Mathematical Approaches to Kobayashi–Warren–Carter type models of grain boundary motions

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1. Kobayashi–Warren–Carter model of grain boundary motion

Keywords: Derivation method of Kobayashi–Warren–Carter model, physical background, settings and assumptions

2. Mathematical approach when $\nu > 0$ (regular case)

Keywords: Dirct subdifferential approach / extended gradient formalism, mathematical results [Ito–Kenmochi–Yamazaki](2008–2011), anisotropic model [Moll–S.–Watanabe](2017)

3. Mathematical approach when $\nu = 0$ (singular case)

Keywords: weighted total variation, variational formulation, mathematical results [Moll, S., Watanabe, Yamazaki](2012–), time-discretization approach

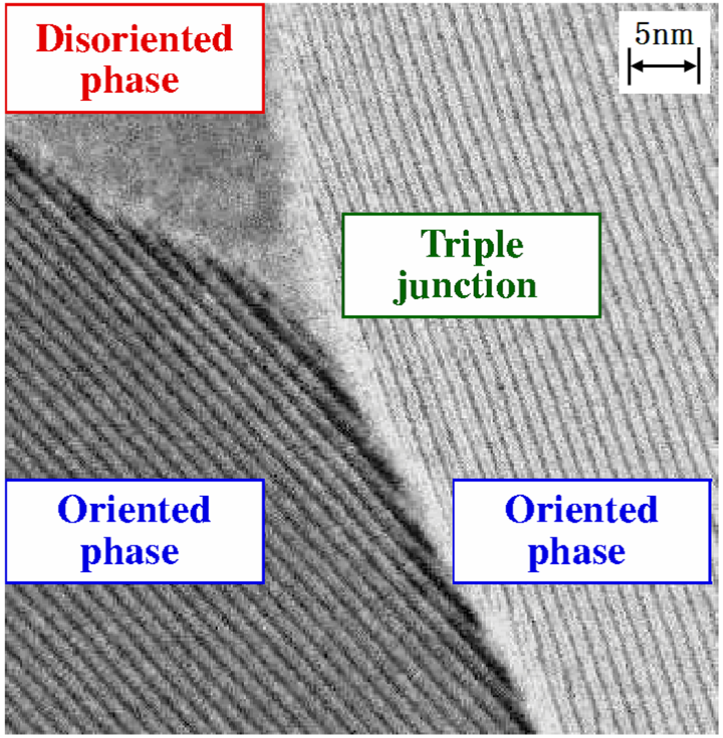
4. Problems in future

Keywords: Structural observations (for steady-state, in time-evolution), further advanced issues (anisotropic singular model, uniqueness)

1. Kobayashi–Warren–Carter model of grain boundary motion

Situation: in a time-interval $(0, \infty)$, a spatial domain $\Omega \subset \mathbb{R}^2$ is occupied by a polycrystal (e.g. Ceramics).

Target: the movement of grain boundaries, i.e. grain boundary motions



← Micrograph (Si_3N_4): UBE Scientific Analysis Laboratory (http://www.ube-ind.co.jp/usal/)

Kobayashi–Warren–Carter model.
[K.–W.–C.](2000) Physica D

System of parabolic equations in $Q := (0, \infty) \times \Omega$, described by:

- $\varpi = \begin{bmatrix} \eta \cos \theta \\ \eta \sin \theta \end{bmatrix}$ mean orientation,
  - $\eta = \eta(t, x)$, $(t, x) \in Q$, orientation order, $0 \leq \eta \leq 1$,

    $$\begin{cases} \eta = 1 \iff \text{oriented}, \\ \eta = 0 \iff \text{disoriented}, \\ \text{otherwise} \iff \text{intermediate}, \end{cases}$$

  - $\theta = \theta(t, x)$, $(t, x) \in Q$, orientation angle.

1.1. Derivation of the model

Gradient flow of the free-energy

$$[\eta, \theta] \in L^2(\Omega)^2 \mapsto \mathscr{F}_\nu(\eta, \theta) := \Psi_0(\eta) + \Phi_\nu(\eta; \theta)$$ Interfacial energy

- $$\eta \mapsto \Psi_0(\eta) := \frac{1}{2} \int_\Omega |D\eta|^2 \, dx + \int_\Omega G(\eta) \, dx$$

- $$[\eta, \theta] \mapsto \Phi_\nu(\eta; \theta) := \int_\Omega \alpha(\eta) |D\theta| \, dx \quad + \quad \frac{\nu^2}{2} \int_\Omega |D\theta|^2 \, dx$$

Total variation | Relaxation

Note that: $\nu = 0 \implies D(\mathscr{F}_\nu) = H^1(\Omega) \times BV(\Omega) \cap L^2(\Omega)$

Kobayashi–Warren–Carter model (KWC)$_\nu$:

$$\left\{ \begin{array}{l} -\eta_t = \nabla_\eta \mathscr{F}_\nu(\eta, \theta) \ \text{ in } Q, \\ -\alpha_0(\eta)\theta_t = \nabla_\theta \mathscr{F}_\nu(\eta, \theta) \ \text{ in } Q, \end{array} \right.$$ (B.C.)+(I.C.)

- $\nu \geq 0$: given small const. • $\alpha_0 = \alpha_0(\eta) > 0$, $\alpha = \alpha(\eta) > 0$: mobilities
- $0 \leq G = G(\eta)$: potential function for the range-constraint $0 \leq \eta \leq 1$

Assumptions.

(A0) $\nu \geq 0$: const., $\Omega \subset \mathbb{R}^N$: b.d.d. domain ($N \in \mathbb{N}$), $\Gamma := \partial\Omega$: smooth

(A1) $0 \leq G \in C^3(\mathbb{R})$, $g = G' \in C^2(\mathbb{R})$ s.t. $g' > 0$ on $[0, 1]$ and $g(1) = 0$

(A2) $\alpha_0 \in C^1(\mathbb{R})$, $\alpha \in C^2(\mathbb{R})$ convex, $\alpha'(0) = 0$, $\delta_* := \inf \alpha_0(\mathbb{R}) \cup \alpha(\mathbb{R}) > 0$

(A3) $[\eta_0, \theta_0]$ belongs to a subclass $D_\nu \subset D(\mathscr{F}_\nu)$, where

$$D_\nu := \left\{ [\tilde{\eta}, \tilde{\theta}] \in D(\mathscr{F}_\nu) \;\middle|\; \begin{array}{c} \tilde{\eta} \in H^1(\Omega),\ 0 \leq \tilde{\eta} \leq 1 \text{ a.e. on } \Omega, \\ \tilde{\theta} \in BV(\Omega) \cap L^\infty(\Omega) \text{ and } \nu\tilde{\theta} \in H^1(\Omega) \end{array} \right\}$$

Typical choices, cf. [Kobayashi–Warren–Carter](2000).

$$\alpha_0(\eta) = \alpha(\eta) = \frac{\eta^2}{2} + \delta_*, \ G(\eta) = \frac{(\eta - 1)^2}{2}, \ g(\eta) = \eta - 1, \ \forall \eta \in \mathbb{R}$$

†. The presences of the constants ν and δ_* were not supposed in the original model

‡. Red conditions are to lead to the range constraint $0 \leq \eta \leq 1$, and this range constraint enables us to suppose Lipschitz continuities for α_0, α, g, without loss of generality

2. Mathematical approach when $\nu > 0$

System $(\mathrm{KWC})_\nu$ with "Neumann-zero B.C." for θ:

$$\begin{cases} \eta_t - \Delta\eta + g(\eta) + \alpha'(\eta)|D\theta| = 0, \ \text{in } Q, \\ \alpha_0(\eta)\theta_t - \mathrm{div}\left(\alpha(\eta)\frac{D\theta}{|D\theta|} + \nu^2 D\theta\right) = 0, \ \text{in } Q, \\ D\eta \cdot n_{\partial\Omega} = 0, \ \left(\alpha(\eta)\frac{D\theta}{|D\theta|} + \nu^2 D\theta\right) \cdot n_{\partial\Omega} = 0, \ \text{on } \Sigma := (0,T) \times \partial\Omega, \\ \eta(0,x) = \eta_0(x), \ \theta(0,x) = \theta_0(x), \ x \in \Omega. \end{cases}$$

◇ **Corresponding interfacial energy (Neumann-zero B.C. for θ)**

$$[\eta, \theta] \in L^2(\Omega)^2 \mapsto \Phi_\nu(\eta;\theta) := \begin{cases} \displaystyle\int_\Omega \left(\alpha(\eta)|D\theta| + \frac{\nu^2}{2}|D\theta|^2\right) dx, \\ \qquad \text{if } \theta \in H^1(\Omega), \\ \infty, \quad \text{otherwise.} \end{cases}$$

Note that: by the range constraint $0 \leq \eta \leq 1$, $\alpha'(\eta)|D\theta|$ can be L^2-function, and $-\mathrm{div}\left(\alpha(\eta)\frac{D\theta}{|D\theta|} + \nu^2 D\theta\right) \approx \partial\Phi_\nu(\eta;\theta)$, where $\partial\Phi_\nu(\eta;\theta)$ is the L^2-subdifferential of $\Phi_\nu(\eta;\theta)$ with respect to θ

2. Mathematical approach when $\nu > 0$

System (KWC)$_\nu$ with "Dirichlet-zero B.C." for θ:

$$\begin{cases} \eta_t - \Delta\eta + g(\eta) + \alpha'(\eta)|D\theta| = 0, \ \text{in } Q, \\ \alpha_0(\eta)\theta_t - \mathrm{div}\left(\alpha(\eta)\dfrac{D\theta}{|D\theta|} + \nu^2 D\theta\right) = 0, \ \text{in } Q, \\ D\eta \cdot n_{\partial\Omega} = 0, \ \theta = 0, \ \text{on } \Sigma := (0,T)\times\partial\Omega, \\ \eta(0,x) = \eta_0(x), \ \theta(0,x) = \theta_0(x), \ x \in \Omega. \end{cases}$$

◇ **Corresponding interfacial energy (Dirichlet-zero B.C. for θ)**

$$[\eta,\theta] \in L^2(\Omega)^2 \mapsto \Phi_\nu(\eta;\theta) := \begin{cases} \displaystyle\int_\Omega \left(\alpha(\eta)|D\theta| + \frac{\nu^2}{2}|D\theta|^2\right) dx, \\ \qquad \text{if } \theta \in H_0^1(\Omega), \text{ i.e. we suppose } \theta = 0 \text{ on } \partial\Omega, \\ \infty, \quad \text{otherwise.} \end{cases}$$

Note that: by the range constraint $0 \leq \eta \leq 1$, $\alpha'(\eta)|D\theta|$ can be L^2-function, and $-\mathrm{div}\left(\alpha(\eta)\frac{D\theta}{|D\theta|} + \nu^2 D\theta\right) \approx \partial\Phi_\nu(\eta;\theta)$, where $\partial\Phi_\nu(\eta;\theta)$ is the L^2-subdifferential of $\Phi_\nu(\eta;\theta)$ with respect to θ

2.1. Direct subidfferential-approach to $(\mathrm{KWC})_\nu$ when $\nu > 0$

Vectorial variable $v \in H$ on a Hilbert space H:

$$H := L^2(\Omega)^2 \text{ and } v := [\eta, \theta] \in H$$

Operator $\mathcal{A} : H \longrightarrow L^2(\Omega)^{2\times 2}$ of mobility:

$$v = [\eta, \theta] \in H \mapsto \mathcal{A}(v) := \begin{bmatrix} 1 & 0 \\ 0 & \alpha_0(\eta) \end{bmatrix}$$

"Total convex energy" $\mathcal{J}_\nu : H \longrightarrow [0, \infty]$ with the subdifferential $\partial\mathcal{J}_\nu \subset H^2$:

$$v = [\eta, \theta] \in D(\mathscr{F}_\nu) \subset H \mapsto \mathcal{J}_\nu(v) := \frac{1}{2}\int_\Omega \left[|D\eta|^2 + \left(\nu|D\theta| + \frac{1}{\nu}\alpha(\eta) \right)^2 \right] dx$$

Lipschitz perturbation $\mathcal{G} : H \longrightarrow H$:

$$v = [\eta, \theta] \in H \mapsto \mathcal{G}(v) := {}^{\mathrm{t}}\!\left[g(\eta) - \frac{1}{\nu}\alpha(\eta)\alpha'(\eta), 0 \right]$$

Reformulation of $(\mathrm{KWC})_\nu$ by a doubly-nonlinear evolution equation on H:

$$(\mathrm{E})_\nu \qquad \mathcal{A}(v(t))v'(t) + \partial\mathcal{J}_\nu(v(t)) + \mathcal{G}(v(t)) \ni 0 \text{ in } H, \ t > 0$$

†. The general theories of [Brézis, Barbu](1972–) are avalirable for the existence result and the uniqueness when $\alpha_0 \equiv \text{Const.}$

‡. The direct subdifferential approach is NOT available when $\nu = 0$

2.2. Mathematical results when $\nu > 0$, cf. [Ito–Kenmochi–Yamazaki](2008–2011)

For simplicity, we suppose the Dirichlet-zero B.C. for θ

Theorem I (Solvability, energy-dissipation and large-time behavior) Under (A0)–(A3) with $\nu > 0$, the system $(\mathrm{KWC})_\nu$ admits a solution $[\eta, \theta]$, defined as follows.

(S1)$_\nu$ $[\eta, \theta] \in W^{1,2}_{\mathrm{loc}}([0, \infty); L^2(\Omega)^2) \cap L^\infty_{\mathrm{loc}}([0, \infty); H^1(\Omega) \times H^1_0(\Omega))$;

$0 \le \eta(t) \le 1$ a.e. in Ω and $|\theta(t)|_{L^\infty(\Omega)} \le |\theta_0|_{L^\infty(\Omega)}$, $\forall t \ge 0$;

$[\eta(0), \theta(0)] = [\eta_0, \theta_0] \in D_\nu$, in $L^2(\Omega)^2$

(S2)$_\nu$ $[\eta, \theta]$ solves the following variational inequalities:

$$\int_\Omega \big(\eta_t(t) + g(\eta(t)) + \alpha'(\eta(t))|D\theta(t)|\big)\varphi \, dx + \int_\Omega D\eta(t) \cdot D\varphi \, dx = 0,$$

$$\int_\Omega \alpha_0(\eta(t))\theta_t(t)\big(\theta(t) - \psi\big) \, dx + \nu^2 \int_\Omega D\theta(t) \cdot D\big(\theta(t) - \psi\big) \, dx$$
$$+ \int_\Omega \alpha(\eta(t))|D\theta(t)| \, dx \le \int_\Omega \alpha(\eta(t))|D\psi| \, dx,$$

$$\forall \varphi \in H^1(\Omega),\ \psi \in H^1_0(\Omega) \ \text{ a.e. } t > 0$$

to be continued ...

... rest of the statement

(S3)$_\nu$ (Energy dissipation) $\mathscr{F}_\nu(\eta(\,\cdot\,), \theta(\,\cdot\,))$ is absolutely continuous in time, and

$$|\eta_t(t)|^2_{L^2(\Omega)} + |\sqrt{\alpha_0(\eta(t))}\theta_t(t)|^2_{L^2(\Omega)} + \frac{d}{dt}\mathscr{F}_\nu(\eta(t), \theta(t)) = 0, \text{ a.e. } t > 0.$$

Moreover, the following convergence holds in the large-time.

$$[\eta(t), \theta(t)] \to [1, 0] \text{ in } L^2(\Omega)^2 \text{ as } t \to \infty$$

In particular, if $\alpha_0 \equiv$ Const., then the solution $[\eta, \theta]$ is unique.

†. The convergent point $[1, 0]$ is the (unique) solution to the steady-state prpblem (S$_\infty$)$_\nu$

(S$_\infty$)$_\nu$:

$$\begin{cases} -\Delta\eta_\infty + g(\eta_\infty) + \alpha'(\eta_\infty)|D\theta_\infty| = 0 \text{ in } \Omega, \text{ with Neumann-zero B.C.,} \\ -\mathrm{div}\left(\alpha(\eta_\infty)\dfrac{D\theta_\infty}{|D\theta_\infty|} + \nu^2 D\theta_\infty\right) = 0, \text{ with Dirichlet-zero B.C.} \end{cases}$$

◇ **Relevant previouis works**

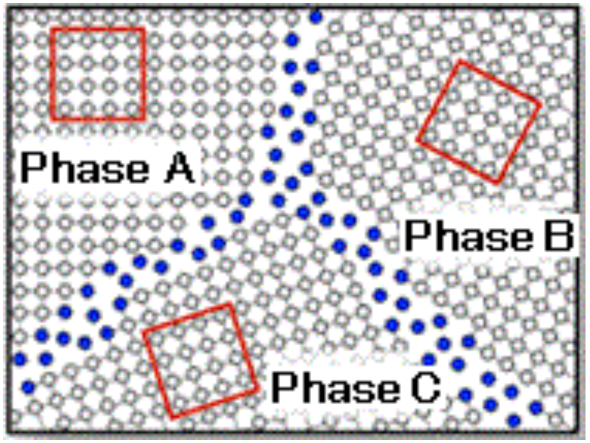
♯1) **Neumann-zero B.C. for θ:** [Moll, S., Watanabe, Yamazaki](2012–)

♯2) **Inhomogeneous Dirichlet B.C. for θ:** [Moll, S., Watanabe](2016–2017)

♯3) Anisotropic system (A-KWC)$_\nu$, cf. [Moll–S.–Watanabe](2016–2017):

$$\begin{cases} \eta_t - \Delta\eta + g(\eta) + \alpha'(\eta)\gamma(R(\theta)D\theta) = 0, \text{ in } Q, \\ \alpha_0(\eta)\theta_t - \mathrm{div}\left(\alpha(\eta)R(-\theta)\partial\gamma(R(\theta)D\theta) + \nu D\theta\right) \\ \qquad\qquad + \alpha(\eta)\partial\gamma(R(\theta)D\theta)\cdot R(\theta+\frac{\pi}{2})D\theta \ni 0 \text{ in } Q, \\ \text{(B.C.)+(I.C.)} \end{cases}$$

- $\Omega \subset \mathbb{R}^2$: b.d.d. domain
- $\partial\gamma$: subdifferential of an anisotropic norm $0 \le \gamma \in W^{1,\infty}(\mathbb{R}^2)$
- $R(\vartheta) := \begin{bmatrix} \cos\vartheta & \sin\vartheta \\ -\sin\vartheta & \cos\vartheta \end{bmatrix}$, $\forall\vartheta \in \mathbb{R}$ (rotation angle)



Anisotropic interfaical energy:

$$[\eta,\theta] \in H^1(\Omega)^2 \mapsto \Phi_\nu(\eta;\theta) := \int_\Omega \alpha(\eta)\gamma(R(\theta)D\theta)\,dx + \frac{\nu^2}{2}\int_\Omega |D\theta|^2\,dx$$

♯3) Anisotropic system (A-KWC)$_\nu$, cf. [Moll–S.–Watanabe](2016–2017):

$$\begin{cases} \eta_t - \Delta\eta + g(\eta) + \alpha'(\eta)\gamma(R(\theta)D\theta) = 0, \quad \text{in } Q, \\ \alpha_0(\eta)\theta_t - \mathrm{div}\left(\alpha(\eta)R(-\theta)\partial\gamma(R(\theta)D\theta) + \nu D\theta\right) \\ \qquad\qquad + \alpha(\eta)\partial\gamma(R(\theta)D\theta)\cdot R(\theta + \tfrac{\pi}{2})D\theta \ni 0 \text{ in } Q, \\ \text{(B.C.)+(I.C.)} \end{cases}$$

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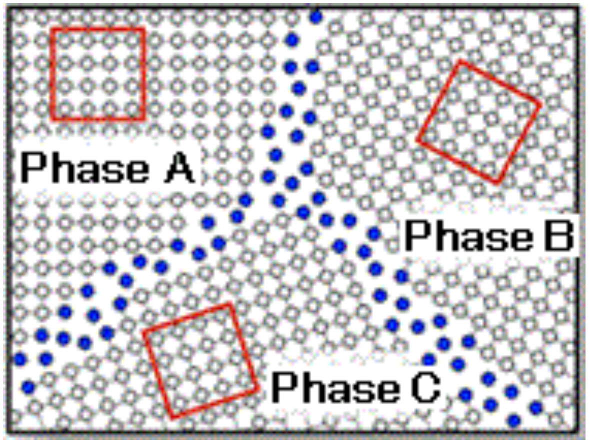


Note that:

Due to the difference of γ and $|\cdot|$, we can NOT apply the direct sudifferential-approach for (A-KWC)$_\nu$, and we need another approach based on the mathematical analysis when $\nu = 0$

3. Mathematical approach when $\nu = 0$

System $(\mathrm{KWC})_0$ with "Neumann-zero B.C." for θ:

$$\begin{cases} \eta_t - \Delta\eta + g(\eta) + \alpha'(\eta)|D\theta| = 0, \ \text{ in } Q, \\ \alpha_0(\eta)\theta_t - \mathrm{div}\left(\alpha(\eta)\dfrac{D\theta}{|D\theta|}\right) = 0, \ \text{ in } Q, \\ D\eta \cdot n_{\partial\Omega} = 0, \ \ (\alpha(\eta)\frac{D\theta}{|D\theta|}) \cdot n_{\partial\Omega} = 0, \ \text{ on } \Sigma := (0,T) \times \partial\Omega, \\ \eta(0,x) = \eta_0(x), \ \theta(0,x) = \theta_0(x), \ \ x \in \Omega. \end{cases}$$

◇ **Corresponding interfacial energy (Neumann-zero B.C. for θ)**

$$[\eta,\theta] \in L^2(\Omega)^2 \mapsto \Phi_0(\eta;\theta) := \begin{cases} \displaystyle\int_\Omega \alpha(\eta)|D\theta| \ \text{(weighted total variation)}, \\ \qquad \text{if } \eta \in H^1(\Omega) \cap L^\infty(\Omega) \text{ and } \theta \in BV(\Omega), \\ \infty, \quad \text{otherwise.} \end{cases}$$

Mathematical focus: $\theta \in BV(\Omega) \Longrightarrow |D\theta|$: measure (not function)

(MF1) Meaningful mathemtaical expression of $\alpha(\eta)|D\theta|$, $\alpha'(\eta)|D\theta|$, e.t.c.,
i.e. the expressions of weighted total varitaions

3. Mathematical approach when $\nu = 0$

System $(\mathrm{KWC})_0$ with "Dirichlet-zero B.C." for θ:

$$\begin{cases} \eta_t - \Delta\eta + g(\eta) + \alpha'(\eta)|D\theta| = 0, & \text{in } Q, \\ \alpha_0(\eta)\theta_t - \mathrm{div}\left(\alpha(\eta)\dfrac{D\theta}{|D\theta|} + \nu^2 D\theta\right) = 0, & \text{in } Q, \\ D\eta \cdot n_{\partial\Omega} = 0, \ \ \theta = 0, & \text{on } \Sigma := (0,T) \times \partial\Omega, \\ \eta(0,x) = \eta_0(x), \ \theta(0,x) = \theta_0(x), & x \in \Omega. \end{cases}$$

◇ **Expected interfacial energy (Dirichlet-zero B.C. for θ)**

$$[\eta,\theta] \in L^2(\Omega)^2 \mapsto \widetilde{\Phi}_0(\eta;\theta) := \begin{cases} \displaystyle\int_\Omega \alpha(\eta)|D\theta| & \text{if } \eta \in H^1(\Omega) \cap L^\infty(\Omega), \\ & \theta \in BV(\Omega) \text{ and } \theta = 0 \text{ on } \partial\Omega, \\ \infty, & \text{otherwise.} \end{cases}$$

Mathematical focus: $\theta \in BV(\Omega)$ may have jumps bet. values on Ω and $\partial\Omega$

$\Longrightarrow$ the B.C. "$\theta = 0$ on $\partial\Omega$" is meaningless in mathematics

3. Mathematical approach when $\nu = 0$

System (KWC)$_0$ with "Dirichlet-zero B.C." for θ:

$$\begin{cases} \eta_t - \Delta\eta + g(\eta) + \alpha'(\eta)|D\theta| = 0, \quad \text{in } Q, \\ \alpha_0(\eta)\theta_t - \operatorname{div}\left(\alpha(\eta)\dfrac{D\theta}{|D\theta|} + \nu^2 D\theta\right) = 0, \quad \text{in } Q, \\ D\eta \cdot n_{\partial\Omega} = 0, \quad \theta = 0, \quad \text{on } \Sigma := (0,T) \times \partial\Omega, \\ \eta(0,x) = \eta_0(x), \ \theta(0,x) = \theta_0(x), \quad x \in \Omega. \end{cases}$$

◇ **Expected interfacial energy (Dirichlet-zero B.C. for θ)**

$$[\eta, \theta] \in L^2(\Omega)^2 \mapsto \widetilde{\Phi}_0(\eta;\theta) := \begin{cases} \displaystyle\int_\Omega \alpha(\eta)|D\theta| \text{ if } \eta \in H^1(\Omega) \cap L^\infty(\Omega), \\ \qquad \theta \in BV(\Omega) \text{ and } \theta = 0 \text{ on } \partial\Omega, \\ \infty, \quad \text{otherwise.} \end{cases}$$

Mathematical focus: the expected energy $\widetilde{\Phi}_0$ is NOT lower semi-continuous

(MF2) The exact formulation of the interfaical energy "$\Phi_0(\eta;\theta)$" for the Dirichlet-zero B.C. for θ

3.1. Preliminaries for $(\mathrm{KWC})_0$ with Dirichlet-zero B.C. for θ

(MF1) Weighted total variation, cf. [Amar, Bellettini, de Cicco, Fusco](1994–)

$\forall \beta \in H^1(\Omega) \cap L^\infty(\Omega)$, $\theta \in BV(\Omega) \cap L^2(\Omega)$, the weighted total variation $[\beta|D\theta|]$ is a finite Radon measure on Ω, s.t.

$$\int_\Omega d[\beta|D\theta|] = \int_\Omega \beta^*|D\theta| \text{ (integral of } \beta^* \text{ w.r.t. } |D\theta|)$$

where β^* is the precise expression of β, $\mathcal{H}^{N-1}$-a.e. in Ω

Proposition 3.1 (Continuous dependence), cf. [Moll–S.](2014) If:

$$\begin{cases} \beta, \rho \in H^1(\Omega) \cap L^\infty(\Omega), \ \{\beta_n, \rho_n\}_{n=1}^\infty \subset H^1(\Omega) \cap L^\infty(\Omega), \\ \theta \in BV(\Omega) \cap L^2(\Omega), \ \{\theta_n\}_{n=1}^\infty \subset BV(\Omega) \cap L^2(\Omega) \end{cases}$$

$$\beta_n \to \beta, \ \rho_n \to \rho \text{ in } L^2(\Omega), \text{ weakly in } H^1(\Omega), \text{ as } n \to \infty,$$

$$\beta_n \geq \exists \delta_\beta > 0 \text{ on } \Omega, \forall n \in \mathbb{N}, \text{ and } \theta_n \to \theta \text{ in } L^2(\Omega), \text{ as } n \to \infty$$

then it holds that:

$$\int_\Omega d[\beta_n|D\theta_n|] \to \int_\Omega d[\beta|D\theta|] \Longrightarrow \int_\Omega d[\rho_n|D\theta_n|] \to \int_\Omega d[\rho|D\theta|], \text{ as } n \to \infty$$

(MF2) Dirichlet-zero B.C. for θ, cf. [Andreu–Ballester–Caselles–Mazón](2001)

$\forall \beta \in H^1(\Omega) \cap L^\infty(\Omega),\ \theta \in BV(\Omega) \cap L^2(\Omega)$, let $[\beta|D\theta|]_0$ be a measure, defined as:

$$\int_B d[\beta|D\theta|]_0 := \int_B [\beta^*]_0^{\mathrm{ex}} |D[\theta]_0^{\mathrm{ex}}| = \int_{B\cap\Omega} \beta^* |D\theta| + \int_{B\cap\partial\Omega} \beta|\theta|\, d\mathcal{H}^{N-1}, \forall B \subset \mathbb{R}^N\text{: Borel}$$

where $[\,\cdot\,]_0^{\mathrm{ex}}$ is the zero-extension of a function

Interfacial energy under Dirichlet-zero B.C. for θ:

$$\Phi_0(\eta;\theta) := \int_{\overline{\Omega}} d[\alpha(\eta)|D\theta|]_0 = \int_\Omega \alpha(\eta^*)|D\theta| + \int_{\partial\Omega} \alpha(\eta)|\theta|\, d\mathcal{H}^{N-1}$$

◇ **Dirichlet type B.C. derived from the subdifferential $\partial\Phi_0(\eta;\,\cdot\,)$ (1st variation)**

$$-\alpha(\eta)\frac{D\theta}{|D\theta|}\cdot n_\Gamma \in \alpha(\eta)\,\mathrm{Sgn}(\theta) \iff \theta \in (\mathrm{Sgn})^{-1}\left(-\frac{D\theta}{|D\theta|}\cdot n_\Gamma\right)$$

$$\begin{cases} \theta = 0, \text{ if } \frac{D\theta}{|D\theta|}\cdot n_\Gamma \in (-1,1), \\ \theta \le 0, \text{ if } \frac{D\theta}{|D\theta|}\cdot n_\Gamma = 1, \\ \theta \ge 0, \text{ if } \frac{D\theta}{|D\theta|}\cdot n_\Gamma = -1, \end{cases} \qquad \text{a.e. on } \Gamma$$

where $(\mathrm{Sgn})^{-1}$ is the inverse of the signal-function Sgn (set-valued)

3.2. Mathematical results when $\nu = 0$, cf. [Moll, S., Watanabe, Yamazaki](2012–)

For simplicity, we suppose the Dirichlet-zero B.C. for θ

Theorem II (Solvability, energy-dissipation and large-time behavior) Under (A0)–(A3) with $\nu = 0$, the system $(\mathrm{KWC})_0$ admits a solution $[\eta, \theta]$, defined as follows.

$(\mathrm{S1})_0$ $\eta \in W^{1,2}_{\mathrm{loc}}([0,\infty); L^2(\Omega)) \cap L^\infty_{\mathrm{loc}}([0,\infty); H^1(\Omega))$, $\eta(0) = \eta_0$ in $L^2(\Omega)$;

$\theta \in W^{1,2}_{\mathrm{loc}}([0,\infty); L^2(\Omega))$, $|D\theta(\,\cdot\,)|(\Omega) \in L^\infty_{\mathrm{loc}}([0,\infty))$, $\theta(0) = \theta_0$ in $L^2(\Omega)$;

$0 \le \eta(t) \le 1$ a.e. in Ω and $|\theta(t)|_{L^\infty(\Omega)} \le |\theta_0|_{L^\infty(\Omega)}$, $\forall t \ge 0$;

$(\mathrm{S2})_0$ $[\eta, \theta]$ solves the following variational inequalities:

$$\int_\Omega \big(\eta_t(t) + g(\eta(t))\big)\varphi\,dx + \int_\Omega D\eta(t)\cdot D\varphi\,dx + \int_{\overline{\Omega}} d\big[\varphi\alpha'(\eta(t))|D\theta(t)|\big]_0 = 0,$$

$$\int_\Omega \alpha_0(\eta(t))\theta_t(t)\big(\theta(t) - \psi\big)\,dx + \int_{\overline{\Omega}} d\big[\alpha(\eta(t))|D\theta(t)|\big]_0 \le \int_{\overline{\Omega}} d\big[\alpha(\eta(t))|D\psi|\big]_0,$$

$$\forall \varphi \in H^1(\Omega) \cap L^\infty(\Omega),\ \psi \in BV(\Omega) \cap L^2(\Omega) \ \text{ a.e. } t > 0$$

to be continued ...

... rest of the statement

(S3)$_0$ (Energy dissipation) $\mathscr{F}_0(\eta(\,\cdot\,), \theta(\,\cdot\,))$ is BV-local function in time, and

$$\int_s^t \left(|\eta_t(t)|^2_{L^2(\Omega)} + |\sqrt{\alpha_0(\eta(t))}\theta_t(t)|^2_{L^2(\Omega)} \right) dt + \mathscr{F}_0(\eta(t), \theta(t)) \leq \mathscr{F}_0(\eta(s), \theta(s)), \text{ a.e. } 0 < s \leq t < \infty \text{ (including } s = 0)$$

Moreover, the following convergence holds in the large-time.

$$[\eta(t), \theta(t)] \to [1, 0] \text{ in } L^2(\Omega)^2 \text{ as } t \to \infty$$

†$_1$. When $\nu = 0$, there is no uniqueness result, yet

†$_2$. The convergent point $[1, 0]$ is the (unique) solution to the steady-state prpblem (S$_\infty$)$_0$

(S$_\infty$)$_0$:

$$\begin{cases} -\Delta\eta_\infty + g(\eta_\infty) + \alpha'(\eta_\infty)|D\theta_\infty| = 0 \text{ in } \Omega, \text{ with Neumann-zero B.C.}, \\ -\mathrm{div}\left(\alpha(\eta_\infty) \dfrac{D\theta_\infty}{|D\theta_\infty|} \right) = 0, \text{ with Dirichlet-zero B.C.} \end{cases}$$

†$_3$. In general, the solution to (S$_\infty$)$_0$ is NOT unique when the Dirichlet boundary source for θ is inhomogeneous

3.3. Proof: Mathematical approach when $\nu = 0$

Keypoint: time-discretization for regular systems $(\mathrm{KWC})_\nu$ when $\nu > 0$

Approximating problem $(\mathbf{AP})_h^\nu$ with $\nu > 0$ and time-step $h > 0$:

$$\begin{cases} \dfrac{\eta_i^\nu - \eta_{i-1}^\nu}{h} - \Delta_N \eta_i^\nu + g(\eta_i^\nu) + \alpha'(\eta_i^\nu)|D\theta_{i-1}^\nu| = 0 \ \text{ in } L^2(\Omega), & \text{(ap.1)} \\ \alpha_0(\eta_i^\nu)\dfrac{\theta_i^\nu - \theta_{i-1}^\nu}{h} + \partial\Phi_\nu(\eta_i^\nu;\theta_i^\nu) \ni 0 \text{ in } L^2(\Omega), \quad i = 1, 2, 3, \dots & \text{(ap.2)} \end{cases}$$

- Δ_N: opeartor of Laplacian with Neumann-zero B.C.
- $\{[\eta_0^\nu, \theta_\nu]\}_{\nu>0} \subset H^1(\Omega)^2$: approximating sequence of $[\eta_0, \theta_0] \in D_0 \subset H^1(\Omega) \times BV(\Omega)$

Key-Lemma (Energy-estimate). There exists $h_* \in (0, 1]$, and for any $\nu > 0$ and any $h \in (0, h_*]$, it follows that:

$$\frac{1}{2h}|\eta_i^\nu - \eta_{i-1}^\nu|_{L^2(\Omega)}^2 + \frac{1}{2h}\left|\sqrt{\alpha_0(\eta_i^\nu)}(\theta_i^\nu - \theta_{i-1}^\nu)\right|_{L^2(\Omega)}^2 + \mathscr{F}_\nu(\eta_i^\nu, \theta_i^\nu) \leq \mathscr{F}_\nu(\eta_{i-1}^\nu, \theta_{i-1}^\nu), \ i = 1, 2, 3, \dots \qquad \text{(ap.3)}$$

†. Analytic methods: theories of compactness (Ascoli type), theory of Γ-convergence (as $h, \nu \to 0$, $t \to \infty$, e.t.c.)

4. Problems in future

(I) Structural observations for steady-states

Keypoint : • one-dimensional case

- radial symmetric cases
- other various structures

(II) Structural observations in time-evolution

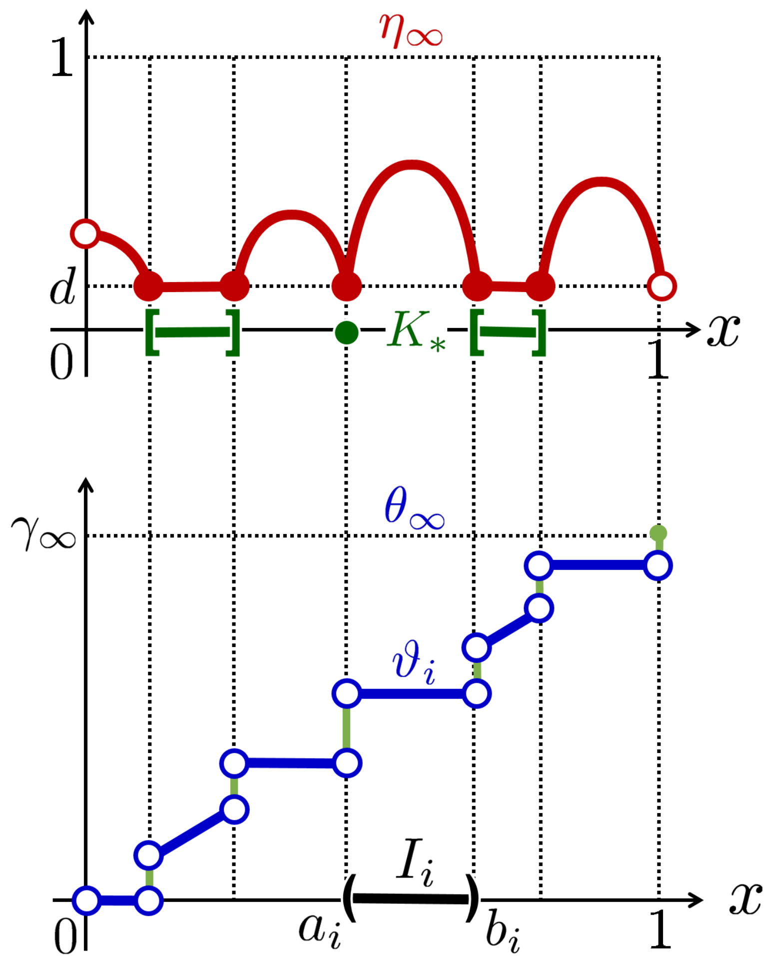
Keypoints: • previous works kindred to our study, e.g. [Andreu–Caselles–Mazón](2004), [Bellettini–Caselles–Novaga](2002), [Kobayashi–Giga](1999), [Giga–Giga–Kobayashi](2001), [Giga–Giga](2010), [Moll](2005–), [Rybka–Mucha](2000–), [S.](2000–) e.t.c.

(III) Anisotropic model when $\nu = 0$

Status : • No advance, yet

(IV) Uniqueness

Status : • No advance, yet



Example of a 1D steady-state