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

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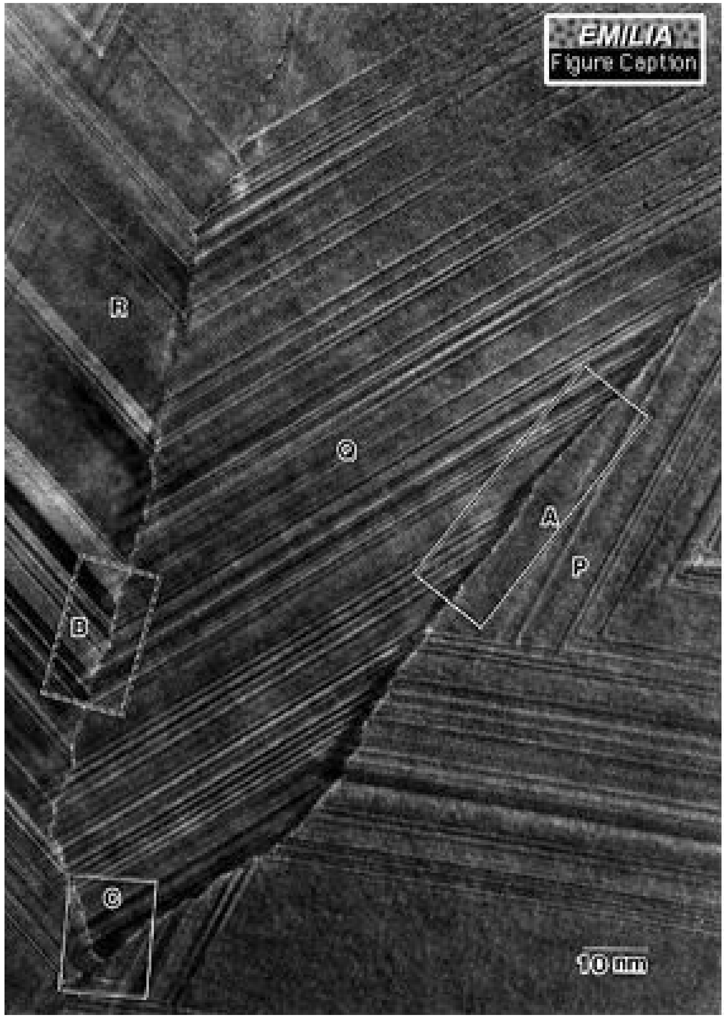
Contents

A Grain Boundary Problem

A grain boundary is the interface between two grains in a polycrystalline material

[Example] Tilt boundary and lattice defect in a SiC composite (Silicon Carbide)



The most simple grain boundary is that of a tilt boundary where the rotation axis is parallel to the boundary plane.

This boundary can be conceived as forming from a single, contiguous crystallite or grain which is gradually bent by some external force.

[http://asma7.tagen.tohoku.ac.jp/EMILIA/html/eg/index.html]

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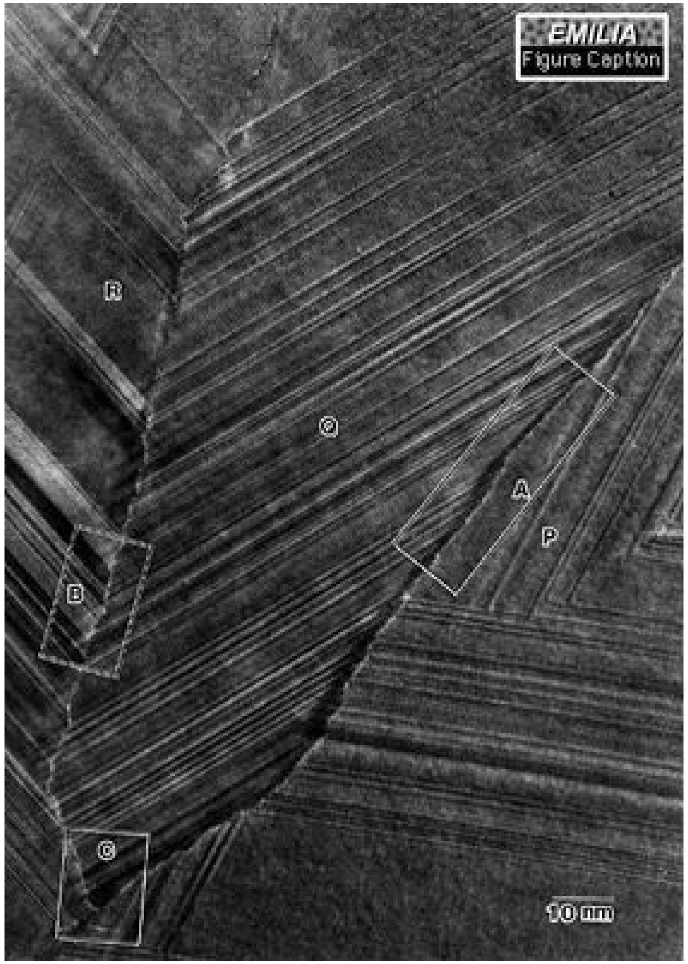
Grain Boundary Problem

- Grain boundaries disrupt the motion of dislocations through a material.

- Grain boundaries are defects in the crystal structure.

So, it is very important to investigate the dynamics of grain rotation and grain boundary motion in material science.



[http://asma7.tagen.tohoku.ac.jp/EMILIA/html/eg/index.html]

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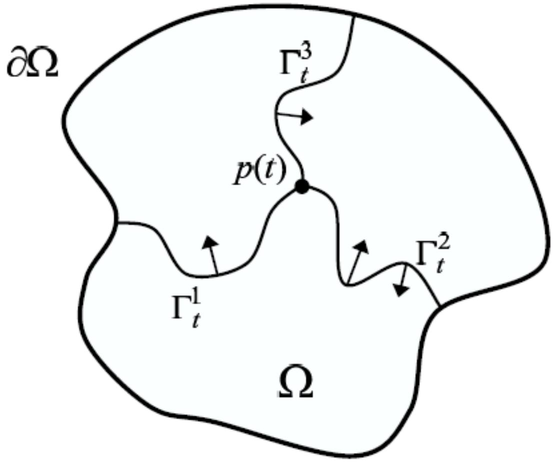
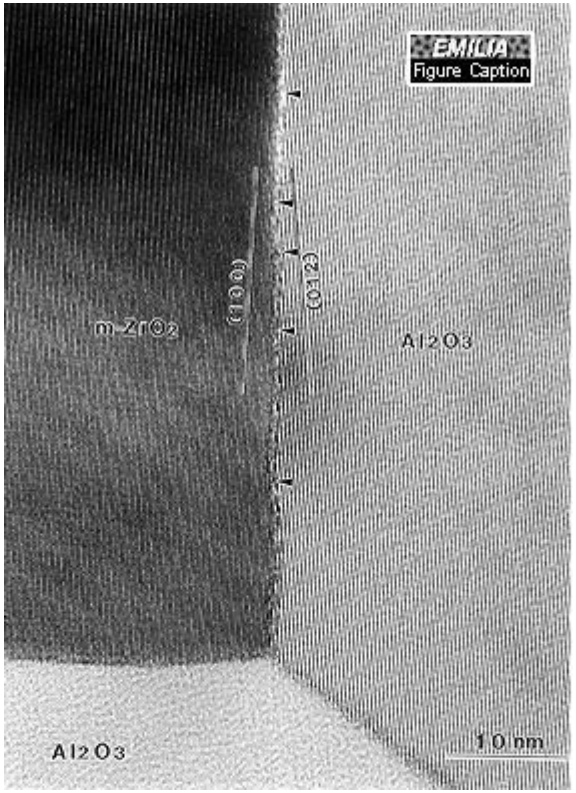
Mathematical Approaches
Surface evolution eq. and Phase-field eq.

[Example] Triple junction problems

Study the curves Γ_t^i $(i = 1, 2, 3)$ and

the triple junction $p(t) \in \Omega$





Garcke–Novick-Cohen ('00), Ito–Kohsaka ('00, '01)

Ikota–Yanagida ('03, '05), Garcke–Ito–Kohsaka ('09)

Garcke–Kohsaka–Ševčovič ('09), $\cdots$ etc.

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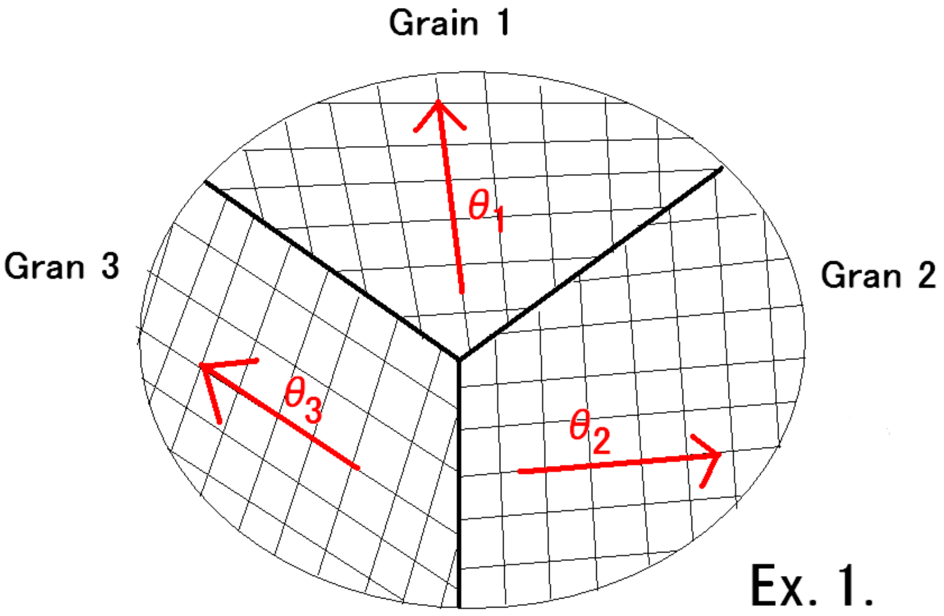
Mathematical Approaches

Surface evolution eq. and Phase-field eq.

- Kobayashi-Warren-Carter [Phys. D, **140**(2000), 141–150] (2-D model)

η : degree of crystalline orientation order

θ : mean orientation



More precisely, in Ex. 1,

$$(\eta\cos\theta, \eta\sin\theta) = \frac{1}{N}\sum_{i=1}^{3} N_i\,(\cos\theta_i, \sin\theta_i)$$

where

$$N = N_1 + N_2 + N_3$$

θ_i is the orientation angle in Grain i $(i = 1, 2, 3)$

N_i is the number of lattice in Grain i $(i = 1, 2, 3)$

Remark • $0 \le \eta \le 1$ • A polar coordinate system (η, θ)

• $\eta = 1$ means a completely oriented state

• $\eta = 0$ is a state where no meaningful value of orientation exists

Isotropic η-θ Grain Boundary Motion Model

- A phase-filed model of Kobayashi-Warren-Carter type

$$\begin{cases} \eta_t - \kappa\Delta\eta + g(\eta) + \alpha'(\eta)|\nabla\theta| = 0 & \text{in } Q_T = \Omega \times (0,T) \\ \alpha_0(\eta)\theta_t - \nu\Delta\theta - \operatorname{div}\left(\alpha(\eta)\dfrac{\nabla\theta}{|\nabla\theta|}\right) + \partial I_{[-\theta^*,\theta^*]}(\theta) \ni 0 & \text{in } Q_T \end{cases}$$

where

- η : order parameter of orientation, θ : orientation angle
- $\partial I_{[-\theta^*,\theta^*]}(\cdot)$ is the subdifferential of the indicator function $I_{[-\theta^*,\theta^*]}(\cdot)$ on the closed interval $[-\theta^*,\theta^*]$ with some constant $\theta^* > 0$
- $\kappa > 0, \nu > 0$: given small constants
- $g(\cdot)$, $\alpha_0(\cdot)$, $\alpha(\cdot)$: given functions on $\mathbb{R}$

Remark Original Kobayashi-Warren-Carter system is a phase-filed model without constraint $\partial I_{[-\theta^*,\theta^*]}(\theta)$ in 2-D domain.

(R. Kobayashi, J. A. Warren and W. C. Carter,
A continuum model of grain boundaries, *Phys. D*, **140**(2000), 141–150)

2. A Grain Boundary Motion Model with constraint

AIM Existence-Uniqueness and Large-time behavior of sol. to (P):

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

where

- η : order parameter of orientation, θ : orientation angle
- Ω is a bounded domain in $\mathbb{R}^N$ $(N \geq 1)$ with smooth boundary $\Gamma := \partial\Omega$
- $\partial I_{[-\theta^*,\theta^*]}(\cdot)$ is the subdifferential of the indicator function $I_{[-\theta^*,\theta^*]}(\cdot)$ on the closed interval $[-\theta^*,\theta^*]$ with some constant $\theta^* > 0$
- $\kappa > 0, \nu > 0$: given small constants
- $g(\cdot)$, $\alpha_0(\cdot)$, $\alpha(\cdot)$: given functions on $\mathbb{R}$

3. Known Results: Modelling

- Grain boundary motion of crystal growth in 2-D case: $\Omega \subset \mathbb{R}^2$

[Kobayashi-Warren-Carter, Phys. D, **140**(2000), 141–150]

$$\begin{cases} \eta_t - \kappa\Delta\eta + g(\eta) + \alpha'(\eta)|\nabla\theta| = 0 & \text{in } Q_T := (0,T)\times\Omega \\ \alpha_0(\eta)\theta_t - \mathrm{div}\left(\alpha(\eta)\dfrac{\nabla\theta}{|\nabla\theta|}\right) = 0 & \text{in } Q_T \end{cases}$$

where

- η : order parameter of orientation, θ : orientation angle
- $\kappa > 0$: given small constant
- $g(\cdot)$, $\alpha_0(\cdot)$, $\alpha(\cdot)$: given functions on $\mathbb{R}$

Remark A polar coordinate system (η, θ)

The free energy functional

$$\mathcal{F}(\eta,\theta) := \frac{\kappa}{2}\int_\Omega |\nabla\eta|^2 dx + \int_\Omega \hat{g}(\eta)dx + \int_\Omega \alpha(\eta)|\nabla\theta|dx$$

Known results : Numerical experiments

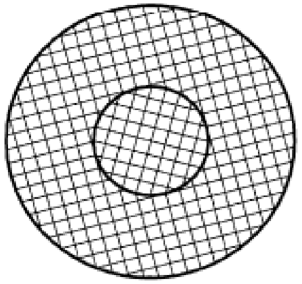
- 2-D case: the unite disk $D \subset \mathbb{R}^2$

  [Kobayashi-Warren-Carter, Phys. D, **140**(2000), 141–150]

$$\begin{cases} \tau\eta_t - \kappa\Delta\eta + g(\eta) + s\alpha'(\eta)|\nabla\theta| = 0 & \text{in } Q_T \\ \alpha_0(\eta)\theta_t - s\,\mathrm{div}\left(\alpha(\eta)\dfrac{\nabla\theta}{|\nabla\theta|}\right) - \nu\Delta\theta = 0 & \text{in } Q_T \\ \dfrac{\partial\eta}{\partial n} = 0, \quad \theta = h & \text{on } \Sigma_T := \partial D \times (0,T) \\ \eta(0) = \eta_0, \quad \theta(0) = \theta_0 & \text{in } D \end{cases}$$

where

- $g(\eta) = \eta - 1, \qquad \alpha_0(\eta) = \alpha(\eta) = \eta^2$
- $\tau = 0.1, \quad \kappa = 4 \times 10^{-4}, \qquad s = 0.2$
- $\nu = 10^{-4}, \quad h = \dfrac{\pi}{3}$
- Initial angle in the inner grain is $\theta_0 = -\dfrac{\pi}{3}$



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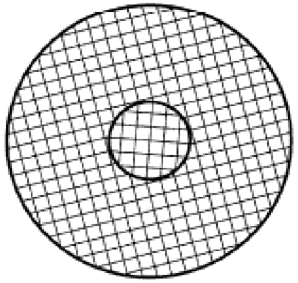

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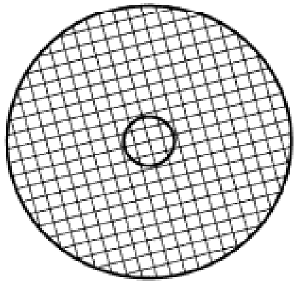
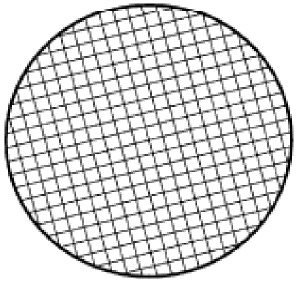


t = 19



t = 24

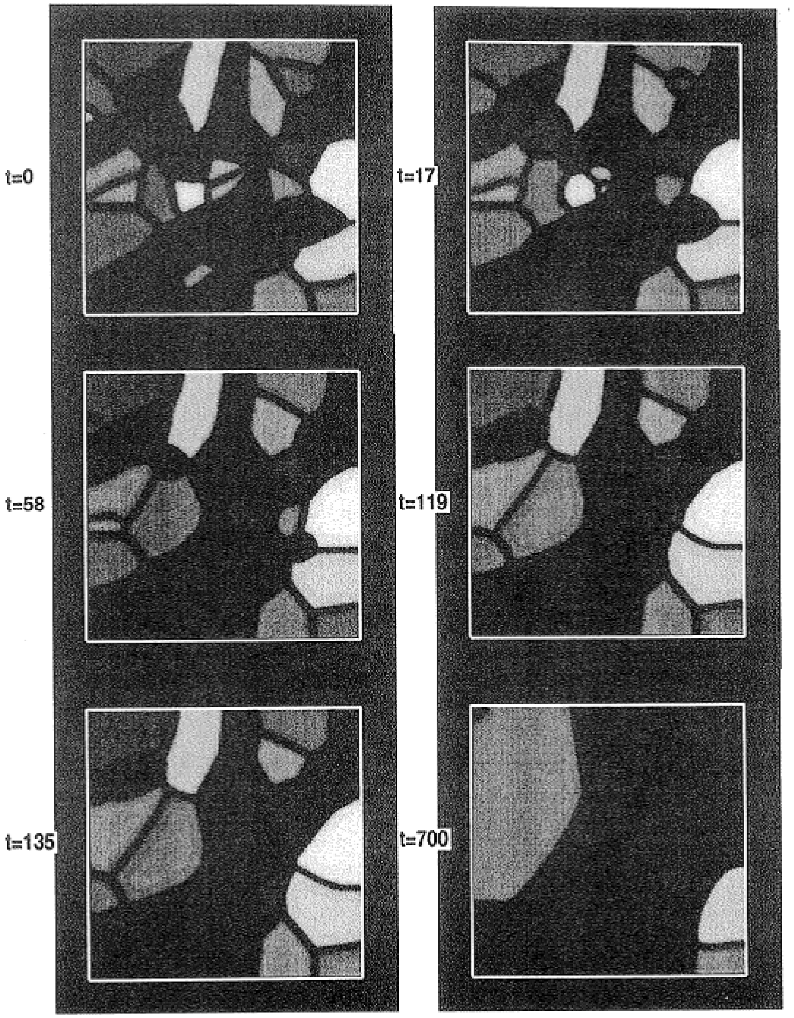
Known results : Numerical experiments

- 2-D case: $\Omega \subset \mathbb{R}^2$

[Kobayashi-Warren-Carter, GAKUTO Internat. Ser. Math. Sci. Appl., **14**(2000)]

$$\begin{cases} \eta_t - \kappa\Delta\eta + g(\eta) + \alpha'(\eta)|\nabla\theta| = 0 & \text{in } Q_T \\ \alpha_0(\eta)\theta_t - \mathrm{div}\left(\alpha(\eta)\dfrac{\nabla\theta}{|\nabla\theta|}\right) - \nu\Delta\theta = 0 & \text{in } Q_T \\ \dfrac{\partial\eta}{\partial n} = 0, \quad \theta = h & \text{on } \Sigma_T := \partial\Omega \times (0,T) \\ \eta(0) = \eta_0, \quad \theta(0) = \theta_0 & \text{in } \Omega \end{cases}$$

where $g(\eta) = \eta - 1, \quad \alpha_0(\eta) = \alpha(\eta) = \eta^2$



Remark

The above system is considered in the physical situation that the whole region is already solidified and filled with some grains.

So we may assume that θ has two threshold values $-\theta^*$ and θ^*, where θ^* is a prescribed positive constant.

Remark: Mathematical study is difficult!

Difficulty Mobility term and Singular diffusivity

$$(\mathrm{P})\begin{cases} \eta_t - \kappa\Delta\eta + g(\eta) + \alpha'(\eta)|\nabla\theta| = 0 & \text{in } Q_T := \Omega \times (0,T) \\ \alpha_0(\eta)\theta_t - \nu\Delta\theta - \mathrm{div}\left(\alpha(\eta)\dfrac{\nabla\theta}{|\nabla\theta|}\right) + \partial I_{[-\theta^*,\theta^*]}(\theta) \ni 0 & \text{in } Q_T \end{cases}$$

Remark The singular diffusion equations,

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

have been studied by a lot of mathematicians:

Andreu–Ballester–Caselles–Mazón ('01),
Andreu–Caselles-Mazón–Moll ('04),
Bellettini–Caselles-Novaga ('02),
Giga–Giga ('10), Giga–Giga–Kobayashi ('01),
Kobayashi–Giga ('99), Kuroda ('09), ··· etc.

Subdifferential Approach

Difficulty Singular diffusivity

$$-\nu\Delta\theta - \mathrm{div}\left(\alpha(\eta)\frac{\nabla\theta}{|\nabla\theta|}\right) + \partial I_{[-\theta^*,\theta^*]}(\theta) \ni -\alpha_0(\eta)\theta_t \quad \text{in } Q_T$$

$$\Longleftrightarrow \qquad \partial\varphi(\eta;\theta) \ni -\alpha_0(\eta)\theta_t \quad \text{in } L^2(\Omega)$$

where $\partial\varphi(\eta(t),z)$ is the subdifferential of $\varphi(\eta(t),z)$ in $z \in L^2(\Omega)$:

$$\varphi(\eta(t);z) := \begin{cases} \displaystyle\int_\Omega \left\{\frac{\nu}{2}|\nabla z|^2 + \alpha(\eta(t))|\nabla z| + I_{[-\theta^*,\theta^*]}(z)\right\} dx & \text{if } z \in H_0^1, \\ \infty & \text{otherwise.} \end{cases}$$

Remark $\varphi(\eta(t);\cdot)$ is a proper, l.s.c. and convex function on $L^2(\Omega)$

Variational inequality

$$\int_\Omega \alpha_0(\eta)\theta_t(\theta - z)dx + \nu\int_\Omega \nabla\theta\cdot\nabla(\theta - z)dx + \int_\Omega \alpha(\eta)|\nabla\theta|dx \le \int_\Omega \alpha(\eta)|\nabla z|dx$$

for a.e. $t \in (0,T)$ and all $z \in H_0^1$ with $|z| \le \theta^*$ a.e. inΩ

A Grain Boundary Motion Model with constraint

AIM Existence-Uniqueness and Large-time behavior of sol. to (P):

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

where

- η : order parameter of orientation, θ : orientation angle
- Ω is a bounded domain in $\mathbb{R}^N$ $(N \geq 1)$ with smooth boundary $\Gamma := \partial\Omega$
- $\partial I_{[-\theta^*,\theta^*]}(\cdot)$ is the subdifferential of the indicator function $I_{[-\theta^*,\theta^*]}(\cdot)$ on the closed interval $[-\theta^*,\theta^*]$ with some constant $\theta^* > 0$
- $\kappa > 0, \nu > 0$: given small constants
- $g(\cdot)$, $\alpha_0(\cdot)$, $\alpha(\cdot)$: given functions on $\mathbb{R}$

Definition of a solution to (P)

A pair $\{\eta, \theta\}$ is called a solution to (P) on $[0,T]$, if (1)–(5) are satisfied:

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

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

(3) $\eta'(t) - \kappa \Delta_N \eta(t) + g(\eta(t)) + \alpha'(\eta(t))|\nabla\theta(t)| = 0$ in L^2 for a.a. $t \in (0,T)$

where $\Delta_N : D(\Delta_N) := \{z \in H^2;\ \frac{\partial z}{\partial n} = 0 \text{ a.e. on } \Gamma\} \longrightarrow L^2$

(4) For a.e. $t \in (0,T)$,

$$\Big(\alpha_0(\eta(t))\theta'(t), \theta(t) - z\Big)_{L^2} + \nu \int_\Omega \nabla\theta(t) \cdot \nabla(\theta(t) - z)dx$$

$$+ \int_\Omega \alpha(\eta(x,t))|\nabla\theta(x,t)|dx \le \int_\Omega \alpha(\eta(x,t))|\nabla z(x)|dx,$$

$\forall z \in H^1_0$ with $|z| \le \theta^*$ a.e. in Ω

(5) $\eta(0) = \eta_0$, $\theta(0) = \theta_0$ in $L^2 := L^2(\Omega)$

Assumptions

(A1) α_0 is a function in $C^2(\mathbb{R})$ such that

$$\alpha_0 \geq \delta_0 \text{ on } \mathbb{R} \text{ for some positive constant } \delta_0$$

(A2) α is a non-negative function in $C^1(\mathbb{R})$ such that

$$\alpha' \text{ is non-decreasing and bounded on } \mathbb{R} \text{ with } \alpha'(0) = 0$$

(A3) g is a Lipschitz continuous function on $\mathbb{R}$ such that

$$g \leq 0 \text{ on } (-\infty, 0] \quad \text{and} \quad g \geq 0 \text{ on } [1, \infty)$$

(A4) κ, ν and θ^* are the fixed positive constants in $\mathbb{R}$.

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

$\theta_0 \in L^2(\Omega)$ with $|\theta_0| \leq \theta^*$ a.e. on Ω.

4. Main Theorem: Existence-Uniqueness of solutions

Theorem 1. [Existence of a solution] [Ito-Kenmochi-Y., '09]

Assume (A1)–(A5). Then there is at least one solution $\{\eta, \theta\}$ of (P), and η satisfies $0 \leq \eta \leq 1$ a.e on Q_T.

Moreover there is a positive constant N_1, independent of the choice of the initial data $\{\eta_0, \theta_0\}$, such that

$$\sup_{t \geq 0} \int_t^{t+1} \mathcal{F}(\eta(\tau), \theta(\tau)) d\tau \leq N_1.$$

Also, for each $\mu \in (0,1]$, there is a positive constant M_μ, independent of the choice of the initial data $\{\eta_0, \theta_0\}$, such that

$$\|\eta'\|^2_{L^2(\mu,\infty;L^2)} + \|\sqrt{\alpha_0(\eta)}\theta'\|^2_{L^2(\mu,\infty;L^2)} + \sup_{t \geq \mu} \mathcal{F}(\eta(t), \theta(t)) \leq M_\mu.$$

- $\mathcal{F}(\cdot, \cdot)$ is the free energy functional defined by

$$\mathcal{F}(\eta, \theta) := \int_\Omega \left\{ \frac{\kappa}{2} |\nabla \eta|^2 + \widehat{g}(\eta) + \frac{\nu}{2} |\nabla \theta|^2 + \alpha(\eta) |\nabla \theta| dx + I_{[-\theta^*, \theta^*]}(\theta) \right\} dx$$

where $\widehat{g}$ is a primitive of g.

Key point of the proof of Theorem 1

Grain Boundary Motion Model with constraint

$$(\mathrm{P})\begin{cases} \eta_t - \kappa\Delta\eta + g(\eta) + \alpha'(\eta)|\nabla\theta| = 0 & \text{in } Q_T \\ \alpha_0(\eta)\theta_t - \nu\Delta\theta - \mathrm{div}\left(\alpha(\eta)\dfrac{\nabla\theta}{|\nabla\theta|}\right) + \partial I_{[-\theta^*,\theta^*]}(\theta) \ni 0 & \text{in } Q_T \\ \dfrac{\partial\eta}{\partial n} = 0, \quad \theta = 0 & \text{on } \Sigma_T \end{cases}$$

$$\Longleftrightarrow \begin{cases} \eta'(t) - \kappa\Delta_N\eta(t) + g(\eta(t)) + \alpha'(\eta(t))|\nabla\theta(t)| = 0 \ \text{ in } L^2 & \text{for } t \in (0,T) \\ \alpha_0(\eta(t))\theta'(t) + \partial\varphi(\eta(t);\theta(t)) \ni 0 \ \text{ in } L^2 & \text{for } t \in (0,T) \end{cases}$$

where $\partial\varphi(\eta(t),z)$ is the subdifferential of $\varphi(\eta(t),z)$ in $z \in L^2$:

$$\varphi(\eta(t);z) := \begin{cases} \displaystyle\int_\Omega \left\{\frac{\nu}{2}|\nabla z|^2 + \alpha(\eta(t))|\nabla z| + I_{[-\theta^*,\theta^*]}(z)\right\} dx & \text{if } z \in H_0^1, \\ \infty & \text{otherwise.} \end{cases}$$

Note that $\varphi(\eta(t);\cdot)$ is a proper, l.s.c. and convex function on L^2

Key points of the proof of Theorem 1

- Approximate Problems $(\mathrm{P})_\varepsilon$ $(\varepsilon \in (0,1])$

$$(\mathrm{P})_\varepsilon \begin{cases} \eta'(t) - \kappa\Delta_N \eta(t) + g(\eta(t)) + \alpha'(\eta(t))|\nabla\theta(t)| = 0 \ \text{ in } L^2 & \text{for } t \in (0,T) \\ \alpha_0((\rho_\varepsilon * \eta)(t))\theta'(t) + \partial\varphi(\eta(t);\theta(t)) \ni 0 \ \text{ in } L^2 & \text{for } t \in (0,T) \\ \eta(x,0) = \eta_0(x), \quad \theta(x,0) = \theta_0(x) & \text{for } x \in \Omega \end{cases}$$

where ρ_ε is a usual one-dimensional mollifier with support $[-\varepsilon,\varepsilon]$ in time

$$(\rho_\varepsilon * \eta)(x,t) := \int_{-\infty}^{\infty} \rho_\varepsilon(t-s)\tilde{\eta}(x,s)ds \qquad \text{for } x \in \Omega,\ t \in [0,T]$$

$$\tilde{\eta}(x,t) := \begin{cases} \eta(x,0) & \text{for } x \in \Omega, \quad t < 0 \\ \eta(x,t) & \text{for } x \in \Omega, \quad 0 \le t \le T \\ \eta(x,T) & \text{for } x \in \Omega, \quad t > T \end{cases}$$

$$\varphi(\eta(t);z) := \begin{cases} \displaystyle\int_\Omega \left\{ \frac{\nu}{2}|\nabla z|^2 + \alpha(\eta(t))|\nabla z| + I_{[-\theta^*,\theta^*]}(z) \right\} dx & \text{if } z \in H_0^1, \\ \infty & \text{otherwise.} \end{cases}$$

Remark $\varphi(\eta(t);\cdot)$ is a proper, l.s.c. and convex function on L^2

Theorem 2. [Uniqueness of a solution] [Ito-Kenmochi-Y., '09]

Assume (A1)–(A4), $\eta_0 \in H^1$ with $0 \le \eta_0 \le 1$ a.e. on Ω, $\theta_0 \in H^1_0$ 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 $\{\eta, \theta\}$ of (P) is unique.

Key point of the proof of Theorem 2

- The embedding $H^1_0 \hookrightarrow L^\infty$ and $H^1 \hookrightarrow L^\infty$

Remark

If the mobility term α_0 is positive constant, i.e., $\alpha_0 \equiv c_0$ for some constant $c_0 > 0$, then the solution $\{\eta, \theta\}$ of (P) is unique in the case when $\{\eta_0, \theta_0\}$ in (A5) and Ω is a bounded domain in $\mathbb{R}^N$ $(N \ge 1)$:

$$\begin{cases} \eta_t - \kappa\Delta\eta + g(\eta) + \alpha'(\eta)|\nabla\theta| = 0 & \text{in } Q_T = \Omega \times (0, T) \\ \alpha_0(\eta)\theta_t - \nu\Delta\theta - \operatorname{div}\left(\alpha(\eta)\dfrac{\nabla\theta}{|\nabla\theta|}\right) + \partial I_{[-\theta^*, \theta^*]}(\theta) \ni 0 & \text{in } Q_T \end{cases}$$

Next Aim : Large-time behavior of solutions to (P)

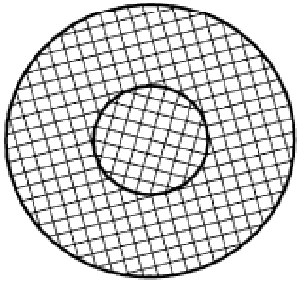
Remark Numerical experiments in 2-D case: the unite disk $D \subset \mathbb{R}^2$

[Kobayashi-Warren-Carter, Phys. D, **140**(2000), 141–150]

$$\begin{cases} \tau\eta_t - \kappa\Delta\eta + g(\eta) + s\alpha'(\eta)|\nabla\theta| = 0 & \text{in } Q_T \\ \alpha_0(\eta)\theta_t - s\,\mathrm{div}\left(\alpha(\eta)\dfrac{\nabla\theta}{|\nabla\theta|}\right) - \nu\Delta\theta = 0 & \text{in } Q_T \\ \dfrac{\partial\eta}{\partial n} = 0, \quad \theta = h & \text{on } \Sigma_T := \partial D \times (0,T) \\ \eta(0) = \eta_0, \quad \theta(0) = \theta_0 & \text{in } D \end{cases}$$

where

- $g(\eta) = \eta - 1, \qquad \alpha_0(\eta) = \alpha(\eta) = \eta^2$
- $\tau = 0.1, \qquad \kappa = 4 \times 10^{-4}, \qquad s = 0.2$
- $\nu = 10^{-4}, \qquad h = \dfrac{\pi}{3}$
- Initial angle in the inner grain is $\theta_0 = -\dfrac{\pi}{3}$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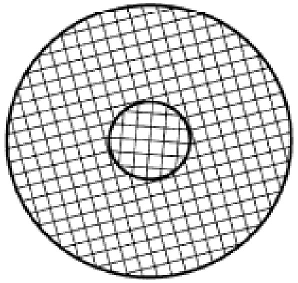
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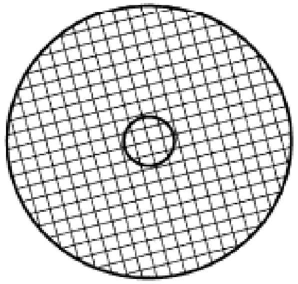
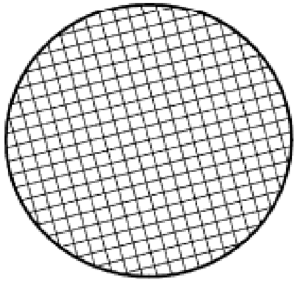

t = 19


t = 24

Steady-state system for (P)

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

Then we easily see that $\{\eta,\theta\}$ is a solution of (S), if and only if

$$\theta = 0 \text{ in } L^2(\Omega) \quad \text{and} \quad -\kappa\Delta_N\eta + g(\eta) = 0 \text{ in } L^2(\Omega).$$

Remark $\quad$ (S) $\Longleftrightarrow$
$$
\begin{cases} -\kappa\Delta_N\eta + g(\eta) + \alpha'(\eta)|\nabla\theta| = 0 & \text{in } L^2(\Omega), \\ 0 \in \partial\varphi(\eta;\theta) \quad \text{in } L^2(\Omega). \end{cases}
$$

In fact, if $\{\eta,\theta\}$ is any solution of (S), then it follows from $0 \in \partial\varphi(\eta;\theta)$ that

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

The above minimum is 0 and is taken at $z = 0$. Hence

$\theta = 0$ in L^2 and the first equation of (S) is $-\kappa\Delta_N\eta + g(\eta) = 0$ in L^2.

Large-time behavior of solutions to (P)

Theorem 3. [Large-time behavior of sol. to (P)] [Kenmochi-Y., '10]

Assume (A1)–(A5). 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

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

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

Key energy inequalities to show Theorem 3

(i) There is a positive constant N_1 such that

$$\sup_{t \ge 0} \int_t^{t+1} \mathcal{F}(\eta(\tau), \theta(\tau)) d\tau \le N_1.$$

(ii) For each $\mu \in (0, 1]$, there is a positive constant M_μ such that

$$\|\eta'\|^2_{L^2(\mu,\infty;L^2)} + \|\sqrt{\alpha_0(\eta)}\theta'\|^2_{L^2(\mu,\infty;L^2)} + \sup_{t \ge \mu} \mathcal{F}(\eta(t), \theta(t)) \le M_\mu.$$

Remark Note that the solution of (S) is not unique, namely, the set S_0 is not a singleton in general, because of the function $g(\cdot)$.

A special case of g (e.g. $g(\eta) = \eta - 1$)

- Asymptotic convergence of all solutions of (P) as $t \to \infty$

Theorem 4. [Kenmochi-Y., '10]

Assume (A1)–(A5).

Additionally, assume 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 $\{1, 0\}$ is a unique steady–state solution of (P),

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

and the above convergence is uniform with respect to $\{\eta_0, \theta_0\}$.

Sketch of the proof of Theorem 4

By the additional assumptions of g, we can show that the set S_0 of steady-state solutions of (P) is a singleton set consisting of the pair $\{1,0\}$, namely, $S_0 = \{\{1,0\}\}$.

Moreover let s be any positive number. Then the following equality holds:

$$\|\eta'(\tau)\|_H^2 + \|\sqrt{\alpha_0(\eta(\tau))}\theta'(\tau)\|_H^2 + \frac{d}{d\tau}\mathcal{F}(\eta(\tau),\theta(\tau)) = 0$$

$$\text{for a.e. } \tau \geq s > 0,$$

which implies that $\mathcal{F}(\eta(t),\theta(t))$ is non-increasing with respect to $t > 0$.

Thus we can show that $\mathcal{F}(1,0) = 0$ and

$\mathcal{F}(\eta(t),\theta(t)) \longrightarrow 0$ uniformly in all global solutions $\{\eta,\theta\}$ as $t \to \infty$,

hence we see that

$$\|\eta(t) - 1\|_{H^1} \longrightarrow 0 \quad \text{and} \quad \|\theta(t)\|_{H_0^1} \longrightarrow 0 \quad \text{as } t \to \infty$$

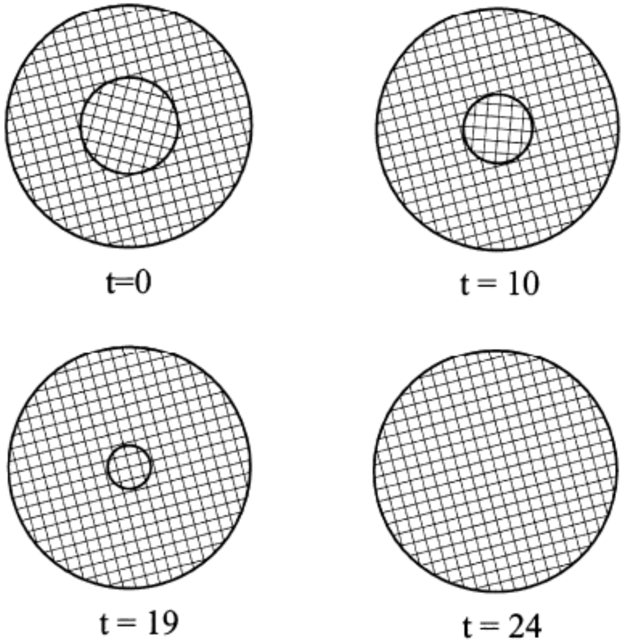
uniformly in all global solutions $\{\eta,\theta\}$ of (P).

Conclusion

We can construct the global solutions to a grain boundary motion models of Kobayashi-Warren-Carter type.

Also we can give the theoretical explanation of numerical results obtained in [Kobayashi-Warren-Carter, Phys. D, **140**(2000), 141–150], although α_0 is strictly positive and there is a constraint $\partial I_{[-\theta_*,\theta_*]}$.

$$\begin{cases} \tau\eta_t - \kappa\Delta\eta + g(\eta) + s\alpha'(\eta)|\nabla\theta| = 0 & \text{in } Q_T \\ \alpha_0(\eta)\theta_t - s\,\mathrm{div}\left(\alpha(\eta)\dfrac{\nabla\theta}{|\nabla\theta|}\right) - \nu\Delta\theta = 0 & \text{in } Q_T \\ \dfrac{\partial\eta}{\partial n} = 0, \quad \theta = h & \text{on } \Sigma_T \\ \eta(0) = \eta_0, \quad \theta(0) = \theta_0 & \text{in } D \end{cases}$$



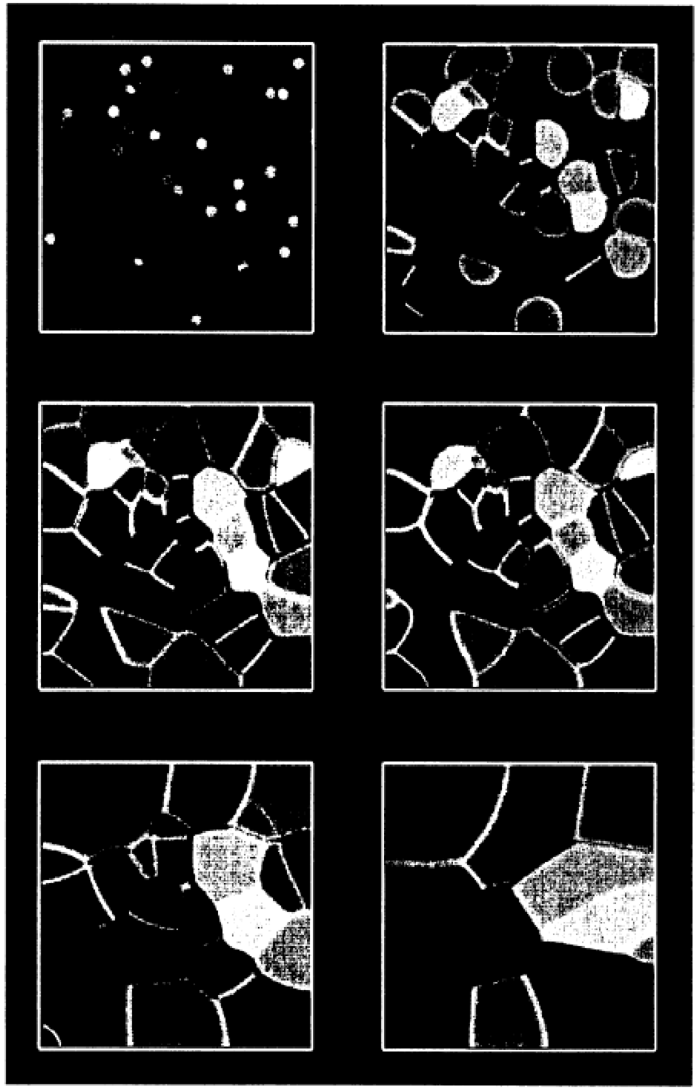
where

- $g(\eta) = \eta - 1, \qquad \alpha_0(\eta) = \alpha(\eta) = \eta^2$
- $\tau = 0.1, \quad \kappa = 4 \times 10^{-4}, \quad s = 0.2, \quad \nu = 10^{-4}, \quad h = \dfrac{\pi}{3}, \quad \theta_0 = -\dfrac{\pi}{3}$

Future Problem

- Liquid-Solid-Grain Boundary Motion Model

$$\begin{cases} \phi_t - \delta\Delta\phi + \phi(\phi-1)(\phi-1/2) - \eta + \phi + \nu\phi|\nabla\theta|^2 = 0 & \text{in } Q_T \\ \eta_t - \kappa\Delta\eta + \eta - \phi + 2\eta|\nabla\theta| = 0 & \text{in } Q_T \\ \eta^2\theta_t - \mathrm{div}\left(\eta^2\dfrac{\nabla\theta}{|\nabla\theta|} - \nu\phi^2\nabla\theta\right) = 0 & \text{in } Q_T \end{cases}$$



where

- ϕ: liquid-solid order parameter
- η : order parameter of orientation
- θ : orientation angle

Reference

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