

COUPLED SURFACE AND GRAIN BOUNDARY MOTION: A TRAVELLING WAVE SOLUTION

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ABSTRACT. Existence and uniqueness are proven for a travelling wave solution for a problem in which motion by mean curvature is coupled with surface diffusion. This problem pertains to a bicrystal in a "quarter-loop" geometry in which one grain grows at the expense of the other, and the internal grain boundary between the two crystals contacts the exterior surface at a "groove root" or "tri-junction" where various balance laws hold. Far in front and behind the groove root the overall height of the bicrystal is assumed to be unperturbed. Whereas in a previous paper [15] a partially linearized formulation was considered for which explicit solutions could be found, here we treat the fully nonlinear problem. Employing an angle formulation and a scaled arc-length parameterization, we reduce the problem to the solution of a third order ODE with a jump condition at the origin. Existence is proven if m , the ratio of the exterior surface energy to the surface energy of the grain boundary, is less than about $\approx .92$. Uniqueness of these solutions is demonstrated within the class of single-valued solutions. A numerical comparison is made with the solution of the partially linearized formulation found earlier for the sake of illustration.

Keywords: Third order ODEs, travelling waves, surface diffusion, motion by mean curvature, grain boundary motion.

1. INTRODUCTION

In this paper, we analyze the coupled motion of a grain boundary which is attached at a "groove root" to an exterior surface which evolves under the influence of surface diffusion. More precisely, we find travelling wave solutions describing grain boundary motion in a bicrystal in the context of the "quarter loop" geometry [9, 10], see Figure 1. In accordance with the manner in which the bicrystal is produced, it is reasonable to assume that the cross-section of the bicrystal is uniform, so that the problem is effectively two-dimensional. And assuming that the cross-sectional dimensions of the specimen are small relative to its length, it is also reasonable to treat the bicrystal as if it were of infinite lateral extent. We assume the grain boundary to evolve according to motion by mean curvature,

$$\mathbf{V} = A\kappa, \tag{1.1}$$

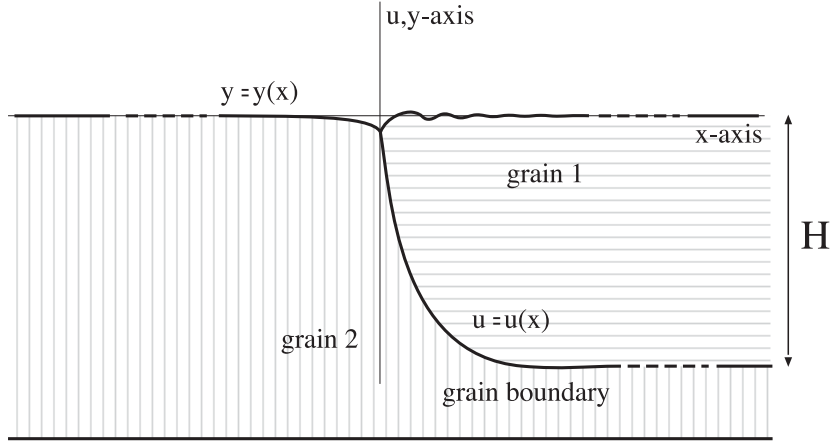


FIGURE 1. The quarter loop bicrystal geometry.

where \mathbf{V} denotes the normal velocity of the surface and κ denotes its mean curvature. Away from the "groove root" or "tri-junction," the evolution of the exterior surface can be assumed to be governed by surface diffusion

$$\mathbf{V} = -B\kappa_{ss}, \quad (1.2)$$

where s denotes an arc-length parameterization of the exterior surface. At the groove root or tri-junction it is reasonable to assume that the boundary conditions are given Young's law, continuity of the surface chemical potentials, and the balance of mass flux. Young's law can be written as

$$\frac{\gamma_{\text{exterior surface}}}{\sin(\theta_{\text{left}})} = \frac{\gamma_{\text{exterior surface}}}{\sin(\theta_{\text{right}})} = \frac{\gamma_{\text{grain boundary}}}{\sin(\theta_{\text{groove root}})} \quad (1.3)$$

where $\gamma_{\text{exterior surface}}$, $\gamma_{\text{grain boundary}}$ denote respectively the surface energies of the exterior surface and of the grain boundary, $\theta_{\text{groove root}}$ denotes the angle at the groove root, and θ_{left} , θ_{right} , denote the angles between the exterior surface and the grain boundary, on the left and on the right respectively. Continuity of the surface chemical potentials and the balance of mass flux can be written as

$$\kappa(0^-) = \kappa(0^+), \quad (1.4)$$

and

$$\kappa_s(0^-) = \kappa_s(0^+), \quad (1.5)$$

where the origin of the arc-length parameterization along the upper surface has been taken to lie at the tri-junction.

In terms of the geometry and the physics, the problem outlined above can be understood as follows. In the "quarter loop geometry" (See Figure 1), the two crystalline grains which comprise the bicrystal begin initially as parallel components in a single block of material. Bicrystals in such an initial configuration can be produced, for example, by an electron beam floating technique [25]. The two grains in the bicrystal are identical in composition and differ only in their relative crystalline orientation. This discrepancy

manifests itself as a grain boundary which moves in order to reduce the surface energy and to heal the orientation mismatch. Since both grains are of the same material, no bulk energetic effects need to be taken into account. Neglecting possible effects of elasticity, anisotropy and defects [12], the net driving force arises from minimization of the surface energies along the exterior and interior surfaces, and implies the laws of motion (1.2) and (1.1) given above. At the groove root tri-junction, Young's law (1.3) reflects a balance of mechanical forces, continuity of the surface chemical potentials (1.4) can be viewed as either a regularity assumption or as an assumption that the groove root does not contribute in a singular fashion to the overall surface chemical potential, and the condition (1.5) reflects an assumption that there is no mass flowing along the grain boundary and up into the groove root and hence that the mass that flows into the groove root from the left is balanced by the flow of mass to the right of the groove root. A discussion of these boundary conditions can be found in [21, 15]. Recently it has been shown that these boundary conditions can also be obtained as the sharp interface limit of a system of Allen-Cahn/Cahn-Hilliard equations [23, 24]. In the quarter loop geometry, the grain boundary configuration is preserved as the grain boundary and groove root progress through the specimen. It is also reasonable to assume that far in front and far behind the groove root, the original height of the bicrystal is preserved. Within this framework, it makes sense to look for travelling wave solutions.

The quarter loop set up can be envisioned as a relatively simple framework in which to focus on the coupling effect of the motion of the exterior surface with that of the grain boundary, though other relatively simple geometries exist, for example the "Sun and Bauer" geometry ([1, 8]) and in grain growth in thin-film arrays ([28]). However, in these latter contexts, the driving force is not constant and hence it does not make sense to look for travelling wave solutions as we shall do here.

Discussions of coupling grain boundary motion to that of an exterior surface have been ongoing ([11]) since the landmark paper of Mullins [21] in 1958. There the problem given above was formulated, though the equations for the exterior surface were considered in a linearized form and the grain boundary itself was only taken into account in as far as it affected the angle at the bottom of the groove root. In later publications, Mullins considered the motion of an exterior surface coupled to a groove root and the motion of a grain boundary connected to a groove root [20, 19], but not the full coupled system. Within the simplified framework within which he treated these problems, fascinatingly enough he proved [21] that only for some specific value of the angle at the groove root can the groove root progress through the bicrystal as a constant velocity travelling wave whose velocity is determined by the groove depth. The paper [21] contains also a number of speculations with regard to "anchoring" of the grain boundary at the groove root and how a combined anchoring and escape mechanism may give rise to "jerky" or "stop and go" motion. It was long believed that even if the groove root did not actually anchor the grain boundary, then at least it should slow it down. This idea is discussed in our recent paper [15], where in the framework of a partially linearized formulation, it is shown that indeed in general there is some degree of slowing down, though remarkably for certain extreme values of the parameters, the coupling to the exterior surface may indeed cause the grain boundary to accelerate. As it were, the grain boundary may be pulled along by

the evolution of the exterior surface. With regard to "jerky motion" indeed despite all the years which have passed since this was first discussed by Mullins, this phenomenon has yet to be resolved and recent reports of this phenomenon can be found in [10, 26, 27]. It is our intuitive understanding that by further study of these nonlinear travelling wave solutions, accompanied by a subsequent (at least numerical) stability study, some of these questions shall be resolved in the near future.

Since it is our goal to identify travelling wave solutions, we adopt the travelling wave variable: $\xi = x - Vt$, where V denotes the wave speed which we assume to be constant. We also introduce the variables $y(x, t)$ and $u(x, t)$, where $y = y(x, t)$ denotes the height of the exterior surface relative to the height of the exterior surface at $\pm\infty$, and $u = u(x, t)$ denotes the height of the grain boundary, again with respect to the height of the exterior (upper) surface at $\pm\infty$. In order to adopt a dimensionless formulation as in [15], we set

$$y \rightarrow y/H, \quad u \rightarrow u/H, \quad x \rightarrow x/H, \quad \xi \rightarrow \xi/H, \quad t \rightarrow \frac{B}{H^4}t,$$

and define

$$a = \frac{AH^2}{B}, \quad m = \frac{\gamma_{\text{grain boundary}}}{\gamma_{\text{exterior surface}}}, \quad w = \frac{H^3}{B}V.$$

Here a is a dimensionless parameter which reflects the relative response rate of the grain boundary and the exterior surface, m measures the relative surface energies, and w is a dimensionless wave speed.

Employing the notation x instead of ξ for simplicity, we arrive at the following formulation:

$$(\mathbf{P}_y) \left\{ \begin{array}{l} 0 = - \left[\frac{1}{(1+y_x^2)^{1/2}} \left[\frac{y_{xx}}{(1+y_x^2)^{3/2}} \right]_x \right] + wy_x, \quad x \in (-\infty, 0^-) \cup (0^+, \infty), \\ 0 = au_{xx}(1+u_x^2)^{-1} + wu_x, \quad x \in (0, \infty), \\ y(0^+) = y(0^-) = u(0^+), \\ \arctan(y_x(0^+)) - \arctan(y_x(0^-)) = 2 \arcsin \left[\frac{m}{2} \right], \\ \arctan(u_x(0^+)) = -\frac{\pi}{2} + \frac{1}{2} [\arctan(y_x(0^+)) + \arctan(y_x(0^-))], \\ \frac{y_{xx}}{(1+y_x^2)^{3/2}} \Big|_{(0^+)} = \frac{y_{xx}}{(1+y_x^2)^{3/2}} \Big|_{(0^-)}, \\ \left[\frac{1}{(1+y_x^2)^{1/2}} \left[\frac{y_{xx}}{(1+y_x^2)^{3/2}} \right]_x \right]_{(0^+)} = \left[\frac{1}{(1+y_x^2)^{1/2}} \left[\frac{y_{xx}}{(1+y_x^2)^{3/2}} \right]_x \right]_{(0^-)}, \\ y(-\infty) = y(+\infty) = 0, \\ u(+\infty) = -1. \end{array} \right.$$

The first two equations in P_y correspond to (1.1) and (1.2), respectively. The first boundary condition at $x = 0$ is a persistence condition that states that it is unphysical for the tri-junction to spontaneously pull apart. The second and third boundary conditions at $x = 0$ reflect Young's law (1.3), and the fourth and fifth boundary conditions at $x = 0$ correspond to (1.4) and (1.5). The two last lines in P_y prescribe the "far-field" boundary conditions. This formulation was first presented in [15].

In line with the philosophy expressed by Mullins in [20, 21, 4], although theoretically the parameter m may vary between 0 and 2, typically, for example in metals, $0 < m < 1/3$, and can be taken to be a small parameter. This implies in turn by the first of the Young's law conditions that the discontinuity in the slopes of the upper surface at the grain groove is small, and hence in conjunction with the far field boundary conditions for y , it is reasonable to assume that the spatial gradients in y along the entire upper surface are small and to linearize the equations for y around the trivial state. However, by considering the far field behavior of u and the fact that the grain boundary must be attached to the upper surface which is fairly flat, gradients in u cannot be assumed to be uniformly small over the entirety of the grain boundary, and hence the equations for u cannot be similarly linearized [4]. This lead us in [15] to consider the following partially linearized formulation:

$$(\mathbf{P}'_y) \left\{ \begin{array}{l} 0 = -y_{xxxx} + wy_x \quad x \in (\infty, 0^-) \cup (0^+, \infty), \\ 0 = au_{xx}(1 + u_x^2)^{-1} + wu_x \quad x > 0, \\ y(0^+) = y(0^-) = u(0^+), \\ y_x(0^+) - y_x(0^-) = m, \\ \arctan(u_x(0^+)) = -\frac{\pi}{2} + \frac{1}{2}[y_x(0^+) + y_x(0^-)], \\ y_{xx}(0^+) = y_{xx}(0^-), \\ y_{xxx}(0^+) = y_{xxx}(0^-), \\ y(+\infty) = y(-\infty) = 0, \\ u(+\infty) = -1. \end{array} \right.$$

Variants of (\mathbf{P}'_y) are also possible to consider. For example, one could consider the system (\mathbf{P}''_y) obtained by replacing the second boundary condition in (\mathbf{P}'_y) by:

$$\arctan(u_x(0^+)) = -\frac{\pi}{2} + \frac{1}{2} \left[\arctan(y_x(0^+)) + \arctan(y_x(0^-)) \right]. \quad (1.6)$$

In [15] we showed that both the systems, (\mathbf{P}'_y) , (\mathbf{P}''_y) , admit unique travelling wave solutions which can be given explicitly in terms of the wave speed w , which is determined as by a cubic equation whose coefficients depend on the dimensionless parameters. (The coefficients are a little different in each of the two cases.)

In [15] we also calculated the shape, u_f , and wave speed, w_f , of a grain boundary which is freely moving; i.e., which is unaffected by modulation of the exterior surface which is assumed in this context to be planar, and show that for typical parameter values, $0 < w < w_f$, though the decrease in speed is usually not great. However for certain extreme values of the parameters, it may also happen that $w_f < w$, in contradiction to previously held notions [11].

The stability of the solutions which were found in [15] was tested numerically [29] and analytically [18] and did not appear to indicate such features as "jerky" motion or "stop and go" motion. However, nonlinear effects may be critical with respect to the onset of instabilities [6, 7]. Thus the emphasis in the present paper is on travelling wave solutions to the full nonlinear formulation.

The outline of our paper is as follows. In §2 we express Problem P_y in terms of angle variables and (scaled) arc-length parameterizations, and demonstrate that u , y , and w can all be determined via a third order ODE with a jump condition at the origin, which we shall refer to as Problem P_Ψ . In §3 we demonstrate that the solution to Problem P_Ψ is unique as long as $-\frac{\pi}{2} \leq \Psi \leq \frac{\pi}{2}$ for arbitrary values of the parameter m , which implies in turn that the solution to Problem P_y is unique within the class of single-valued functions. In §4 we demonstrate existence of a solution to Problem P_Ψ for sufficiently small values of m . Our analysis here relies on the structure of the stable and unstable manifolds of the governing equation and on some simple transversality arguments. The methodology here is somewhat similar to that employed for example in [2], though there the analysis is simpler since there the problem formulation does not contain jumps. In §5 we treat Problem P_Ψ via integral formulations using the Green functions corresponding to the linearizations of P_Ψ at $\pm\infty$ respectively, and existence and uniqueness of solutions for $0 < m < \approx .92$ is proven using iteration arguments. Uniqueness follows from §3 once the necessary bounds are demonstrated for the solution. While preparing this manuscript, we also approached the fully nonlinear problem using shooting methods and were able in [16] to prove existence for all $m \in [0, 2)$. We believe however that the proof of §5 is of interest in its own right, in that it presents an original methodology for solving ODEs with jumps and it also provides a possible computational framework for calculating solutions. In the final section, §6 we present some numerical solutions to Problems P_Ψ and P_y for the sake of illustration, comparing them with the solutions of the partially linearized problem which was treated in [15]. Further numerics can be found in [17].

2. AN ANGLE FORMULATION

In this section we express Problem P_y in terms of angle variables and (scaled) arc-length parameterizations. In this fashion we obtain a certain third order ODE on the whole real line with a jump condition at zero whose solution determines u , y , and w . With this in mind and since we are looking for single valued solutions, we define

$$\Phi = \arctan u_x \quad \text{and} \quad \Psi = \arctan y_x, \quad (2.1)$$

and we require that

$$-\frac{\pi}{2} \leq \Phi \leq 0 \quad \text{and} \quad -\frac{\pi}{2} \leq \Psi \leq \frac{\pi}{2}. \quad (2.2)$$

We introduce arc-length parameterizations of the exterior surface and the grain boundary by defining

$$s_1 = \int_0^x \sqrt{1 + u_x^2} dx, \quad x \in (0, \infty), \quad \text{and} \quad s_2 = \int_0^x \sqrt{1 + y_x^2} dx, \quad x \in (-\infty, \infty). \quad (2.3)$$

See Figure 2. Note that $s_1 = s_2 = 0$ at the triple junction, and that s_2 is an "arc-length parameterization" which assumes negative values along the exterior surface for $x \leq 0$.

We shall now express Problem P_y in terms of

$$\Phi = \Phi(s_1, t), \quad s_1 \in (0, \infty), \quad \text{and} \quad \Psi = \Psi(s_2, t), \quad s_2 \in (-\infty, 0) \cup (0, \infty).$$

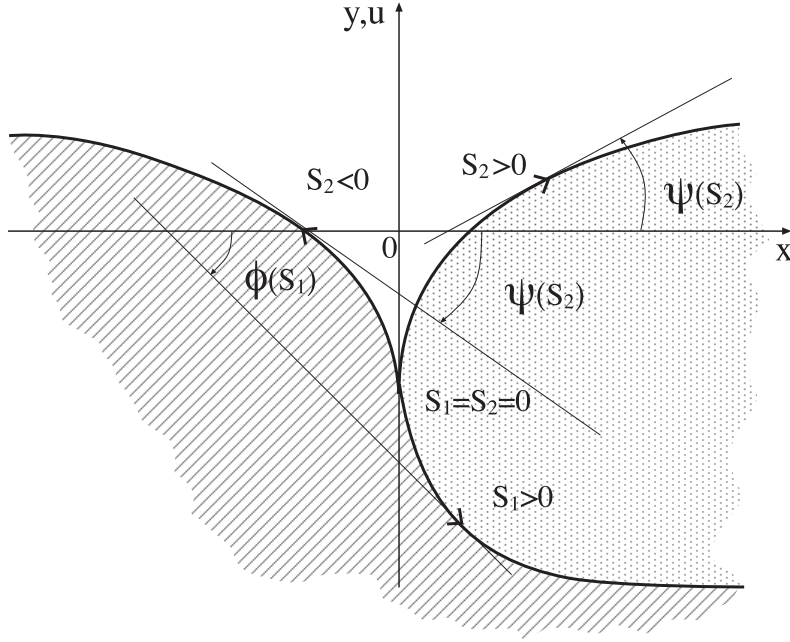


FIGURE 2. The variables Φ , Ψ and s_1 , s_2 .

Substituting (2.1) and (2.3) into the governing equations for u and y from Problem P_y ,

$$a \frac{\partial \Phi}{\partial s_1} = -w \sin \Phi, \quad s_1 \in (0, \infty). \quad (2.4)$$

$$\frac{\partial^3 \Psi}{\partial s_2^3} = w \sin \Psi, \quad s_2 \in (-\infty, 0) \cup (0, \infty), \quad (2.5)$$

With respect to the second, third, fourth, and fifth boundary conditions at zero which are given in Problem P_y , we may write

$$\Psi(0^+) - \Psi(0^-) = 2 \arcsin(m/2), \quad (2.6)$$

$$\Phi(0^+) = -\frac{\pi}{2} + \frac{1}{2}[\Psi(0^+) + \Psi(0^-)], \quad (2.7)$$

$$\frac{\partial \Psi}{\partial s_2}(0^+) = \frac{\partial \Psi}{\partial s_2}(0^-), \quad (2.8)$$

$$\frac{\partial^2 \Psi}{\partial s_2^2}(0^+) = \frac{\partial^2 \Psi}{\partial s_2^2}(0^-). \quad (2.9)$$

The far field boundary conditions in Problem P_y imply that

$$\Phi(+\infty) = \Psi(\pm\infty) = 0. \quad (2.10)$$

In order to express the remaining (first) boundary condition in Problem P_y at the triple junction in terms of Φ and Ψ , we first note that by (2.1)–(2.3), and the far field conditions

on u and y

$$u(s_1) = -1 - \int_{s_1}^{\infty} \sin \Phi ds, \quad s_1 \in (0, \infty), \quad y(s_2) = - \int_{s_2}^{\infty} \sin \Psi ds, \quad s_2 \in (-\infty, \infty). \quad (2.11)$$

Substituting (2.11) into the first boundary condition at the triple junction and using the far field conditions on u and y , we obtain the integral constraint

$$-1 - \int_0^{\infty} \sin \Phi ds = - \int_0^{\infty} \sin \Psi ds. \quad (2.12)$$

Employing (2.4),(2.5), and (2.10) in (2.12),

$$\frac{a}{w} \Phi(0^+) = -1 - \frac{1}{w} \frac{\partial^2 \Psi}{\partial s_2^2}(0^+). \quad (2.13)$$

Solving (2.4) in conjunction with (2.10)

$$\Phi(s_1) = 2 \arctan \left(\tan \left[\frac{1}{2} \Phi(0^+) \right] e^{-(w/a)s_1} \right), \quad (2.14)$$

and recalling (2.7), it follows that

$$\Phi = \Phi(s_1; \Psi(0^+), \Psi(0^-), w). \quad (2.15)$$

and can be decoupled from the governing system of equations.

It remains now to solve the equations governing Ψ and w :

$$\frac{\partial^3 \Psi}{\partial s_2^3} = w \sin \Psi, \quad s_2 \in (-\infty, 0) \cup (0, \infty), \quad (2.16)$$

$$\Psi(0^+) - \Psi(0^-) = 2 \arcsin(m/2), \quad (2.17)$$

$$\frac{\partial \Psi}{\partial s_2}(0^+) = \frac{\partial \Psi}{\partial s_2}(0^-), \quad (2.18)$$

$$\frac{\partial^2 \Psi}{\partial s_2^2}(0^+) = \frac{\partial^2 \Psi}{\partial s_2^2}(0^-), \quad (2.19)$$

$$\Psi(\pm\infty) = 0, \quad (2.20)$$

together with the constraint

$$-1 - \frac{1}{w} \frac{\partial^2 \Psi}{\partial s_2^2}(0^+) = \frac{a}{w} \left[-\frac{\pi}{2} + \frac{1}{2} [\Psi(0^+) + \Psi(0^-)] \right] \quad (2.21)$$

which follows from (2.7) and (2.13).

Note that the equations given above may be decoupled from the constraint (2.21), by introducing the rescaled variable $s = w^{1/3}s_2$. In terms of the variable s , we may write (2.16)–(2.20) as:

$$\frac{\partial^3 \Psi}{\partial s^3} = \sin \Psi, \quad s \in (-\infty, 0) \cup (0, \infty), \quad (2.22)$$

$$\Psi(0^+) - \Psi(0^-) = 2 \arcsin(m/2), \quad (2.23)$$

$$\frac{\partial \Psi}{\partial s}(0^+) = \frac{\partial \Psi}{\partial s}(0^-), \quad (2.24)$$

$$\frac{\partial^2 \Psi}{\partial s^2}(0^+) = \frac{\partial^2 \Psi}{\partial s^2}(0^-), \quad (2.25)$$

$$\Psi(\pm\infty) = 0. \quad (2.26)$$

Similarly from (2.21), we obtain

$$-1 - \frac{1}{w^{1/3}} \frac{\partial^2}{\partial s^2} \Psi(0^+) = \frac{a}{w} \left[-\frac{\pi}{2} + \frac{1}{2} [\Psi(0^+) + \Psi(0^-)] \right]. \quad (2.27)$$

Note that in terms of $\lambda = w^{1/3}$, (2.27) may be written as

$$f(\lambda) := \lambda^3 + \lambda^2 \frac{\partial^2}{\partial s^2} \Psi(0^+) - a \left[\frac{\pi}{2} - \frac{1}{2} [\Psi(0^+) + \Psi(0^-)] \right] = 0,$$

which parallels equation (11) obtained in [15]. In [15] we noted that the wave speed was uniquely determined by (11) since $f(0)$ could shown there to be negative. In the present context

$$f(0) = -a \left[\frac{\pi}{2} - \frac{1}{2} [\Psi(0^+) + \Psi(0^-)] \right],$$

and the assumption $a > 0$ and the constraint (2.2) imply that $f(0)$ is negative unless

$$\Psi(0^-) = \Psi(0^+) = \frac{\pi}{2}. \quad (2.28)$$

However, by (2.23), if m is assumed to be a small positive parameter, then (2.28) is only possible if $m = 0$, and if $m = 0$ then (2.22)–(2.26) admits the trivial solution $\Psi \equiv 0$. This, in conjunction with uniqueness which will be demonstrated in §3, implies that (2.28) cannot occur in the context of single-valued solutions. Hence, modulo the details of uniqueness which have been postponed, we conclude that the wave speed w is uniquely determined by (2.27).

Therefore,

$$w = w(\Psi; a),$$

where by (2.22)–(2.26), $\Psi = \Psi(m)$, and hence by (2.15)

$$\Phi = \Phi(s_1; \Psi, a).$$

Thus the solution to Problem P_y is completely determined by the system

$$(\mathbf{P}_\Psi) \begin{cases} \Psi_{sss} = \sin \Psi, & s \in (-\infty, 0) \cup (0, \infty), \\ \Psi(0^+) - \Psi(0^-) = 2 \arcsin(m/2), \\ \Psi_s(0^+) = \Psi_s(0^-), \\ \Psi_{ss}(0^+) = \Psi_{ss}(0^-), \\ \Psi(\pm\infty) = 0. \end{cases}$$

The remainder of this paper is devoted to the solution of the system P_Ψ , which we will refer to as Problem P_Ψ , though in the last section we will return to give some numerical portraits of the solutions in terms of the original variables $u = u(x)$ and $y = y(x)$.

3. UNIQUENESS

Theorem 1. *Let $m \in [-2, 2]$ be arbitrary. Then there exists at most one solution $\Psi \in \mathcal{C}^3((-\infty, 0) \cup (0, \infty))$ to Problem P_Ψ such that $-\frac{\pi}{2} \leq \Psi \leq \frac{\pi}{2}$.*

Remark: Note that, though m is allowed to be arbitrary, the above theorem implies uniqueness of the solution to Problem P_y only within the class of single-valued functions.

Proof. Suppose that there exist two solutions to Problem P_Ψ , which we denote by Ψ_1, Ψ_2 , such that $\Psi_1, \Psi_2 \in \mathcal{C}^3((-\infty, 0) \cup (0, \infty))$ and $-\frac{\pi}{2} \leq \Psi_1, \Psi_2 \leq \frac{\pi}{2}$. Defining

$$\tilde{\Psi} := \Psi_1 - \Psi_2,$$

it follows that

$$\tilde{\Psi}_{sss} = \sin \Psi_1 - \sin \Psi_2, \tag{3.1}$$

$\tilde{\Psi} \in \mathcal{C}^3((-\infty, \infty))$, and $\tilde{\Psi}, \tilde{\Psi}_s, \tilde{\Psi}_{ss} \rightarrow 0$ as $s \rightarrow \pm\infty$. Multiplying (3.1) by $\tilde{\Psi}$, using a little trigonometry, and integrating over the interval $(-\infty, \infty)$,

$$\int_{-\infty}^{\infty} \tilde{\Psi} \tilde{\Psi}_{sss} ds = 4 \int_{-\infty}^{\infty} \left[\frac{\tilde{\Psi}}{2} \sin\left(\frac{\tilde{\Psi}}{2}\right) \right] \cos\left(\frac{\Psi_1 + \Psi_2}{2}\right) ds. \tag{3.2}$$

Integrating by parts

$$\int_{-\infty}^{\infty} \tilde{\Psi} \tilde{\Psi}_{sss} ds = \left[\tilde{\Psi} \tilde{\Psi}_{ss} \right]_{-\infty}^{\infty} - \int_{-\infty}^{\infty} \tilde{\Psi}_s \tilde{\Psi}_{ss} ds = \left[\tilde{\Psi} \tilde{\Psi}_{ss} - \frac{1}{2} (\tilde{\Psi}_s)^2 \right]_{-\infty}^{\infty} = 0.$$

Hence

$$4 \int_{-\infty}^{\infty} \left[\frac{\tilde{\Psi}}{2} \sin\left(\frac{\tilde{\Psi}}{2}\right) \right] \cos\left(\frac{\Psi_1 + \Psi_2}{2}\right) ds = 0. \tag{3.3}$$

Note now that the constraint $-\frac{\pi}{2} \leq \Psi_1, \Psi_2 \leq \frac{\pi}{2}$ implies that $-\frac{\pi}{2} \leq \frac{1}{2}\tilde{\Psi} \leq \frac{\pi}{2}$ and $-\frac{\pi}{2} \leq \frac{1}{2}(\Psi_1 + \Psi_2) \leq \frac{\pi}{2}$. Therefore

$$\frac{\tilde{\Psi}}{2} \sin\left(\frac{\tilde{\Psi}}{2}\right) \geq 0, \quad \cos\left(\frac{\Psi_1 + \Psi_2}{2}\right) \geq 0.$$

Returning to (3.3), we see that for almost all $s \in (-\infty, \infty)$, either $\tilde{\Psi}(s) = 0$ or $\frac{1}{2}(\Psi_1 + \Psi_2) = \pm\frac{\pi}{2}$. The latter possibility implies that $\Psi_1 + \Psi_2 = \pm\pi$, which implies in turn by virtue of the assumed range of Ψ that $\Psi_1 = \Psi_2 = \pm\frac{\pi}{2}$. Hence $\tilde{\Psi} \equiv 0$, from which uniqueness follows. \square

4. EXISTENCE FOR $0 < m \ll 1$

In this section we give a proof of existence which relies on the structure of the stable and unstable manifold of the trivial solution $\Psi = 0$ and on the autonomy of the governing equations. We obtain a necessary and sufficient condition for a solution on the unstable manifold for $s < 0$ and a solution on the stable manifold for $s > 0$ to meet at the origin and to satisfy there the boundary conditions from Problem P_Ψ . Using the implicit function theorem, we demonstrate that for m positive and sufficiently small, this condition

is satisfied. By the construction, the solution thus obtained satisfies $-\frac{\pi}{2} \leq \Psi \leq \frac{\pi}{2}$, and therefore it is unique in the sense of Theorem 1 from §3.

Theorem 2. *For m positive and sufficiently small, there exists a solution to P_Ψ .*

Proof. First we study the properties of the stable and unstable manifolds of the trivial solution, in order to find solutions on the right ($s > 0$) and solutions on the left ($s < 0$) which satisfy the "far-field" condition, $\Psi(\pm\infty) = 0$.

On the right, we may write the governing equation in P_Ψ as:

$$\vec{x}_t^R = A^R \vec{x}^R + \vec{f}^R(\vec{x}^R), \quad \vec{x}^R(0^+) = \vec{x}_0^R, \quad (4.1)$$

where $t = s \in (0, \infty)$, $(\vec{x}^R(t))^T = (x_1^R, x_2^R, x_3^R)(t) := (\Psi(t), \Psi_s(t), \Psi_{ss}(t))$,

$$A^R = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}, \quad \vec{f}^R(\vec{x}^R) = \begin{pmatrix} 0 \\ 0 \\ \sin x_1^R - x_1^R \end{pmatrix}, \quad \vec{x}^R(0^+) = \begin{pmatrix} \Psi(0^+) \\ \Psi_s(0^+) \\ \Psi_{ss}(0^+) \end{pmatrix}. \quad (4.2)$$

Similarly on the left, we may write the governing equation as:

$$\vec{x}_t^L = A^L \vec{x}^L + \vec{f}^L(\vec{x}^L), \quad \vec{x}^L(0^+) = \vec{x}_0^L, \quad (4.3)$$

where $t = -s \in (0, \infty)$, $(\vec{x}^L(t))^T = (x_1^L, x_2^L, x_3^L)(t) := (\Psi(-t), \Psi_s(-t), \Psi_{ss}(-t))$,

$$A^L = \begin{pmatrix} 0 & -1 & 0 \\ 0 & 0 & -1 \\ -1 & 0 & 0 \end{pmatrix}, \quad \vec{f}^L(\vec{x}^L) = \begin{pmatrix} 0 \\ 0 \\ -\sin x_1^L + x_1^L \end{pmatrix}, \quad \vec{x}^L(0^+) = \begin{pmatrix} \Psi(0^-) \\ \Psi_s(0^-) \\ \Psi_{ss}(0^-) \end{pmatrix}. \quad (4.4)$$

In order to capture the behavior of the unstable manifolds near $(0, 0, 0)$, it is useful to introduce the change of variables:

$$\vec{y}^R := P^R \vec{x}^R \quad \text{and} \quad \vec{y}^L := P^L \vec{x}^L, \quad (4.5)$$

where

$$P^R = \begin{pmatrix} -\frac{1}{6} & -\frac{1}{6} & \frac{1}{3} \\ \frac{1}{2\sqrt{3}} & -\frac{1}{2\sqrt{3}} & 0 \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \end{pmatrix}, \quad \text{and} \quad P^L = \begin{pmatrix} \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \\ \frac{1}{2\sqrt{3}} & -\frac{1}{2\sqrt{3}} & 0 \\ -\frac{1}{6} & -\frac{1}{6} & \frac{1}{3} \end{pmatrix}.$$

In terms of \vec{y}^R and \vec{y}^L we may write (4.1)–(4.4) as:

$$\vec{y}_t^R = B^R \vec{y}^R + \vec{g}^R(\vec{y}^R), \quad \vec{y}^R(0^+) = \vec{y}_0^R, \quad (4.6)$$

where $\vec{y}_0^R = P^R \vec{x}_0^R$,

$$B^R = \begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} & 0 \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \vec{g}^R(\vec{y}^R) = [\sin(-y_1^R + \sqrt{3}y_2^R + y_3^R) - (-y_1^R + \sqrt{3}y_2^R + y_3^R)] \begin{pmatrix} \frac{1}{3} \\ 0 \\ \frac{1}{3} \end{pmatrix}, \quad (4.7)$$

and

$$\vec{y}_t^L = B^L \vec{y}^L + \vec{g}^L(\vec{y}^L), \quad \vec{y}^L(0^+) = \vec{y}_0^L, \quad (4.8)$$

where $\bar{y}_0^L = P^L \bar{x}_0^L$,

$$B^L = \begin{pmatrix} -1 & 0 & 0 \\ 0 & \frac{1}{2} & \frac{\sqrt{3}}{2} \\ 0 & -\frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix}, \quad \bar{g}^L(\bar{y}^L) = [-\sin(y_1^L + \sqrt{3}y_2^L - y_3^L) + (y_1^L + \sqrt{3}y_2^L - y_3^L)] \begin{pmatrix} \frac{1}{3} \\ 0 \\ \frac{1}{3} \end{pmatrix}. \quad (4.9)$$

Since $\bar{g}^R(0) = \bar{g}^L(0) = 0$, $\bar{g}^R(\bar{y}^R), \bar{g}^L(\bar{y}^L)$ are analytic, and since for any $\epsilon > 0$ there exists a $\delta > 0$ such that

$$|\bar{g}^R(\bar{y}^R) - \bar{g}^R(\tilde{y}^R)| \leq \epsilon |\bar{y}^R - \tilde{y}^R|, \quad |\bar{g}^L(\bar{y}^L) - \bar{g}^L(\tilde{y}^L)| \leq \epsilon |\bar{y}^L - \tilde{y}^L|,$$

if $|\bar{y}^R|, |\tilde{y}^R| \leq \delta$ and $|\bar{y}^L|, |\tilde{y}^L| \leq \delta$, it follows from Theorem 4.1 and Theorem 4.2 in [5, Section 13] that in the neighborhood of the origin $(0, 0, 0)$, $y^R(t)$ has a two-dimensional stable manifold, \mathcal{S}^R , and $y^L(t)$ has a one-dimensional stable manifold, \mathcal{S}^L , and the stable manifolds can be prescribed in the form

$$\mathcal{S}^R = (y_1^R, y_2^R, Y_3^R(y_1^R, y_2^R)), \quad \mathcal{S}^L = (y_1^L, Y_2^L(y_1^L), Y_3^L(y_1^L)), \quad (4.10)$$

where Y_3^R, Y_2^L , and Y_3^L are defined and analytic in a neighborhood of the origin. Moreover,

$$Y_3^R(0, 0) = Y_2^L(0) = Y_3^L(0) = 0, \quad (4.11)$$

$$\frac{\partial}{\partial y_1^R} Y_3^R(0, 0) = \frac{\partial}{\partial y_2^R} Y_3^R(0, 0) = 0, \quad \text{and} \quad \frac{\partial}{\partial y_1^L} Y_2^L(0) = \frac{\partial}{\partial y_1^L} Y_3^L(0) = 0. \quad (4.12)$$

Returning to Problem P_Ψ , we see that we should like to take initial conditions for \bar{y}^R on \mathcal{S}^R and initial conditions for \bar{y}^L on \mathcal{S}^L . If the boundary conditions at the origin in P_Ψ are to be satisfied, then referring to the definitions of \bar{x}^R, \bar{x}^L and B^R, B^L , in terms of $\bar{y}^R(0^+)$ and $\bar{y}^L(0^+)$ this implies that

$$y_1^R(0^+) = Y_3^L(y_1^L(0^+)) - \frac{1}{3} \arcsin\left(\frac{m}{2}\right), \quad (4.13)$$

$$y_2^R(0^+) = Y_2^L(y_1^L(0^+)) + \frac{1}{\sqrt{3}} \arcsin\left(\frac{m}{2}\right), \quad (4.14)$$

$$Y_3^R(y_1^R(0^+), y_2^R(0^+)) = y_1^L(0^+) + \frac{2}{3} \arcsin\left(\frac{m}{2}\right). \quad (4.15)$$

From (4.13)–(4.15) it follows that the existence of a solution to Problem P_Ψ is guaranteed if a value for $y_1^L(0^+)$ can be found such that $G(y_1^L(0^+), m) = 0$ where

$$G(\bar{y}_1, m) := Y_3^R(Y_3^L(\bar{y}_1) - \frac{1}{3} \arcsin\left(\frac{m}{2}\right), Y_2^L(\bar{y}_1) + \frac{1}{\sqrt{3}} \arcsin\left(\frac{m}{2}\right)) - \bar{y}_1 - \frac{2}{3} \arcsin\left(\frac{m}{2}\right).$$

Noting that

$$\frac{\partial}{\partial \bar{y}_1} G(0, 0) = \frac{\partial}{\partial y_1^R} Y_3^R(0, 0) \frac{\partial}{\partial y_1^L} Y_3^L(0) + \frac{\partial}{\partial y_2^R} Y_3^R(0, 0) \frac{\partial}{\partial y_1^L} Y_2^L(0) - 1, \quad (4.16)$$

$$\frac{\partial}{\partial m} G(0, 0) = \frac{1}{2} \left[-\frac{1}{3} \frac{\partial}{\partial y_1^R} Y_3^R(0, 0) + \frac{1}{\sqrt{3}} \frac{\partial}{\partial y_2^R} Y_3^R(0, 0) - \frac{2}{3} \right], \quad (4.17)$$

it follows from the definition of G and (4.11)–(4.12) that

$$G(0, 0) = 0, \quad \frac{\partial}{\partial y_1} G(0, 0) = -1, \quad \text{and} \quad \frac{\partial}{\partial m} G(0, 0) = -\frac{1}{3}, \quad (4.18)$$

and local solvability is implied for m sufficiently small. \square

5. EXISTENCE FOR $0 < m < .92$

In this section, we obtain an integral representation for solutions of the governing equation in P_Ψ which lie on the unstable manifold of $\Psi = 0$ for $s < 0$, and for solutions which lie on the stable manifold for $s > 0$. Then, essentially expressing the condition $G(y_1^L(0^+), m) = 0$ from the previous section in terms of these integral representations, existence is demonstrated by iteration. We prove

Theorem 3. *Suppose that*

$$0 < m < \hat{m}, \quad (5.1)$$

where $\hat{m} \approx .92068702$. Then there exists a unique solution to Problem P_Ψ which satisfies $|\Psi| < \pi/2$.

Remark: The inequality $|\Psi| < \pi/2$ can be shown to imply that the profiles $u = u(x)$, $y = y(x)$ are well-defined for $-\infty < x < \infty$.

Proof. By Theorem 4.5 [5, Chapter 13], all solutions of

$$\Psi_{sss} = \sin \Psi, \quad (5.2)$$

which satisfy the far field condition, $\Psi(-\infty) = 0$, must also satisfy

$$\Psi(s) = O(e^s) \quad \text{as} \quad s \rightarrow -\infty. \quad (5.3)$$

Similarly, all solutions of (5.2) which satisfy $\Psi(+\infty) = 0$, must also satisfy

$$\Psi(s) = O(e^{-\frac{1}{2}s}) \quad \text{as} \quad s \rightarrow +\infty. \quad (5.4)$$

Global existence for (5.2) together with the estimates (5.3), (5.4) and Theorem 4.1 [5, Chapter 13], can then easily be shown to imply that all solutions of (5.2) on the interval $(-\infty, 0)$ satisfying $\Psi(-\infty) = 0$ may be written in the form:

$$\Psi(s) = C_0 e^s + \frac{1}{3} \int_{-\infty}^s g(\Psi(\tilde{s})) G(s - \tilde{s}) d\tilde{s}, \quad -\infty < s < 0, \quad (5.5)$$

and all solutions of (5.2) on the interval $(0, \infty)$ satisfying $\Psi(+\infty) = 0$ may be written in the form:

$$\Psi(s) = e^{-\frac{1}{2}s} (C_1 \cos \frac{\sqrt{3}}{2}s + C_2 \sin \frac{\sqrt{3}}{2}s) - \frac{1}{3} \int_s^\infty g(\Psi(\tilde{s})) G(s - \tilde{s}) d\tilde{s}, \quad 0 < s < \infty, \quad (5.6)$$

where C_0, C_1 , and C_2 are arbitrary constants, and

$$g(u) := \sin u - u, \quad (5.7)$$

$$G(\xi) := e^\xi - 2e^{-\frac{1}{2}\xi} \sin \left(\frac{\sqrt{3}}{2}\xi + \frac{\pi}{6} \right). \quad (5.8)$$

Note that

$$G'(\xi) = e^\xi + 2e^{-\frac{1}{2}\xi} \sin\left(\frac{\sqrt{3}}{2}\xi - \frac{\pi}{6}\right), \quad (5.9)$$

$$G''(\xi) = e^\xi + 2e^{-\frac{1}{2}\xi} \cos\frac{\sqrt{3}}{2}\xi, \quad (5.10)$$

$$G(\xi) + G'(\xi) + G''(\xi) = 3e^\xi, \quad (5.11)$$

$$G(0) = G'(0) = 0, \quad (5.12)$$

$$G''(0) = 3. \quad (5.13)$$

Thus solving P_Ψ has been reduced to finding C_0, C_1 , and C_2 so that the boundary conditions at the origin in P_Ψ are satisfied. We formally find C_0, C_1 , and C_2 by imposing the boundary conditions at the origin, treating $\psi = \Psi(0^-)$ as a parameter and m as a function of the parameter ψ . We get in this manner integral equations which must hold on the intervals $(-\infty, 0)$, and $(0, \infty)$ respectively. We then solve these equations by iteration and obtain a solution to P_Ψ under the condition that

$$\hat{\psi} < \psi < 0, \quad (5.14)$$

where $\hat{\psi}$ is a number such that $m(\hat{\psi}) \approx .92068702$. We complete the proof by showing that conditions (5.1) and (5.14) are equivalent. The proof relies on the following lemmas.

Lemma 5.1. *Let*

$$g(u) := \sin u - u, \quad \Delta u := u_2 - u_1, \quad \text{and} \quad \Delta g := g(u_2) - g(u_1),$$

then

$$|\Delta g| \leq \frac{1}{6} |\Delta u| (u_1^2 + u_1 u_2 + u_2^2). \quad (5.15)$$

Proof. Noting that

$$\Delta g = \int_0^1 \frac{d}{d\mu} g(u_1 + \mu \Delta u) d\mu = -2\Delta u \int_0^1 \sin^2\left(\frac{u_1 + \mu \Delta u}{2}\right) d\mu,$$

we obtain

$$|\Delta g| \leq 2|\Delta u| \int_0^1 \frac{1}{4} (u_1 + \mu \Delta u)^2 d\mu = \frac{1}{6} |\Delta u| (u_1^2 + u_1 u_2 + u_2^2).$$

□

Lemma 5.2. *Suppose that*

$$a_{n+1} = a + qa_n^3, \quad n = 0, 1, 2, \dots, \quad (5.16)$$

where $a_0 = 0$, and a, q are positive constants such that

$$a = \frac{2}{3\sqrt{3}q}. \quad (5.17)$$

Then

$$a_n \leq \frac{3}{2}a, \quad n = 0, 1, 2, \dots \quad (5.18)$$

Proof. Clearly (5.18) holds for $n = 0$. Suppose that (5.18) holds for some fixed $n \in N$. Then (5.16)-(5.18) imply that

$$a_{n+1} \leq a(1 + q\frac{27}{8}a^2) \leq a\left(1 + q\frac{27}{8}\left(\frac{4}{27q}\right)\right) = \frac{3}{2}a.$$

Hence (5.18) holds for all $n \in N$. □

Consider now the following problem:

$$\Psi_{sss} = \sin \Psi, \quad -\infty < s < 0, \quad (5.19)$$

$$\Psi(-\infty) = 0, \quad \Psi(0^-) = \psi, \quad (5.20)$$

where ψ is a real parameter.

Lemma 5.3. *Suppose that*

$$-\sqrt{56/45} < \psi < 0. \quad (5.21)$$

Then there exists a solution $\Psi = \Psi(s; \psi) \in C^3(-\infty, 0)$ to Problem (5.19)-(5.20) such that

$$|\Psi(s)| \leq \frac{3}{2}|\psi|e^s, \quad -\infty < s < 0. \quad (5.22)$$

Proof. All solutions to Problem (5.19)-(5.20), if they exist, may be written in the form (5.5). We may find C_0 using condition (5.20), and formally write the solution as:

$$\Psi(s) = \psi e^s + \frac{1}{3} \int_{-\infty}^s g(\Psi(\tilde{s}))G(s-\tilde{s})d\tilde{s} - \frac{1}{3}e^s \int_{-\infty}^0 g(\Psi(\tilde{s}))G(-\tilde{s})d\tilde{s}, \quad -\infty < s < 0. \quad (5.23)$$

Thus the problem (5.19)-(5.20) is reduced to the integral equation (5.23), which we solve by considering the iterative system:

$$\Psi_0(s) = 0, \quad \Psi_1(s) = \psi e^s, \quad (5.24)$$

$$\Psi_{n+1}(s) = \Psi_1(s) + \frac{1}{3} \int_{-\infty}^s g(\Psi_n(\tilde{s}))G(s-\tilde{s})d\tilde{s} - \frac{1}{3}e^s \int_{-\infty}^0 g(\Psi_n(\tilde{s}))G(-\tilde{s})d\tilde{s}, \quad n = 1, 2, \dots, \quad (5.25)$$

on the interval $-\infty < s < 0$. Let us first estimate $|\Psi_n(s)|$, $n = 0, 1, 2, \dots$. We have from (5.24) that for $-\infty < s < 0$

$$|\Psi_n(s)| \leq a_n e^s, \quad n = 0, 1, \quad (5.26)$$

with

$$a_0 = 0, \quad a_1 = |\psi|. \quad (5.27)$$

We now proceed by iteration. Suppose that (5.26) holds for some fixed $n \in N$ and a_n . We may estimate $|\Psi_{n+1}(s)|$ as follows. Lemma 5.1 with $u_1 = 0$ and $u_2 = \Psi_n(s)$ implies that

$$|g(\Psi_n)| \leq \frac{1}{6}|\Psi_n|^3. \quad (5.28)$$

Formulas (5.25), (5.8) and (5.26), (5.28) imply after some elementary estimates that

$$|\Psi_{n+1}(s)| \leq a_{n+1}e^s,$$

for $-\infty < s < 0$, where

$$a_{n+1} = |\psi| + \frac{5}{42}a_n^3, \quad n \in N. \quad (5.29)$$

It follows from condition (5.21) that $|\psi| < \frac{2}{3\sqrt{3q}}$, where $q = \frac{5}{42}$. Hence (5.27),(5.29) imply by Lemma 5.2 that

$$a_n \leq \frac{3}{2}|\psi|, \quad n = 0, 1, \dots \quad (5.30)$$

Thus (5.26) holds for any $n \in N$, where a_n satisfies (5.30). Therefore, for $-\infty < s < 0$,

$$|\Psi_n(s)| \leq \frac{3}{2}|\psi|e^s, \quad \text{for } n \in N. \quad (5.31)$$

Now we prove that the sequence $\Psi_n(s)$ converges in $C(-\infty, 0)$. It follows from (5.25) that

$$\Delta\Psi_{n+1}(s) := \Psi_{n+1}(s) - \Psi_n(s) = \frac{1}{3} \int_{-\infty}^s \Delta g_n(\tilde{s})G(s - \tilde{s})d\tilde{s} - \frac{1}{3}e^s \int_{-\infty}^0 \Delta g_n(\tilde{s})G(-\tilde{s})d\tilde{s}, \quad (5.32)$$

for $-\infty < s < 0$, where

$$\Delta g_n(\tilde{s}) := g(\Psi_n(\tilde{s})) - g(\Psi_{n-1}(\tilde{s})).$$

Lemma 5.1 implies that

$$|\Delta g_n(\tilde{s})| \leq \frac{1}{6}|\Delta\Psi_n(\tilde{s})|(\Psi_{n-1}^2 + \Psi_{n-1}\Psi_n + \Psi_n^2). \quad (5.33)$$

It follows from (5.31), (5.33) that for $-\infty < \tilde{s} < 0$,

$$|\Delta g_n(\tilde{s})| \leq \frac{9}{8}|\Delta\Psi_n(\tilde{s})|\psi^2 e^{2\tilde{s}}. \quad (5.34)$$

Setting

$$\Theta_n := \sup_{-\infty < s < 0} (e^{-s}|\Delta\Psi_n(s)|), \quad n = 1, 2, \dots, \quad (5.35)$$

it follows from (5.24) that $\Theta_1 = |\psi|$. We get from (5.32) by elementary estimates, using (5.34), (5.35), and (5.8), that for $-\infty < s < 0$

$$|\Delta\Psi_{n+1}(s)| \leq \frac{45}{56}\psi^2\Theta_n e^s, \quad n = 1, 2, \dots \quad (5.36)$$

Formulas (5.35) and (5.36) imply that

$$\Theta_{n+1} \leq \frac{45}{56}\psi^2\Theta_n, \quad n = 1, 2, \dots \quad (5.37)$$

Condition (5.21) guarantees that

$$\frac{45}{56}\psi^2 < 1. \quad (5.38)$$

We have from (5.31),(5.36)-(5.38), and (5.25) that

$$\Psi_n(s) \rightarrow \Psi(s) \quad \text{uniformly on } (-\infty, 0], \quad \text{as } n \rightarrow \infty,$$

where $\Psi(s)$ is solution of (5.23). Moreover, Ψ satisfies (5.22). It follows from (5.22) and (5.23) that $\Psi(s)$ is in fact a solution of (5.19)-(5.20) which belongs to $C^3(-\infty, 0)$. \square

Let us now formally consider solutions $\Psi(s) = \tilde{\Psi}(s; \psi)$ of (5.2) which satisfy the far field condition on the right, $\Psi(\infty) = 0$, which coincide for $-\infty < s < 0$ with the solution $\Psi(s; \psi)$ which was found in Lemma 5.3 for some ψ satisfying (5.21), and which satisfy the boundary conditions from Problem P_Ψ at the origin, where the jump in the angles at the origin, $\Psi_m = \Psi(0^+) - \Psi(0^-)$, which should be equal to $2 \arcsin(m/2)$, is taken to be determined by the parameter ψ . Such solutions may be written in the form (5.6). Differentiating (5.6) and using (5.12) and the boundary conditions at the origin, we get the following algebraic system for C_1 and C_2 :

$$C_1 - \frac{1}{3} \int_0^\infty g(\Psi(\tilde{s}))G(-\tilde{s})d\tilde{s} = \psi + \Psi_m, \quad (5.39)$$

$$-\frac{1}{2}C_1 + \frac{\sqrt{3}}{2}C_2 - \frac{1}{3} \int_0^\infty g(\Psi(\tilde{s}))G'(-\tilde{s})d\tilde{s} = \psi_1(\psi), \quad (5.40)$$

$$-\frac{1}{2}C_1 - \frac{\sqrt{3}}{2}C_2 - \frac{1}{3} \int_0^\infty g(\Psi(\tilde{s}))G''(-\tilde{s})d\tilde{s} = \psi_2(\psi), \quad (5.41)$$

where in (5.40),(5.41) we have set

$$\psi_1(\psi) := \Psi_s(0^-; \psi) \text{ and } \psi_2(\psi) := \Psi_{ss}(0^-; \psi). \quad (5.42)$$

Solving the system (5.40)-(5.41) for C_1 and C_2 , and substituting these values into (5.6), we obtain using (5.8)-(5.11) and some elementary transformations and trigonometry that

$$\Psi(s) = \Psi_1(s) - \frac{1}{3} \int_s^\infty g(\Psi(\tilde{s}))G(s - \tilde{s})d\tilde{s} - \frac{2}{3}e^{-\frac{1}{2}s} \int_0^\infty g(\Psi(\tilde{s}))H_0(s, \tilde{s})d\tilde{s}, \quad (5.43)$$

for $0 < s < \infty$, where

$$\Psi_1(s) := e^{-\frac{1}{2}s} [(-\psi_1(\psi) - \psi_2(\psi)) \cos \frac{\sqrt{3}}{2}s + \frac{1}{\sqrt{3}}(\psi_1(\psi) - \psi_2(\psi)) \sin \frac{\sqrt{3}}{2}s], \quad (5.44)$$

and

$$H_0(s, \tilde{s}) := e^{-\tilde{s}} \cos \frac{\sqrt{3}}{2}s - e^{\frac{1}{2}\tilde{s}} \sin \left(\frac{\sqrt{3}}{2}(s - \tilde{s}) + \frac{\pi}{6} \right). \quad (5.45)$$

Adding (5.39)-(5.41) and using (5.11), we get that

$$\Psi_m = -\psi - \psi_1(\psi) - \psi_2(\psi) - \int_0^\infty g(\Psi(\tilde{s}))e^{-\tilde{s}}d\tilde{s}. \quad (5.46)$$

We now transform (5.44) and (5.46) into a more convenient form. Differentiating (5.23) and using (5.12),(5.42), we get that

$$\psi_1(\psi) = \psi + \frac{1}{3} \int_{-\infty}^0 g(\Psi(\tilde{s}))(G'(-\tilde{s}) - G(-\tilde{s}))d\tilde{s}, \quad (5.47)$$

$$\psi_2(\psi) = \psi + \frac{1}{3} \int_{-\infty}^0 g(\Psi(\tilde{s}))(G''(-\tilde{s}) - G(-\tilde{s}))d\tilde{s}. \quad (5.48)$$

Substituting (5.47) and (5.48) into (5.44) and (5.46), and using (5.8)-(5.11), we get the following formulas:

$$\Psi_1(s) = e^{-\frac{1}{2}s} \left[-2\psi \cos\left(\frac{\sqrt{3}}{2}s\right) + \frac{2}{3} \int_{-\infty}^0 g(\Psi(\tilde{s})) H_1(s, \tilde{s}) d\tilde{s} \right], \quad (5.49)$$

for $0 < s < \infty$, and

$$\Psi_m = -3\psi + 2 \int_{-\infty}^0 g(\Psi(\tilde{s})) e^{\frac{1}{2}\tilde{s}} \sin\left(\frac{\sqrt{3}}{2}\tilde{s} - \frac{\pi}{6}\right) d\tilde{s} - \int_0^{\infty} g(\Psi(\tilde{s})) e^{-\tilde{s}} d\tilde{s}, \quad (5.50)$$

where

$$H_1(s, \tilde{s}) := e^{\frac{1}{2}\tilde{s}} \left[2 \cos\left(\frac{\sqrt{3}}{2}s\right) \sin\left(\frac{\sqrt{3}}{2}\tilde{s} - \frac{\pi}{6}\right) - \sin\left(\frac{\sqrt{3}}{2}(s - \tilde{s}) + \frac{\pi}{6}\right) \right].$$

Thus we see that solving Problem P_Ψ for some m in the interval given in (5.1) has been reduced to finding ψ and $\tilde{\Psi}(s; \psi)$, with ψ in the interval (5.21), which solve the system (5.43), (5.49), and such that Ψ_m given by (5.50) satisfies

$$\Psi_m = 2 \arcsin(m/2). \quad (5.51)$$

Let us continue, for the moment, to treat ψ as an independent parameter. It is easy to obtain from (5.49), using Lemma 5.1 and the estimate (5.22), that

$$|\Psi_1(s)| \leq b(\psi) e^{-\frac{1}{2}s}, \quad (5.52)$$

for $0 < s < \infty$, where

$$b(\psi) := 2|\psi|(1 + \frac{9}{56}|\psi|^2). \quad (5.53)$$

Lemma 5.4. *Suppose that*

$$\psi < 0 \quad \text{and} \quad b(\psi) < \frac{2}{3} \sqrt{\frac{15}{13}}. \quad (5.54)$$

Then there exists a solution $\Psi(s) = \tilde{\Psi}(s; \psi)$ of (5.2) on the interval $0 < s < \infty$, satisfying

$$\Psi_s(0^+) = \psi_1(\psi), \quad \Psi_{ss}(0^+) = \psi_2(\psi), \quad \Psi(+\infty) = 0, \quad (5.55)$$

such that

$$|\Psi(s)| \leq \frac{3}{2} b(\psi) e^{-\frac{1}{2}s}, \quad 0 < s < \infty. \quad (5.56)$$

Moreover, if ψ' , ψ'' satisfy (5.54), then for $0 < s < \infty$

$$|\tilde{\Psi}(s, \psi') - \tilde{\Psi}(s, \psi'')| \leq C|\psi' - \psi''|, \quad (5.57)$$

where C depends on $\max\{|\psi'|, |\psi''|\}$.

Lemma 5.4 provides us with an estimate for (5.43) and (5.49). Note that (5.54) is equivalent to the condition

$$\tilde{\psi} < \psi < 0, \quad (5.58)$$

where $\tilde{\psi} \approx -0.35110155$ is defined as the unique real negative solution of $b(\tilde{\psi}) = \frac{2}{3} \sqrt{\frac{15}{13}}$, and hence condition (5.58) implies (5.21). The problem of solving (5.2), (5.55) has been reduced to solving the integral equation (5.43) with (5.49). The proof of existence in

Lemma 5.4 is analogous to the proof of Lemma 5.3. The continuous dependence result in Lemma 5.4 may be obtained by a straight forward iteration argument, using (5.43), (5.49), and Lemma 5.1.

Now we prove Theorem 3. Lemmas 5.3 and 5.4 imply that there exists a solution $\Psi = \tilde{\Psi}(s; \psi)$ to Problem P_Ψ with $m(\psi) = 2 \sin(\Psi_m/2)$ where $\Psi_m = \Psi_m(\psi)$ is defined by (5.50), if ψ satisfies condition (5.58). It remains now to clarify the connection between the interval (5.58) and the implied attained values of $m(\psi)$:

$$\{m(\psi) \mid \tilde{\psi} < \psi < 0\}.$$

It follows from (5.50) and (5.57) that Ψ_m is a continuous function of ψ for $\tilde{\psi} < \psi < 0$. Hence, $m(\psi)$ is also continuous for $\tilde{\psi} < \psi < 0$.

We now demonstrate that $m(\psi)$ is also strictly monotone on the interval $(\tilde{\psi}, 0)$. Suppose that $m(\psi)$ was not strictly monotone on the interval $(\tilde{\psi}, 0)$. Then there would exist two values, $\psi_1, \psi_2, \psi_1 \neq \psi_2$, such that $m(\psi_1) = m(\psi_2)$. Then by Lemmas 5.3 and 5.4, there exist two solutions, $\tilde{\Psi}(s; \psi_1)$ and $\tilde{\Psi}(s; \psi_2)$ to Problem P_Ψ with $m(\psi_1) = m(\psi_2)$. Note now that the estimates (5.22), (5.56), and (5.58) imply that

$$|\tilde{\Psi}(s; \psi_1)|, |\tilde{\Psi}(s; \psi_2)| < \frac{\pi}{2}, \quad \text{for } -\infty < s < 0 \text{ and } 0 < s < \infty. \quad (5.59)$$

But the uniqueness in the "single-valued" sense which was proven in Theorem 1 for a fixed value of m now implies that the solutions $\tilde{\Psi}(s; \psi_1)$ and $\tilde{\Psi}(s; \psi_2)$ must be identical. However, by construction, $\tilde{\Psi}(0^-; \psi_1) = \psi_1$ and $\tilde{\Psi}(0^-; \psi_2) = \psi_2$, and $\psi_1 \neq \psi_2$. Therefore a contradiction is obtained, and it follows that $m(\psi)$ is indeed strictly monotone. Moreover (5.51) and the bound (5.59) imply that Ψ_m is also strictly monotone.

Next, let us note that Lemma 5.1 with $u_1 = 0$ and $u_2 = \psi$, together with the estimates (5.22) and (5.56), implies that

$$\left| \int_{-\infty}^0 g(\Psi(\tilde{s})) e^{\frac{1}{2}\tilde{s}} \sin\left(\frac{\sqrt{3}}{2}\tilde{s} - \frac{\pi}{6}\right) d\tilde{s} \right| < \frac{9}{56} |\psi|^3, \quad \tilde{\psi} \leq \psi < 0, \quad (5.60)$$

$$\left| \int_0^\infty g(\Psi(\tilde{s})) e^{-\tilde{s}} d\tilde{s} \right| < \frac{9}{40} b^3(\psi), \quad \tilde{\psi} \leq \psi < 0. \quad (5.61)$$

Formulas (5.50), (5.60), and (5.61) imply that

$$P^-(\psi) < \Psi_m(\psi) < P^+(\psi), \quad \tilde{\psi} \leq \psi < 0, \quad (5.62)$$

where

$$P^\pm(\psi) = 3|\psi| \left(1 \pm \frac{3}{28} |\psi|^2 \right) \pm \frac{9}{40} b^3(\psi).$$

Note in particular that the above estimate implies that $\Psi_m(0) = 0$, and therefore that $m(0) = 0$. It follows from (5.62) and from the continuity and strict monotonicity of m and Ψ_m that there exists a unique point $\hat{\psi} \in (\tilde{\psi}, 0)$ such that

$$\hat{m} := m(\hat{\psi}) = 2 \sin\left(\frac{1}{2} P^-(\tilde{\psi})\right) \approx 0.92068702,$$

and inequalities (5.14) and $0 < m(\psi) < \hat{m}$ are equivalent.

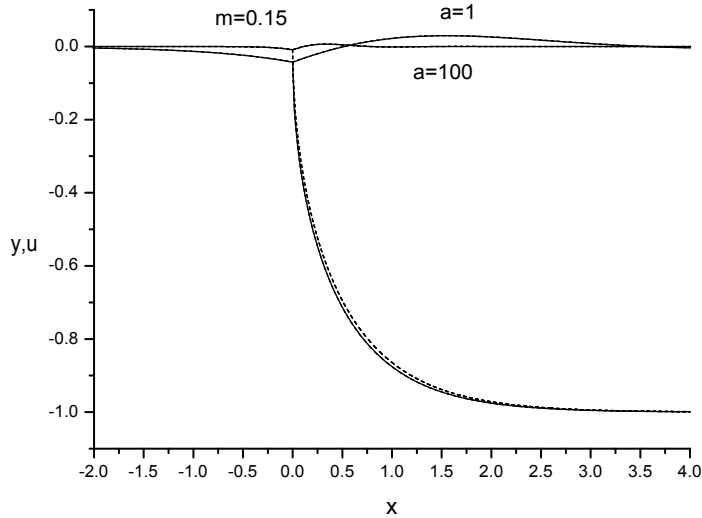


FIGURE 3. Profiles of u and y when $m = 0.15$ and $a = 1, 100$. The solid line indicates solutions to the fully nonlinear problem and the dashed line indicates solutions to the partially linearized formulation.

Thus for any m in the interval (5.1) there exists a corresponding unique solution of P_ψ , which we denote by $\Psi = \tilde{\Psi}(s; \psi)$ where ψ is determined by $m = m(\psi)$ for $\hat{\psi} < \psi < 0$, and the proof of Theorem 3 is completed. \square

6. CONCLUSION

For the sake of illustration we conclude with some numerical solutions to the fully nonlinear formulation as well as to the partially linearized formulation in Figures 3-6 below. In calculating the numerical solutions, an iterative procedure has been used based on starting with a small value of m , which has been taken here as $m = 0.01$, calculating the solution of the fully nonlinear formulation for this value of m by using the solution to the partially linearized formulation as an initial approximation, then solving the fully nonlinear problem for $m = 0.02$ by using the solution for $m = 0.01$ as an initial approximation. This procedure is repeated until the value $m = 2$ is reached.

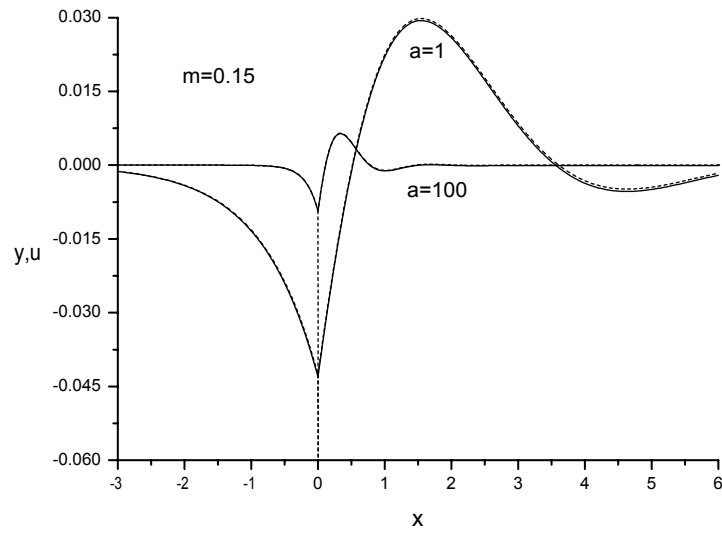


FIGURE 4. A magnification of the profiles in Figure 3 in the vicinity of the groove root.

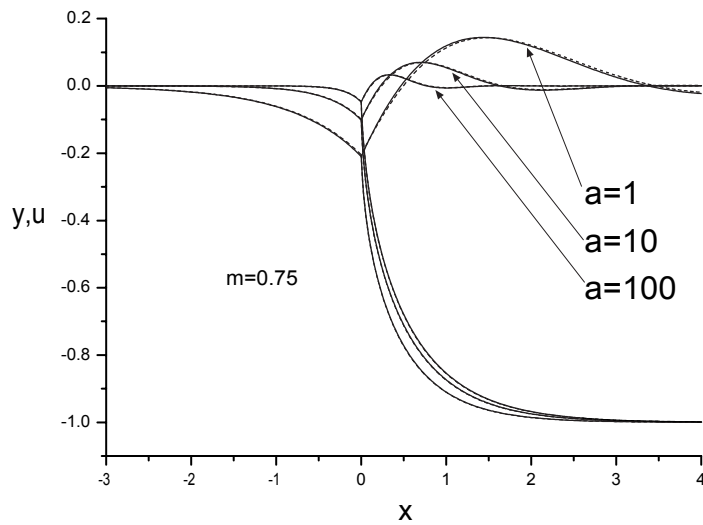


FIGURE 5. Profiles of u and y when $m = 0.75$ and $a = 1, 10, 100$. The solid line indicates solutions to the fully nonlinear problem and the dashed line indicates solutions to the partially linearized formulation.

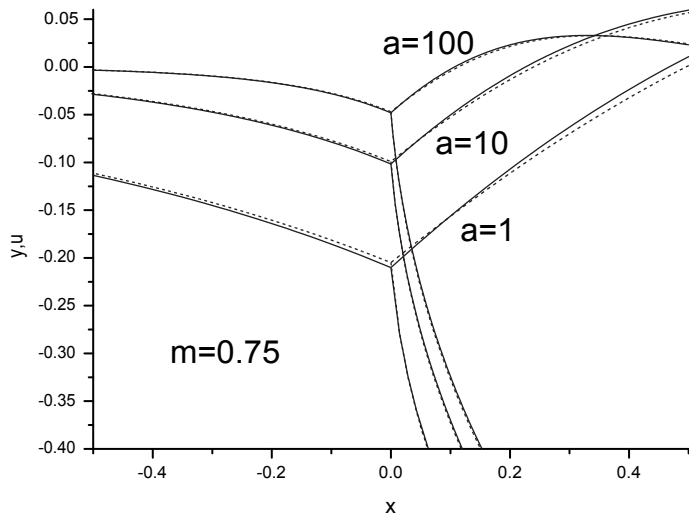


FIGURE 6. A magnification of the profiles in Figure 5 in the vicinity of the groove root.

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REFERENCES

- [1] Aristov, V.Y., Fradkov, V.E. & Shvindlerman, L.S., Detachment of the migration grain-boundary half-loop from an absorbed impurity cloud, *Soviet Phys. Solid St.* **22**, (1980), 1055-1059.
- [2] Akveld, M.E. & Hulshof, J., Travelling wave solutions of a fourth-order semilinear diffusion equation, *Appl. Math. Lett.*, **11**, vol. 3, (1998), 115-120.
- [3] Bailey, G.L.J. & Watkins, H.C., *Proc. Phys. Soc.*, **B 63**, (1950), 350.
- [4] Brokman, A., Kris, R., Mullins, W., & Vilenkin, A., Analysis of boundary motion in thin films, *Scripta Mater.*, **32**, (1995), 1341-1346.
- [5] Coddington & Levinson, *Theory of Ordinary Differential Equations*, McGraw Hill, 1955.
- [6] Coleman, B., Falk, R. & Moakher, M., Stability of cylindrical bodies in the theory of surface diffusion, *Physica D*, **89**, (1995), 123-135.
- [7] Coleman, B., Falk, R. & Moakher, M., Space-time finite element methods for surface diffusion with application to the theory of the stability of cylinders, *SIAM J. Sci. Comput.*, **17**, (1996), 1434-1448.
- [8] Di Prinzio, C.L., Nasello, O.B., Studies of grain boundary motion in ice bicrystals, *J. Phys. Chem. B* **101**, (1997), 7687-7690.
- [9] Dunn, C.G., Daniels, F.W. & Bolton, M.J., *Trans. Am. Inst. Min. Engrs.*, **185**, (1949), 708.
- [10] Furtkamp, M., Gottstein, G., Molodov, D.A., Semenov, V.N. & Shvindlerman, L.S., Grain boundary migration in Fe-3.5% Si bicrystals with [001] tilt boundaries, *Acta Mater.*, **46**, (1998), 4103-4110.
- [11] Gottstein, G., Czubayko, U., Molodov, D.A., Shvindlerman, L.S. & Wunderlich, W., In situ observations of grain boundary migration, *Materials Science Forum*, 1996, Vols. 204-206, 99-108.
- [12] Gottstein, G. & Shvindlerman, L.S., *Grain boundary migration in metals: thermodynamics, kinetics, applications*, CRC Press, 1999.
- [13] Hackney, S.A., Periodic behavior in surface limited grain growth, *Scripta Mater.*, **34**, (1996), 1021-1026.
- [14] Hackney, S.A., Nonlinear effects in periodic surface limited grain growth, *Scripta Mater.*, **35**, (1996), 29-34.
- [15] Kanel, J., Novick-Cohen, A. & Vilenkin, A., A traveling wave solution for coupled surface and grain boundary motion, *Acta Mater.*, **51**, (2003), 1981-1989.
- [16] Kanel, J., Novick-Cohen, A. & Vilenkin, A., Coupled surface and grain boundary motion: Nonclassical traveling wave solutions, *Adv. Diff. Eqns.*, **9** (2004) 299-327.
- [17] Kanel, J., Novick-Cohen, A. & Vilenkin, A., A numerical study for grain boundary motion in bicrystals, submitted.
- [18] Kanel, J., Novick-Cohen, A. & Vilenkin, A., Stability of traveling wave solutions for grain boundary motion, in preparation.
- [19] Mullins, W.W., Two-dimensional motion of ideal grain boundaries, *J. Appl. Phys.*, **27**, (1956), 900-904.
- [20] Mullins, W.W., Theory of thermal grooving, *J. Appl. Physics*, **28**, (1957), 333-339.
- [21] Mullins, W.W., The effect of thermal grooving on grain boundary motion, *Acta Metall.*, **6**, (1958), 414-427.
- [22] Novick-Cohen, A., Order-disorder and phase separation: modeling grain sintering, pp 56-67 in "CMDS99 Proceedings of the 9th International Symposium," Istanbul, 1998, editors: E. Inan & K.Z. Markov, World Scientific Pub. Co., 1999.
- [23] Novick-Cohen, A., Triple-junction motion for an Allen-Cahn/Cahn-Hilliard system, *Physica D*, **137**, (2000), 1-24.

- [24] Novick-Cohen, A. & Peres Hari, L., Geometric motion for a degenerate Allen-Cahn/Cahn-Hilliard system: the partial wetting case, submitted.
- [25] Semenov, V.N., Straumal, B.B., Glebovsky, V.G. & Gust, W.J., *J. Crystal Growth*, **151**, (1995), 180-186.
- [26] Solorzano, G. , El-Boragy, M., Gust, W. & Predel, B., In situ study of discontinuous precipitation in Al-15at.% Zn, *Scripta Mater.*, **34**, (1996), 1431.
- [27] Rabkin, E., Semenov, V., Izyumova, T., Jerky motion of grain boundaries in NiAl: an atomic force microscopy study, *Scripta Mater.*, **42**, (2000), 359-365.
- [28] Vilenkin, A.J., Kris, R. & Brokman, A., Breakup and grain growth in thin-film array, *J. Appl. Phys.*, **81**, (1997), 238-245.
- [29] Vilenkin, A. et al., A numerical study of stability of grain boundary motion in a bicrystal, in preparation.

7. FIGURE CAPTIONS

Figure 1. The quarter loop bicrystal geometry.

Figure 2. The variables Φ , Ψ , and s_1 , s_2 .

Figure 3. Profiles of u and y when $m = 0.15$ and $a = 1, 100$. The solid line indicates solutions to the fully nonlinear problem and the dashed line indicates solutions to the partially linearized formulation.

Figure 4. A magnification of the profiles in Figure 3 in the vicinity of the groove root.

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