A Phase-Field Model for Diffusion-Induced Grain Boundary Motion

Klaus Deckelnick

Abstract. We consider a phase-field model for diffusion-induced grain boundary motion. This model couples a parabolic variational inequality to a degenerate diffusion equation. We summarize recent results on existence and uniqueness, sharp interface limits and numerical discretization.

1. Introduction

The aim of this note is to review recent work on the mathematical study of diffusion-induced grain boundary motion. This kind of motion is observed when a thin polycrystalline film of metal is exposed to vapor consisting of another metal. Atoms from the vapor diffuse into the film along the grain boundaries that separate the crystals inducing the migration of the boundary. As it advances, the solute atoms are left behind the boundary, which changes the concentration of the growing crystal (see [6] and the references in [2]). The following thermodynamically consistent phase-field system was suggested in [2] (see also [5]) in order to describe this phenomenon:

$$\rho\epsilon\phi_t - \epsilon\Delta\phi - \frac{1}{\epsilon}\phi + \beta(\phi) + p_\phi(\phi,u) \ni 0 \qquad (1)$$

$$\epsilon u_t - \nabla\cdot\big(D(\phi)\nabla w\big) = 0\,. \qquad (2)$$

The system (1), (2) is in nondimensionalized form, with the constants ρ and ϵ satisfying

$$0 < \rho \le 1, 0 < \epsilon \ll 1\,.$$

Furthermore, ϕ is an order parameter, which has the value +1 in one crystal and -1 in the other. Within the grain boundary we have $|\phi| < 1$. The constraint $|\phi| \le 1$ is realized in (1) by the use of the subdifferential β of

$$I_{[-1,1]}(s) := \begin{cases} 0 & \text{if } s \in [-1,1]\,, \\ +\infty & \text{otherwise}\,. \end{cases}$$

Thus,

$$\beta(s) = \partial I_{[-1,1]}(s) = \begin{cases} (-\infty,0] & \text{if } s = -1\,, \\ 0 & \text{if } |s| < 1\,, \\ [0,\infty) & \text{if } s = 1\,. \end{cases}$$

The function $\Psi(s) := I_{[-1,1]}(s) + \frac{1}{2}(1-s^2)$ is the well-known double obstacle potential (see [1]).

The variable u denotes the concentration of the solute atoms, while

$$w = u + \frac{\hat{\epsilon}}{\pi} p_u(\phi, u) \qquad (0 < \hat{\epsilon} \ll 1)\,.$$

The coupling term p is given by

$$p(\phi, u) = \frac{\pi}{8}(1+\phi)^2 u^2$$

and models elastic interaction. Finally, the diffusivity is much larger in the grain boundary than in the crystals, so that a reasonable ansatz for D is

$$D(\phi) = \frac{2}{\pi}(1-\phi^2)\,.$$

Note that $D(\phi)$ vanishes within the grains. Thus, (1), (2) couples a parabolic variational inequality to a degenerate diffusion equation leading to challenging mathematical problems.

Let us briefly outline the plan of this note: in § 2 we shall review an existence and uniqueness result for the above system in a two-dimensional slab. § 3 is concerned with results on the sharp-interface limit $\epsilon \to 0$. Finally, in § 4 we briefly introduce a numerical method for the problem studied in § 2 and present some computations.

2. Existence and Uniqueness for the Phase-Field System

We consider the following two-dimensional geometry, which models a metal plate that is surrounded by vapor: for $H > 0$ let $\Omega = \mathbb{R} \times (-H, H)$, where we think of the vapor as being above $x_2 = H$ and below $x_2 = -H$. Instead of (1), (2) we consider the following slightly modified system (which still retains all the mathematical difficulties):

$$\epsilon \phi_t - \epsilon \Delta \phi - \frac{1}{\epsilon}\phi + \beta(\phi) + \frac{\pi}{4}u^2 \ni 0 \qquad (3)$$

$$\epsilon u_t - \nabla \cdot \big(D(\phi)\nabla u\big) = 0 \qquad (4)$$

together with the boundary and initial conditions

$$\frac{\partial \phi}{\partial n} = 0 \qquad \text{on } \partial\Omega \times (0,T), \qquad (5)$$

$$D(\phi)\frac{\partial u}{\partial n} + \alpha D(\phi)^2 (u-1) = 0 \qquad \text{on } \partial\Omega \times (0,T), \qquad (6)$$

$$\phi(.,0) = \phi_0, u(.,0) = u_0 \qquad \text{in } \Omega\,. \qquad (7)$$

The fact that $D(\phi)^2$ (rather than $D(\phi)$) appears in (6) has a technical reason, namely to ensure an a-priori estimate needed for the existence proof. Nevertheless, (6) approximates for large α the condition $u = 1$ on $\{(x_1, x_2) \mid D(\phi) \neq 0, x_2 = \pm H\}$ which is used in [2].

We assume that the initial functions (ϕ_0, u_0) satisfy

$$\begin{aligned}
&\phi_0 \in W^{2,2}_{\text{loc}}(\bar{\Omega})\,, \qquad -1 \le \phi_0 \le 1 \qquad \text{in} \quad \Omega\,, \quad \frac{\partial \phi_0}{\partial n} = 0 \quad \text{on} \quad \partial\Omega\,, \\
&u_0 \in H^1_{\text{loc}}(\bar{\Omega})\,, \qquad 0 \le u_0 \le 1 \qquad \text{in} \quad \Omega
\end{aligned}$$

and that there exists $R_0 > 0$ such that

$$\begin{aligned}
\phi_0(x) &= 1 \quad \text{for} \quad x_1 \ge R_0, \quad \phi_0(x) = -1 \quad \text{for} \quad x_1 \le -R_0\,, \\
u_0(x) &= 0 \quad \text{for} \quad |x_1| \ge R_0\,.
\end{aligned}$$

Furthermore, we define

$$K := \{v \in H^1_{\text{loc}}(\bar{\Omega}) \mid |v| \le 1 \quad \text{a.e. in } \Omega, \quad \exists R = R(v) \quad v(x) = \pm 1, \quad \pm x_1 \ge R\}$$

as well as the space-time function spaces

$$\begin{aligned}
X_1 &:= \{\phi \in L^\infty(\Omega_T) | \nabla\phi \in L^2(0,T;H^1(\Omega) \cap L^\infty(\Omega)),\ \phi_t \in L^2(0,T;H^1(\Omega))\}\,, \\
X_2 &:= L^2(0,T;H^1(\Omega)) \cap W^{1,2}(0,T;L^2(\Omega))\,.
\end{aligned}$$

Definition 2.1. *The pair $(\phi, u) \in X_1 \times X_2$ is called a solution of (3)–(7) provided that*

$$\begin{aligned}
&\phi(0) = \phi_0\,, \quad u(0) = u_0 \ \textit{in}\ \Omega, \\
&\phi(t) \in K \ \textit{for}\ t \in (0,T) \quad \textit{and} \quad \frac{\partial \phi}{\partial n} = 0 \ \textit{on}\ \partial\Omega \times (0,T)\,, \\
&\epsilon \int_\Omega \phi_t(\zeta - \phi) + \epsilon \int_\Omega \nabla\phi \cdot \nabla(\zeta - \phi) - \frac{1}{\epsilon} \int_\Omega \phi(\zeta - \phi) + \frac{\pi}{4} \int_\Omega u^2(\zeta - \phi) \ge 0\,, \\
&\epsilon \int_\Omega u_t \eta + \int_\Omega D(\phi) \nabla u \cdot \nabla \eta + \alpha \int_{\partial\Omega} D(\phi)^2 (u-1)\eta = 0\,,
\end{aligned}$$

for all $\zeta \in K$, all $\eta \in H^1(\Omega)$ and for almost all $t \in (0,T)$.

Theorem 2.2. *Under the above assumptions there exists a solution of (3)–(7) in the sense of definition 2.1.*

Proof. We briefly outline the main ideas and difficulties refering the reader to [3] for a detailed proof.

1. One introduces a regularized strictly parabolic system, in which the subdifferential β and the diffusivity D are replaced by functions β_δ and D_δ in such a way that $\beta_\delta \to \beta, D_\delta \to D$ as $\delta \to 0$ in a suitable sense. In order to avoid difficulties related to the unboundedness of Ω, the system is initially considered on $(-L, L) \times (-H, H) \times (0, T)$, where L is chosen sufficiently large depending on ϵ, R_0 and T.
2. The procedure in step 1 yields a family (ϕ_δ, u_δ) of approximate solutions, for which $0 \le u_\delta \le 1$ and higher norms of ϕ_δ can be estimated independently of δ (by the maximum principle and parabolic regularity theory respectively). The

main difficulty consists in obtaining uniform bounds on derivatives of u_δ. Note that the usual energy estimate for (2) formally reads

$$\sup_{0 \le t \le T} \|u(t)\|^2_{L^2} + \int_0^T \int_\Omega D(\phi)|\nabla u|^2 + \alpha \int_0^T \int_{\partial\Omega} D(\phi)^2 |u|^2 \le C\,,$$

which only provides information on ∇u in the interior of the boundary layer. To obtain a bound on ∇u_δ it is therefore natural —although rather complicated— to work with the evolution equations for $u_{\delta,x_k}, k = 1,2$.

3. Using the a-priori estimates of step 2 and standard compactness results one obtains a subsequence $(\phi_{\delta_k}, u_{\delta_k}), (\delta_k \to 0)$, which converges to a pair (ϕ, u) satisfying the variational identities of definition 2.1 for $(-L,L) \times (-H,H)$ instead of Ω. A comparison argument shows that

$$\phi(x,t) = \pm 1, \quad u(x,t) = 0 \quad \text{ for } \pm x_1 > \frac{L}{2},\ 0 < t < T\,,$$

provided that L is chosen large enough. By extending (ϕ, u) appropriately for $|x_1| \ge L$ one obtains a solution in the sense of definition 2.1.

□

Unfortunately we are not able to show that the above solution is unique within the class $X_1 \times X_2$. However, if we assume slightly more regularity we can prove a uniqueness result, which relies on a duality argument applied to the diffusion equation. Details can again be found in [3].

Theorem 2.3. *Let $(\phi_1, u_1), (\phi_2, u_2) \in X_1 \times X_2$ be two solutions in the sense of definition 2.1 which in addition satisfy*

$$\Delta\phi_i \in L^1(0,T; L^\infty(\Omega)), \quad \nabla u_i \in L^2(0,T; L^p(\Omega)), \quad i = 1,2$$

for some $p > 2$. Then $(\phi_1, u_1) \equiv (\phi_2, u_2)$.

3. Sharp-Interface Limits

In [5] formal asymptotics are used to derive the following moving free boundary problem for the sharp interface $\Gamma(t)$ as $\epsilon \to 0$:

$$\begin{aligned} \rho v &= \kappa + u^2 \qquad \text{on} \quad \Gamma(t) \\ u_{ss} &= vu \qquad\quad\ \ \text{on} \quad \Gamma(t)\,. \end{aligned} \tag{8}$$

Here, v is the normal velocity of $\Gamma(t)$, κ is its curvature and s denotes arclength. The system (8) couples forced curve shortening flow to an elliptic equation on $\Gamma(t)$. If one considers the limit problem for the geometry treated in § 2, boundary conditions have to be added to (8), namely that the curve $\Gamma(t)$ meets the lines $\mathbb{R} \times \{\pm H\}$ orthogonally and that $u = 1$ at these contact points. At $t = 0$, $\Gamma(0)$ is prescribed, while the values $u_0 = u(.,0)$ have to satisfy the compatibility condition

$$u_{0,ss} - \frac{1}{\rho}\big(\kappa(.,0) + u_0^2\big)u_0 = 0 \quad \text{on} \quad \Gamma(0)\,.$$

Apart from deriving the sharp interface limit, [5] also investigates the existence of traveling wave solutions to (8) for the infinite slab. Two types of waves are considered: the first type of solution connects the two faces $x_2 = H$ and $x_2 = -H$, while the second type does not reach the other side of the plate and trails behind.

Including terms of order $O(\epsilon)$ in the derivation of the sharp interface limit, one obtains the following more accurate system for $\Gamma(t)$ (see again [5]):

$$\begin{aligned} \rho v &= \kappa(1+\epsilon C) + u^2\big(1+\epsilon(B+Au^2)\big) && \text{on} \quad \Gamma(t) \\ \epsilon^* \frac{du}{dt} &= \big(u_s(1+\epsilon\alpha u^2)\big)_s - vu - \epsilon^* uv\kappa && \text{on} \quad \Gamma(t) \end{aligned} \tag{9}$$

for certain constants A, B, C, α, g_1 and $\epsilon^* = \frac{\epsilon\pi}{1+\epsilon g_1}$. The symbol $\frac{du}{dt}$ denotes differentiation along flow lines that are perpendicular to $\Gamma(t)$ (see [7] for a precise definition). Due to the presence of $\epsilon^* uv\kappa$ in the second equation of (9), the system is fully nonlinear. In [7], [8] local existence and uniqueness of classical solutions to (9) is proved for a geometry, in which the grain boundary is modeled by a closed curve in the plane (with vapor in the third dimension).

4. Numerical Discretization

In this final section we briefly present a numerical method, which was used in [4] to calculate solutions of (3)–(7). We consider the problem on the rectangle $\Omega_L = (-L, L) \times (-H, H)$ (cf. step 1 of the Proof of theorem 2.2) and introduce a triangulation $\mathcal{T}_h$ of Ω_L as well as the corresponding space of linear finite elements

$$X_h := \{v_h \in C^0(\bar\Omega_L) \mid v_h \in P_1(T) \text{ for all } T \in \mathcal{T}_h\}\,.$$

Furthermore, let

$$K_h := \{v_h \in X_h \mid |v_h(x)| \le 1 \text{ for all } x \in \Omega_L\}$$

and $\Delta t > 0$ the timestep. Denoting by $\phi_h^0 = I_h(\phi_0)$ and $u_h^0 = I_h(u_0)$ the Lagrange interpolants of ϕ_0 and u_0 the numerical algorithm reads as follows: for $0 \le n \le [\frac{T}{\Delta t}]$ find $(\phi_h^n, u_h^n) \in K_h \times X_h$ such that

$$\begin{aligned} \frac{\rho\epsilon}{\Delta t}\int_{\Omega_L} \big(\phi_h^{n+1} - \phi_h^n\big)\big(\zeta_h - \phi_h^{n+1}\big) + \epsilon \int_{\Omega_L} \nabla\phi_h^n \cdot \nabla\big(\zeta_h - \phi_h^{n+1}\big) \\ - \frac{1}{\epsilon}\int_{\Omega_L} \phi_h^n\big(\zeta_h - \phi_h^{n+1}\big) + \frac{\pi}{4}\int_{\Omega_L} (u_h^n)^2\big(\zeta_h - \phi_h^{n+1}\big) \ge 0 \end{aligned}$$

$$\frac{\epsilon}{\Delta t}\langle u_h^{n+1} - u_h^n, \eta_h\rangle_{\Omega_L}^h + \int_{\Omega_L} D(\phi_h^n)\nabla u_h^{n+1} \cdot \nabla\eta_h + \alpha\langle D(\phi_h^n)(u_h^{n+1} - 1), \eta_h\rangle_{\partial\Omega_L}^h = 0$$

for all $\zeta_h \in K_h$ and all $\eta_h \in X_h$. Here, the discrete inner products are defined by

$$\langle f, g\rangle_{\Omega_L}^h = \int_{\Omega_L} I_h\big(fg\big), \qquad \langle f, g\rangle_{\partial\Omega_L}^h = \int_{\partial\Omega_L} I_h\big(fg\big)\,.$$

If we assume in addition, that the triangulation is weakly acute, then the use of numerical integration in the second equation combined with the fact that $0 \le u_0 \le 1$ ensures that $0 \le u_h^n \le 1$ for all $0 \le n \le [\frac{T}{\Delta t}]$.

Figures 1 and 2 show examples of calculated solutions ϕ_h and u_h. The initial conditions were chosen as

$$\phi_0(x) := \begin{cases} -1\,, & x_1 \le -\dfrac{\epsilon\pi}{2} \\ \sin(\dfrac{x_1}{\epsilon})\,, & -\dfrac{\epsilon\pi}{2} < x_1 < \dfrac{\epsilon\pi}{2} \\ +1\,, & x_1 \ge \dfrac{\epsilon\pi}{2} \end{cases}$$

and $u_0 \equiv 0$. The computations were carried out on a uniform grid with $H = 2$, $h = \frac{1}{100}$, $\Delta t = \frac{h^2}{100}$, $\epsilon = 20h$, $\rho = 0.8$ and the numerical solutions are shown at $t = 0.2$. While the function ϕ_h keeps its sinusoidal shape, the interfacial region has width $\approx 0.6 \approx \pi\epsilon$ and is moving in the positive x_1-direction. The concentration u_h, which initially was identically zero, now has non-zero values in the region through which the interface has passed. Once a point has been left behind the interfacial region, the values of u_h at this point do not change at later times. We remark that it is sufficient to carry out the computations in a small neighborhood of the discrete free boundary $|\phi_h| < 1$.

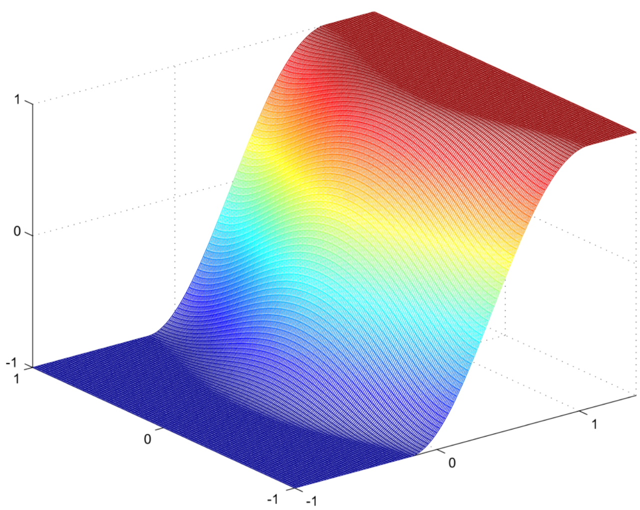

FIGURE 1. $\phi_h(\mathbf{x}, t)$

Apart from presenting calculations for the phase-field model, [4] also investigates the convergence as $\epsilon \to 0$ to the sharp interface limit (8) from a numerical point of view. Furthermore, convergence to traveling wave solutions as $t \to \infty$ is studied.

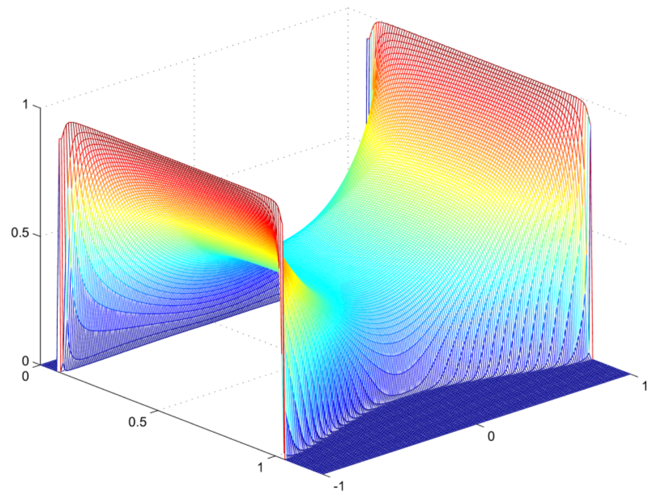

FIGURE 2. $u_h(\mathbf{x}, t)$

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Centre for Mathematical Analysis and Its Applications,
School of Mathematical Sciences,
University of Sussex,
Falmer, Brighton BN1 9QH, England
E-mail address: `k.p.deckelnick@sussex.ac.uk`