Mathematical Analysis of Grain Boundary Motion Models of Kobayashi-Warren-Carter Type

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1 Introduction

This is a joint work with Akio Ito[1] and Nobuyuki Kenmochi[2].

In this talk we consider the following phase-field model of grain boundaries with constraint, denoted by (P):

$$
\text{(P)}\begin{cases}
\eta_t - \kappa\Delta\eta + g(\eta) + \alpha'(\eta)|\nabla\theta| = 0 & \text{a.e. in } Q_T := \Omega \times (0,T), \\
\alpha_0(\eta)\theta_t - \nu\Delta\theta - \operatorname{div}\left(\alpha(\eta)\dfrac{\nabla\theta}{|\nabla\theta|}\right) + \partial I_{[-\theta^*,\theta^*]}(\theta) \ni 0 & \text{a.e. in } Q_T, \\
\dfrac{\partial\eta}{\partial n} = 0, \quad \theta = 0 & \text{a.e. on } \Sigma_T := \Gamma \times (0,T), \\
\eta(x,0) = \eta_0(x), \quad \theta(x,0) = \theta_0(x) & \text{for a.e. } x \in \Omega,
\end{cases}
$$

where Ω is a bounded domain in $\mathbf{R}^N$ ($N \geq 1$) with regular boundary $\Gamma := \partial\Omega$, $T > 0$ is a fixed finite time, $\kappa > 0$ and $\nu > 0$ are given small constants, $g(\cdot)$, $\alpha(\cdot)$ and $\alpha_0(\cdot)$ are given functions on $\mathbf{R}$, $\partial I_{[-\theta^*,\theta^*]}(\cdot)$ is the subdifferential of the indicator function $I_{[-\theta^*,\theta^*]}(\cdot)$ on the closed interval $[-\theta^*,\theta^*]$ with some constant $\theta^* > 0$, $\partial/\partial n$ is the outward normal derivative on Γ, and $\eta_0(x)$, $\theta_0(x)$ are given initial data.

The system (P) is called a grain boundary motion model of Kobayashi-Warren-Carter type [12, 13]. In the dynamics of grain structure in various materials, the variable θ is an indicator of the mean orientation of crystallines and the variable η is an order parameter for the degree of crystalline orientational order; $\eta = 1$ implies the completely oriented state and $\eta = 0$ is the state where no meaningful value of orientation exists. There are many mathematical models of grain boundary formation. For some related works, we refer to [3, 4, 15, 16].

In connection with this subject, the singular diffusion equations,

$$
u_t = \operatorname{div}\left(\frac{\nabla u}{|\nabla u|}\right), \quad \text{more generally,} \quad u_t = \frac{1}{b(x)}\operatorname{div}\left(a(x)\frac{\nabla u}{|\nabla u|}\right),
$$

kindred to the second equation of (P), have been studied by a lot of mathematicians from various view-points (cf. [1, 2, 5, 11, 14, 17]).

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Kobayashi et al. [12] considered η and θ as a polar coordinate system (η, θ) in two dimensional space, and they proposed a grain boundary motion model (P) without constraint $\partial I_{[-\theta^*,\theta^*]}(\cdot)$. Moreover, in [12, 13], some numerical experiments were obtained when $\hat{g}(\eta) := \frac{1}{2}(1-\eta)^2$, $\alpha_0(\eta) = \alpha(\eta) = \eta^2$ and Ω is a bounded domain in $\mathbf{R}^2$.

Recently assuming that $\{\eta_0, \theta_0\}$ is a pair of good initial data in $H^1(\Omega) \times H_0^1(\Omega)$, system (P) without constraint $\partial I_{[-\theta^*,\theta^*]}(\cdot)$ was studied in [6, 7, 8] from the theoretical point of view. In the case when $\alpha_0 \geq \delta(> 0)$ on $\mathbf{R}$ for a positive constant δ, Ito et al. [6] showed the existence-uniqueness of solutions to the one-dimensional model (P) without $\partial I_{[-\theta^*,\theta^*]}(\cdot)$ and with $-\kappa\Delta\eta$ replaced by $-(\sigma\eta_t + \kappa\eta)_{xx}$, $0 < \sigma < \infty$, in the first equation. Also in the case when $\alpha_0 \geq \delta(> 0)$ on $\mathbf{R}$, the authors [7] showed the existence of a global solution to (P) without $\partial I_{[-\theta^*,\theta^*]}(\cdot)$ in higher dimensional spaces and the uniqueness in one dimensional space. Furthermore the authors [8] constructed global weak solutions to (P) without $\partial I_{[-\theta^*,\theta^*]}(\cdot)$ in the case when $\alpha_0 \geq 0$ on $\mathbf{R}$ (namely, α_0 is possibly degenerate) and Ω is a bounded domain in $\mathbf{R}^N$ $(1 \leq N \leq 3)$.

In this talk we consider the problem (P) in the physical situation that the whole region is already solidified and filled with some grains, so that we may assume that the orientation angle θ has two threshold values $-\theta^*$ and θ^*, where θ^* is a prescribed positive constant. Hence we take account of $\partial I_{[-\theta^*,\theta^*]}(\cdot)$ in the second equation of (P).

The main object of this talk is to show the global existence of a weak solution to (P) in the case when $[\eta_0, \theta_0]$ is the initial data in $L^2(\Omega) \times L^2(\Omega)$. Moreover we establish a result on the large-time behavior of solutions to (P), which was suggested by numerical experiments in [12, 13].

2 Existence-uniqueness of solutions for (P)

Here we assume the following conditions:

(A1) α_0 is a function in $C^2(\mathbf{R})$ such that $\alpha_0 \geq \delta_0$ on $\mathbf{R}$ for a positive constant δ_0.

(A2) α is a non-negative function in $C^1(\mathbf{R})$, whose derivative α' is non-decreasing and bounded on $\mathbf{R}$ such that $\alpha'(0) = 0$.

(A3) g is a Lipschitz continuous function on $\mathbf{R}$. Suppose that $g \leq 0$ on $(-\infty, 0]$ and $g \geq 0$ on $[1, \infty)$. Also we denote by $\hat{g}$ a primitive of g, and assume that $\hat{g}$ is non-negative on $\mathbf{R}$.

(A4) κ, ν and θ^* are real positive constants.

(A5) $\eta_0 \in L^2(\Omega)$ with $0 \leq \eta_0 \leq 1$ a.e. on Ω, and $\theta_0 \in L^2(\Omega)$ with $|\theta_0| \leq \theta^*$ a.e. on Ω.

Next we give a weak formulation for (P) in the variational sense.

Definition 2.1. Let $0 < T < \infty$. Then, given initial data $\{\eta_0, \theta_0\} \in L^2(\Omega) \times L^2(\Omega)$, a pair $\{\eta, \theta\}$ of functions $\eta : [0, T] \to L^2(\Omega)$ and $\theta : [0, T] \to L^2(\Omega)$ is called a solution of (P) on $[0, T]$, if the following conditions are satisfied:

(i) $\eta \in C([0, T]; L^2(\Omega)) \cap W^{1,2}_{loc}((0, T]; L^2(\Omega)) \cap L^\infty_{loc}((0, T]; H^1(\Omega)) \cap L^2_{loc}((0, T]; H^2(\Omega))$.

(ii) $\theta \in C([0,T]; L^2(\Omega)) \cap W^{1,2}_{loc}((0,T]; L^2(\Omega)) \cap L^\infty_{loc}((0,T]; H^1_0(\Omega))$, and $|\theta| \le \theta^*$ a.e. on Q_T.

(iii) The following parabolic equation holds:

$$\eta'(t) - \kappa\Delta_N \eta(t) + g(\eta(t)) + \alpha'(\eta(t))|\nabla\theta(t)| = 0 \quad \text{in } L^2(\Omega) \quad \text{for a.e. } t \in (0,T),$$

where $\eta' := \frac{d\eta}{dt}$ and $\Delta_N : D(\Delta_N) := \{z \in H^2(\Omega); \frac{\partial z}{\partial n} = 0 \text{ a.e. on } \Gamma\} \longrightarrow L^2(\Omega)$ is the Laplacian with homogeneous Neumann boundary condition.

(iv) For a.e. $t \in (0,T)$ the following variational inequality holds:

$$\begin{aligned}&(\alpha_0(\eta(t))\theta'(t), \theta(t) - z) + \nu\,(\nabla\theta(t), \nabla\theta(t) - \nabla z)\\ &+ \int_\Omega \alpha(\eta(x,t))|\nabla\theta(x,t)|dx \le \int_\Omega \alpha(\eta(x,t))|\nabla z(x)|dx,\\ &\qquad\qquad \forall z \in H^1_0(\Omega) \text{ with } |z| \le \theta^* \text{ a.e. in } \Omega,\end{aligned}$$

where $\theta' := \frac{\partial\theta}{\partial t}$ and $(\cdot,\cdot)$ is the standard inner product in $L^2(\Omega)$.

(v) $\eta(0) = \eta_0$ and $\theta(0) = \theta_0$ in $L^2(\Omega)$.

A pair $\{\eta, \theta\}$ of functions $\eta : [0,\infty) \to L^2(\Omega)$ and $\theta : [0,\infty) \to L^2(\Omega)$ is called a solution of (P) on $[0,\infty)$ or a global (in time) solution of (P), if it is a solution of (P) on $[0,T]$ for every finite $T > 0$.

The first main result of this talk is concerned with an existence of solutions for (P).

Theorem 2.2 (cf. [9]). *Assume* (A1)–(A5) *hold, and let T be any finite positive real number. Then there is at least one solution $\{\eta,\theta\}$ of* (P) *on $[0,T]$ in the sense of Definition 2.1, and η satisfies $0 \le \eta \le 1$ a.e on Q_T.*

Also the next main result is concerned with a uniqueness of solutions for (P).

Theorem 2.3 (cf. [9]). *Assume* (A1)–(A4), *$\eta_0 \in H^1(\Omega)$ with $0 \le \eta_0 \le 1$ a.e. on Ω, $\theta_0 \in H^1_0(\Omega)$ with $|\theta_0| \le \theta^*$ a.e. on Ω, and the space dimension of Ω is one, i.e., $\Omega = (-L, L)$ for a positive number L. Then the solution $\{\eta,\theta\}$ obtained by Theorem 2.2 is unique.*

3 Large-time behavior of solutions to (P)

In this section we discuss the large-time behavior of solutions to (P) as $t \to \infty$.

Now we consider the steady-state system for (P), which is of the form:

$$(\mathrm{S})\begin{cases} -\kappa\Delta\eta + g(\eta) + \alpha'(\eta)|\nabla\theta| = 0 & \text{in } \Omega\\ -\nu\Delta\theta - \operatorname{div}\left(\alpha(\eta)\dfrac{\nabla\theta}{|\nabla\theta|}\right) + \partial_{[-\theta^*,\theta^*]}(\theta) \ni 0 & \text{in } \Omega\\ \dfrac{\partial\eta}{\partial n} = 0, \quad \theta = 0 & \text{on } \Gamma\end{cases}$$

A pair of functions $\{\eta, \theta\}$ is a solution of (S), called a steady-state solution of (P), if and only if $\theta = 0$ in $L^2(\Omega)$ and $-\kappa\Delta_N\eta + g(\eta) = 0$ in $L^2(\Omega)$. In fact, let $\{\eta, \theta\}$ be any solution of (S). Then it follows from the second equation of (S) that

$$\frac{\nu}{2}\|\nabla\theta\|^2_{L^2(\Omega)} + \int_\Omega \alpha(\eta)|\nabla\theta|dx = \min_{z\in H^1_0}\left\{\frac{\nu}{2}\|\nabla z\|^2_{L^2(\Omega)} + \int_\Omega \alpha(\eta)|\nabla z|dx + \int_\Omega I_{[-\theta^*,\theta^*]}(z)dx\right\},$$

where $\|\cdot\|_{L^2(\Omega)}$ is the inner product in $L^2(\Omega)$. The above minimum is 0 and is taken at $z = 0$. Hence $\theta = 0$ and the first equation of (S) is $-\kappa\Delta_N\eta + g(\eta) = 0$ in $L^2(\Omega)$. Also it is clear that any pair of functions $\theta = 0$ and η satisfying $-\kappa\Delta_N\eta + g(\eta) = 0$ in $L^2(\Omega)$ is a solution of (S).

Here, for simplicity, we denote by S_0 the set of all solutions of (S), namely

$$S_0 := \{\{\eta, 0\}; \eta \in D(\Delta_N), -\kappa\Delta_N\eta + g(\eta) = 0 \text{ in } L^2(\Omega)\}.$$

Then we have the following third main result of this talk, which is concerned with the large-time behavior of solutions to (P) as $t \to \infty$.

Theorem 3.1 (cf. [10]). *Assume* (A1)–(A5) *hold, and let* $\{\eta, \theta\}$ *be a solution of* (P) *on* $[0, \infty)$. *Denote by* $\omega(\eta, \theta)$ *the* ω*-limit set of* $\{\eta(t), \theta(t)\}$ *as* $t \to \infty$*, namely*

$$\omega(\eta,\theta) := \left\{\{\xi, z\} \in L^2(\Omega)\times L^2(\Omega) \;\middle|\; \begin{array}{c} \eta(t_n) \to \xi \textit{ in } L^2(\Omega),\ \theta(t_n) \to z \textit{ in } L^2(\Omega) \\ \textit{for some } t_n \textit{ with } t_n \uparrow \infty \end{array}\right\}.$$

Then $\omega(\eta, \theta) \subset S_0$.

Note that the solution of (S) is not unique, namely, the set S_0 is not a singleton in general, because of the term $g(\eta)$. So, we assume the additional condition for g. Then we have the following main result, which is concerned with the asymptotic convergence of all solutions of (P) as $t \to \infty$ in a special case of g.

Theorem 3.2 (cf. [10]). *In addition to* (A1)–(A5)*, suppose that* $g < 0$ *on* $[0, 1)$ *and* $g(1) = \hat{g}(1) = 0$. *Let* $\{\eta, \theta\}$ *be any solution of* (P) *on* $[0, \infty)$. *Then*

$$\eta(t) \longrightarrow 1 \textit{ in } H^1(\Omega) \quad \textit{and} \quad \theta(t) \longrightarrow 0 \textit{ in } H^1_0(\Omega) \quad \textit{as } t \to \infty, \tag{3.1}$$

and the convergence (3.1) *is uniform with respect to all the initial data* $\{\eta_0, \theta_0\}$*, and* $\{1, 0\}$ *is a unique steady–state solution of* (P).

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