}$$

If θ and u satisfy (3.2), (3.3), (3.7), (3.8), then (3.39) holds for all s.

Proof. We define

$$p(s) \doteq \frac{\rho c\cos\theta(s)}{\theta(s)+\pi/2}.$$

Clearly

$$\frac{2\rho c}{\pi} < p(s) < \rho c \qquad \boxed{\text{hineq}} \tag{3.40}$$

for all s. The equation (3.2) can be written

$$\theta' - p(s)(\theta+\frac{\pi}{2}) = -u^2. \qquad \boxed{\text{newth}} \tag{3.41}$$

Multiplying (3.41) by the integrating factor $e^{-\int p\,ds}$, we learn that $\int_0^S e^{-\int_0^s p(t)dt}u^2(s)ds = \frac{\pi}{2}\left(1-e^{-\int_0^S p(s)ds}\right)$ and

$$\theta(s)+\frac{\pi}{2} = \int_s^S \exp\left[\int_t^s p(\tau)d\tau\right]u^2(t)dt + \frac{\pi}{2}e^{-\int_s^S p(t)dt} \qquad \boxed{\text{exp-th}} \tag{3.42}$$

$$= \int_s^S (u^2(t)-u^2(s))\exp\left[\int_t^s p(\tau)d\tau\right]dt + u^2(s)q(s)+\frac{\pi}{2}e^{-\int_s^S p(t)dt}, \qquad \boxed{\text{exp-th1}} \tag{3.43}$$

where by (3.40) $q(s) = \int_s^S \exp\left[-\int_s^t p(\tau)d\tau\right]dt > \frac{1}{\rho c}\left(1-e^{-\rho c(S-s)}\right)$. Since $u\le 1$, the last term in (3.43) $\ge u^2(s)\frac{\pi}{2}e^{-\rho c(S-s)}$, hence since $\rho c<1$ from Lemma 1(d), the sum of the last two terms $\ge u^2(s)$.

Using the convexity of u^2, we may replace the factor $u^2(t)-u^2(s)$ in the integrand of (3.43) by $(t-s)(u^2)'(s)$, thereby converting (3.43) into an inequality with "$\ge$". We note that $(u^2)'(s) = 2u(s)u'(s)<0$. Since (from (3.40))

$$2\int_s^\infty (t-s)\exp\left[-\int_s^t p(\tau)d\tau\right]dt \le \frac{\pi^2}{2\rho^2c^2},$$

we get from (3.43)

$$\theta(s) + \frac{\pi}{2} \geq u^2(s) + \frac{\pi^2}{2\rho^2 c^2} u(s) u'(s).$$

Therefore

$$c \cos\theta \geq \frac{2c}{\pi}(\theta + \pi/2) \geq \frac{2c_*}{\pi} u^2 + \frac{\pi}{\rho^2 c_*} u u'. \tag{3.44}$$

Hence the desired conclusion (3.39).

This proves the lemma in the case $S < \infty$. The other case is when (3.2), (3.3) hold for all $s > 0$. The proof in this case is obtained by simply replacing S by ∞ in the above proof. $\diamond$

Proof of Thm. 2(b) Let $c_* = \inf \hat{C}$, where $\hat{C}$ is the set of all possible velocities c for solutions of Prob. I or II, for fixed ρ. Since $\rho c \in (0, 1)$, we have $c_* \geq 0$. We have only to show strict inequality here. There exists a sequence (θ_k, c_k, u_k) of solutions with $c_k \downarrow c_*$. Let $S_k \leq \infty$ be the associated values of S. We may also require that $S_k \to S_\infty$. Now $S_\infty > 0$ (it may be infinite) because an easy argument shows that c is near $\frac{1}{\rho}$ when S is small.

The common bounds for all the functions θ_k and u_k and equations (3.2) and (3.3) imply their second derivatives are uniformly bounded and equicontinuous. A standard compactness argument shows that there is a subsequence converging to a solution of Prob. I or II on $(0, S_\infty)$, where $0 < S_\infty \leq \infty$, with velocity $c = c_*$. If the latter were 0, then $u \equiv 1$ by (3.3), and in view of (3.2), our limit solution of (3.2) could not satisfy (3.4) or (3.7). $\diamond$

Proof of Thm. 2(c) Lemma 6 guarantees that the solution satisfies the hypotheses of Lemma 5, where we set $\psi = c\cos\theta$. The upper bound (3.37) so obtained on u shows the first part of (3.13) and that $\int_0^\infty u^2(s) ds < \infty$. Integrating (3.2), we find that for all s,

$$\theta(s) = \rho c \int_0^s \cos\theta(t) dt - \int_0^s u^2(t) dt.$$

Passing to the limit as $s \to \infty$, we obtain (3.12). The last part of (3.13) follows from $\theta' = \rho c \cos\theta - u^2 < 0$. $\diamond$

Proof of Thm. 2(a) The conclusion (3.37) of Lemma 5 implies that $\int_0^S u^2(s) ds$ is bounded independently of S. The upper bound H^* on H follows from this, the fact that $H = \frac{2}{\rho c} \int_0^S u^2(s) ds$, and the lower bound $c \geq c_*$ in (3.11). $\diamond$

3.3 Critical value of H

bulge

For fixed $\rho > 0$, we expect that there is a value $H_c(\rho)$ of H such that a solution of Problem I exists if and only if $H < H_c$. Theorem 1(b) would then provide a lower bound: $H_c \geq \sqrt{\rho}$, although it will be shown below that there may be reason to believe it is much larger when ρ is small. It is also reasonable that for H slightly less than H_c, the upper part of the grain boundary can be approximated by the solution of Problem II, which extends to infinity in the direction of the positive x-axis. The mirror image of such a configuration would be attached to the bottom of the plate. What would result is a long bulge in the middle of the plate, where the two approximate solutions of Prob. II are connected one with the other. In the region of this bulge, points on the grain boundary will correspond to arclengths which are very large, so that solute material would have to diffuse far from the sources on the plate faces. It will then be reasonable to neglect the solution concentration (and therefore the solute motive force) in that region. Setting $u = 0$ in (3.2), approximating the bulge by one of infinite extent, and resetting the origins of both s and x_2 to the midpoint of the bulge, we obtain the following equation, with boundary conditions, for $\theta(s)$:

$$\theta'(s) = \rho c \cos\theta(s), \tag{3.45}$$

$$\theta(0) = 0, \quad \theta(\pm\infty) = \pm\frac{\pi}{2}. \tag{3.46}$$

This can be solved immediately in the form

$$\theta(s) = -\rho c x_2(s), \qquad \boxed{\text{th=y}} \tag{3.47}$$

since (3.1) $x_2 = -\int_0^s \cos\theta(s')ds'$. Thus x_2 passes from $\frac{\pi}{2\rho c}$ to $-\frac{\pi}{2\rho c}$ as s goes from $-\infty$ to ∞. Note that this approximation is only for the part of the grain boundary far to the right. In it, the speed c is assumed to be known. It will be (approximately) the value associated with Prob. II.

To summarize, the configuration will consist of two solutions of Prob. II, one the mirror image of the other and each penetrating a distance H_∞, together with a bulge of thickness $\frac{\pi}{\rho c}$ connecting them. Recalling that H is defined as the half-thickness of the plate, we obtain the following conjecture about the value of H_c:

Conjecture: There exists a solution of Prob. I if and only if $H < H_\infty + \frac{\pi}{2\rho c}$, where c and H_∞ are the speed and penetration depth corresponding to Problem II.

3.4 Slow and fast motion when $\rho \ll 1$

$\boxed{\text{slofst}}$

When ρ is small, Thm. 1(b) gives the existence of a spanning configuration moving with high speed, when the thickness H is small, namely less that $\sqrt{\rho}$. The reason the speed is large can be seen from the proof of that part of the theorem. In fact (3.25) gives the lower bound $c \geq \frac{c_0}{\rho}$, and (3.32) yields $c_0 = g(2T/\sqrt{\rho}) \geq C\sqrt{\rho}$ for some C, small enough ρ, and fixed T (if ρ is small enough, we may select a fixed T to satisfy (3.26)). Therefore $c \geq \frac{C}{\sqrt{\rho}} \gg 1$.

These highly mobile boundaries have the property that the curvature term on the left of (3.2) is neglible compared to the others, so that $c \approx \frac{\bar{u^2}}{\rho}$, bar denoting some average. Since H is small, u is not too small, due to its sources at the faces of the thin plate. Therefore c is large.

On the other hand, the bulging solutions whose existence we surmised in the previous section have moderate speed. Their speed, in fact, is determined approximately by that for the trailing solution of Prob. II with $\rho = 0$. In the trailing parts of the configuration, the left side of (3.2) balances the last term on the right, the first term on the right being neglible.

In the bulging part, however, the concentration is negligible and the curvature term on the left of (3.2) balances the first term on the right, which (since c is now a known $O(1)$ quantity) is $O(\rho)$. The bulge therefore has small curvature and width of the order $\frac{1}{\rho}$.

We therefore have two kinds of solutions when $\rho \ll 1$: rapid ones when H is sufficiently small, and slower ones when H takes large values in a certain range. The existence of solutions for values of H intermediate between these ranges is an open question.

4 Discussion

disc

We began the modeling process by a set of phase field equations (2.1-(2.3) in which the following dimensional parameters appeared:

$$\begin{aligned}
\delta &= \text{a length characteristic for the gradient contributions to the free energy, and} \\
& \text{also a measure of the grain boundary width} \\
\hat{\epsilon} &= \text{a nondimensional product of elastic modulus and Vegard's law coefficient} \\
D_m &= \text{an average diffusivity of solute in the grain boundary} \\
u^* &= \text{ a characteristic value for the concentration} \\
\tau &= \text{a relaxation time for crystallization}
\end{aligned}$$

In terms of these, our asymptotic analysis proceeded under the assumption that

$$\hat{\epsilon} u^* \ll 1. \qquad \boxed{\text{delass}} \tag{4.1}$$

This, then, was our basic order of magnitude assumption. Another was that $\rho = \frac{\hat{\epsilon}(u^*)^2 D_m \tau}{\delta^2} \le O(1)$.

Our most basic characteristic lengths were δ, which is comparable to the grain boundary width, and $L = \frac{\delta}{\hat{\epsilon}(u^*)^2} \gg \delta$, which in many cases is the length associated with variations along the grain boundary. A characteristic time is $T = \frac{\tau}{\rho \hat{\epsilon}^2 (u^*)^4}$.

We find a solution of Problem II (for the semiinfinite plate) representing a grain boundary which lags behind the motion at the source (which is at the moving intersection of the grain boundary with the face of the plate), so that its shape becomes parallel to the face of the plate at a penetration distance of the order of L. Its speed is of the order L/T.

At a special plate thickness, there is also a steady moving grain boundary spanning the plate which consists of a pair of lagging configurations as described, connected by a much thicker bulge with width of the order $\frac{L}{\rho} = \frac{\delta A}{\epsilon^2 (u^*)^4}$. Finally, there are faster grain boundaries with speed $O(L/(T\sqrt{\rho})$ spanning very thin films of thickness $O(\sqrt{\rho} L)$.

The following reasonable orders of magnitudes for these quantities follow from the estimates given in [4]:

$$\delta \approx 10^{-9}\text{m.}, \quad \epsilon \approx 10^{-3}, \quad L \approx 10^{-6}\text{m.},$$
$$\rho \approx 10^{-3}, \quad L/T \approx 10^{-4}\text{m/sec.}$$

A typical penetration distance will then be $L \approx 10^{-6} m$, and the thickness of plates supporting the slow boundaries indicated in Sec. 3.4 will be of the order $L/\rho \approx 10^{-3}$m, with speed $O(10^{-4})$m/sec. The fast ones will travel 10-100 times faster.

When $\rho \ll 1$, one is tempted to approximate the free boundary evolution problem (2.57), (2.58) by formally setting $\rho = 0$. However, such a resulting problem is likely to be ill posed as an evolution problem. The small parameter ρ apparently serves as a regularizing parameter for the ill-posed problem which must be kept, even though small.

Passing to the steady problem considered in Sec. 3, one has additional difficulties in setting $\rho = 0$. In fact in that case there will never be a solution of Problem I, in which the grain boundary spans the plate, because (3.2) implies that every solution $\theta(s)$ is monotone. The grain boundary could not turn back to meet the other face. However, there is a reasonable solution of the infinite plate problem; this is apparently the only case in which the approximation $\rho = 0$ is reasonable when $\rho \ll 1$.

Many other problems suggest themselves by the treatment given here. The modeling can be extended to the motion of other grain boundary surfaces in a 3D material. Then the "curvature" κ in (2.57) will denote twice the mean curvature, and the diffusion term in (2.58) will be 2D diffusion in the surface. Corresponding plate problems with reservoir boundary conditions are formulated in a straightforward manner. For example one analog of the steady problem considered here would be the nonsteady expansion of a grain boundary which is radially symmetric with respect to an axis perpendicular to the plate.

The unidirectional nature of the model here, i.e. our assumption that $v > 0$ (end of Sec. 2.1), excludes many interesting phenomena such as double-seam configurations [10, 2]. When a boundary begins to propagate into a grain which has already been changed by a DIGM motion, the basic equations will change somewhat, because the concentration u_0 appearing in (2.4) will no longer be 0. Modeling and analysis can no doubt be performed to handle this situation as well.

The steady problem considered in Sec. 3 involved a source of solute at one or two boundaries of the moving grain boundary $\Gamma(t)$. One can also formulate problems in which Γ is a closed curve and therefore has no boundaries or sources. For example suppose it is a circle with changing radius, and that u is uniform on the circle. The compatibility condition for initial conditions for (2.57), (2.58) then state that initially either $v = 0$ or $u = 0$. A transient solution such as in Sec. 2.7 will bring arbitrary initial distributions to that condition. Whether v or u vanishes depends on whether the circle is expanding or contracting. In the former case, the transient brings it to rest with no further motion. In the latter, the circle will shrink to a point according to motion by curvature.

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Appendix: Comparison of notation and assumptions

The model considered in [3] is the same as that in our section 3, namely (3.2) and (3.3), except that an additional effect of grooving is incorporated.

For reference, our equations (2.57), (2.58) take the following form when written in dimensional form:

$$\frac{\tau}{\delta}\hat{v} = \delta\hat{\kappa} + \hat{\epsilon}\hat{u}^2, \tag{4.2}$$

$$\hat{u}_{\hat{s}\hat{s}} - \frac{1}{\delta D_m}\hat{v}\hat{u} = 0. \tag{4.3}$$

They are equivalent to equations used in [3]. In the two papers, dimensionless constants A are used which are identical if one identifies the average diffusivity $\bar{D}$ in [3] with $\frac{D_m}{\pi}$. The usages of the parameter δ are the same, and except for factors involving u^*, the parameters ϵ are also the same.

Except for the difference in ϵ, the parameter assumptions given in [3] are the same as our (2.12). The notation and scaling in the two papers differ, however. The most important difference is in the length scale: in [3], the dimensionless length is given by

$$X = Ax/\delta$$

rather than by $x = \epsilon\hat{x}/\delta$ as in our (2.8).

We use another dimensionless parameter ρ (2.6), and such a parameter v is used in [3]. They are related, disregarding the above-mentioned difference in ϵ and a factor 2π, by

$$\rho \approx v^2.$$

Conjectures are made in the two papers about the maximal width of specimen thickesses admitting a steady moving grain boundary spanning the faces. This is H_c in our notation; see Section 3.3. It is proposed as a function of ρ or v. In the present paper, the conjecture is in order of magnitude only, but it agrees with that in [3]. On the other hand, a lower bound is proved in our Thm. 1(b). If ρ is small, this lower bound is far from the conjectured value.