

SPHERICALLY SYMMETRIC SOLUTIONS TO A MODEL FOR INTERFACE MOTION BY INTERFACE DIFFUSION

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Abstract

The existence of spherically symmetric solutions is proved for a new phase-field model that describes the motion of an interface in an elastically deformable solid, here the motion is driven by configurational forces. The model is an elliptic-parabolic coupled system which consists of a linear elasticity system and a non-linear evolution equation of the order parameter. The non-linear equation is non-uniformly parabolic and is of fourth order. One typical application is sintering.

1. Introduction

A central tenet in materials science is that many properties of materials are determined by microstructure. Microstructure can be defined as the totality of all thermodynamic non-equilibrium lattice defects on a space scale ranging from Ångströms to meters. By their dimension, defects can be arranged in the following hierarchy: i) zero-, ii) one-, iii) two-, iv) three-dimensional defects. Their typical examples are, respectively, point defects, dislocations, grain boundaries and voids. The driving forces for the evolution of defects are of the Eshelby type that is radically different to the Newton type.

We shall study, in this paper, the evolution of two-dimensional defects, taking grain boundary as an example, by employing a phase-field approach that is still young but has been shown powerful and important for both theoretical and numerical investigations, especially for multi-dimensional problems, see, e.g. [8, 10, 13]. Starting from a sharp interface model based on a formula of configurational forces in terms of the Eshelby tensor, Alber and Zhu [1, 2] have formulated a new phase-field model which differs from the famous Cahn-Hilliard model (see [7]) by a non-smooth gradient term. An application of our model is to describe sintering, a technique for making a material from powders.

To state the new model we now introduce some notations. Let Ω be an open subset in \mathbb{R}^3 . It stands for the set of material points of a solid body. The different

phases of a solid are indicated by an order parameter $S(t, x) \in \mathbb{R}$: That S takes values near to zero or one means the solid is in phase γ or γ' . Other unknowns are the displacement $u(t, x) \in \mathbb{R}^3$ of the material point x at time t and the Cauchy stress tensor $T(t, x) \in \mathcal{S}^3$. Here \mathcal{S}^3 denotes the set of symmetric 3×3 -matrices. We shall investigate the quasi-static process, the unknowns thus must satisfy the following equations

$$-\operatorname{div}_x T(t, x) = b(t, x), \quad (1)$$

$$T(t, x) = D(\varepsilon(\nabla_x u) - \bar{\varepsilon}S)(t, x), \quad (2)$$

$$S_t(t, x) = c \operatorname{div}_x \left(\nabla_x (\psi_S(\varepsilon(\nabla_x u), S) - \nu \Delta_x S) |\nabla_x S| \right)(t, x), \quad (3)$$

for $(t, x) \in (0, \infty) \times \Omega$, and the boundary and initial conditions

$$u(t, x) = \gamma(t, x), \quad (t, x) \in [0, \infty) \times \partial\Omega, \quad (4)$$

$$\frac{\partial}{\partial n} S(t, x) = 0, \quad (t, x) \in [0, \infty) \times \partial\Omega, \quad (5)$$

$$\frac{\partial}{\partial n} (\psi_S(\varepsilon, S) - \nu \Delta_x S) |\nabla_x S|(t, x) = 0, \quad (t, x) \in [0, \infty) \times \partial\Omega, \quad (6)$$

$$S(0, x) = S_0(x), \quad x \in \bar{\Omega}. \quad (7)$$

Here n is the unit outward normal vector, $\nabla_x u$ denotes the 3×3 -matrix of first order derivatives of u , the deformation gradient, and

$$\varepsilon(\nabla_x u) = \frac{1}{2}(\nabla_x u + (\nabla_x u)^T)$$

is the strain tensor, where $(\nabla_x u)^T$ denotes the transposed matrix. Further, $\bar{\varepsilon} \in \mathcal{S}^3$ is a given matrix, the transformation strain. The elasticity tensor $D : \mathcal{S}^3 \rightarrow \mathcal{S}^3$ is a linear, symmetric, positive definite mapping, and ψ_S is the derivative with respect to S of the free energy

$$\psi^*(\varepsilon, S, \nabla_x S) = \psi(\varepsilon, S) + \frac{\nu}{2} |\nabla_x S|^2 = \frac{1}{2} (D(\varepsilon - \bar{\varepsilon}S)) \cdot (\varepsilon - \bar{\varepsilon}S) + \hat{\psi}(S) + \frac{\nu}{2} |\nabla_x S|^2, \quad (8)$$

where for $\hat{\psi} : \mathbb{R} \rightarrow [0, \infty)$ we choose a double well potential with minima at points $S \leq 0$ and $S \geq 1$. The scalar product of two matrices is $A \cdot B = \sum_{i,j=1}^3 a_{ij} b_{ij}$. Thus,

$$\psi_S(\varepsilon, S) = -T \cdot \bar{\varepsilon} + \hat{\psi}'(S). \quad (9)$$

Given are the positive constant c , the small positive constant ν , the volume force $b : [0, \infty) \times \Omega \rightarrow \mathbb{R}^3$ and the boundary and initial data $\gamma : [0, \infty) \times \partial\Omega \rightarrow \mathbb{R}^3$, $S_0 : \Omega \rightarrow \mathbb{R}$.

We thus complete the formulation of an initial-boundary value problem. The equations (1) and (2) differ from the system of linear elasticity only by the term $\bar{\varepsilon}S$,

which couples this system to equation (3). The evolution equation (3) for the order parameter S is non-uniformly parabolic because of the term $\operatorname{div}_x(|\nabla_x S| \nabla_x \Delta_x S)$.

Statement of the main result. Since we shall look for spherically symmetric solutions to problem (1)–(7), we can make suitable assumptions to reduce the problem to its one space dimensional form. To this end we now assume that the body force boundary and initial data and the unknowns, which are defined in the domain $\Omega \times (0, T_e)$, have the following form

$$b(t, x) = \hat{b}(t, r) \frac{x}{r}, \quad \gamma(t, x) = \hat{\gamma}(t, r), \quad S_0(x) = \hat{S}_0(r)$$

and

$$u(t, x) = \hat{u}(t, r) \frac{x}{r}, \quad S(t, x) = \hat{S}(t, r),$$

respectively, where T_e is a positive constant which denotes the life-span of weak solutions, $r = |x|$, $\Omega = \{x \in \mathbb{R}^3 \mid a < r < d\}$ for two positive constant a, d satisfying $a < d$, and $\hat{b}, \hat{\gamma}, \hat{S}_0$ are given functions and \hat{u}, \hat{S} are scalar functions to be determined, which depend only on t, r . We write

$$x = (x_i), \quad u = (u_i), \quad T = (T_{ij}), \quad D = (D_{kl}^{ij}),$$

hereafter, $i, j, k, l = 1, 2, 3$, and we assume that D satisfies the properties of symmetry: $D_{kl}^{ij} = D_{ij}^{kl} = D_{lk}^{ji} = D_{kl}^{ji}$. Moreover we assume that the material is isotropic, namely we have

$$D_{kl}^{ij} = \mu_1 \delta_{ik} \delta_{jl} + \frac{\mu_2}{3} \delta_{ij} \delta_{kl}, \quad (10)$$

where δ_{ij} is the Kronecker delta, and $\mu_1 > 0, \mu_2 \geq 0$ are constants. For $\bar{\varepsilon}$, we assume that

$$\bar{\varepsilon}_{ij} = \lambda \delta_{ij}. \quad (11)$$

Then it follows that

$$D\varepsilon = \mu_1 \varepsilon + \frac{\mu_2}{3} \operatorname{Trace}(\varepsilon) I, \quad D\bar{\varepsilon} = \mu_1 \lambda I + \frac{\mu_2}{3} \operatorname{Trace}(\lambda I), \quad I = (\mu_1 + \mu_2) I, \quad (12)$$

here for a matrix A , $\operatorname{Trace}(A)$ denotes the trace of A . Hence,

$$D\varepsilon \cdot \varepsilon = \mu_1 \varepsilon \cdot \varepsilon + \frac{\mu_2}{3} (\operatorname{Trace}(\varepsilon))^2 > 0 \quad \forall \varepsilon \neq 0. \quad (13)$$

Under these assumptions, equations (1)–(3) are reduced to

$$\hat{u}_{rr} + \frac{2}{r} \hat{u}_r - \frac{2}{r^2} \hat{u} = \mathcal{G}, \quad (14)$$

$$\frac{\partial}{\partial t} \hat{S} + c \frac{\partial}{\partial r} \left((\nu \hat{S}_{rrr} + \mathcal{F}_2) |\hat{S}_r| \right) = -\frac{2c}{r} (\nu \hat{S}_{rr} + \mathcal{F}_1) |\hat{S}_r|, \quad (15)$$

with $\mathcal{F}_1, \mathcal{F}_2, \mathcal{G}$ being nonlinear functions defined by

$$\mathcal{G} = \mathcal{G}(\hat{S}_r, \hat{b}) = \frac{\lambda}{\mu} \hat{S}_r + \frac{\hat{b}}{\mu}, \quad (16)$$

$$\begin{aligned} \mathcal{F}_1 &= \mathcal{F}_1(\hat{u}, \hat{u}_r, \hat{u}_{rr}, \hat{S}, \hat{S}_r) \\ &= \lambda \left(\hat{u}_r + \frac{2}{r} \hat{u} \right) + \frac{2\nu}{r} \hat{S}_r - D\bar{\varepsilon} \cdot \bar{\varepsilon} \hat{S} - \hat{\psi}'(\hat{S}), \end{aligned} \quad (17)$$

$$\mathcal{F}_2 = \mathcal{F}_2(\hat{u}, \hat{u}_r, \hat{u}_{rr}, \hat{S}, \hat{S}_r, \hat{S}_{rr}) = \mathcal{F}_{1,r}. \quad (18)$$

Since eq. (14) is linear, the inhomogeneous Dirichlet boundary condition for \hat{u} can be reduced to the homogeneous one. So we may assume for simplicity that $\hat{\gamma} = 0$. Hence, simple computations show that (14) can be rewritten as

$$\hat{u}_r + \frac{2}{r} \hat{u} = \frac{\lambda}{\mu} \hat{S} + \frac{1}{\mu} \int_a^r \hat{b}(t, y) dy + C(t), \quad (19)$$

here, $C(t)$ is a constant depending on t and $\hat{\gamma}(t, r)$ which is zero by assumption. It thus follows from formula (19) and the boundary conditions for \hat{u} that

$$\begin{aligned} \hat{u} &= \frac{1}{r^2} \left(\frac{\lambda}{\mu} \int_a^r y^2 \hat{S}(t, y) dy + \frac{1}{\mu} \int_a^r x^2 \int_a^x \hat{b}(t, y) dy dx \right) \\ &\quad - \frac{1}{r^2} \frac{r^3 - a^3}{d^3 - a^3} \left(\frac{\lambda}{\mu} \int_a^d y^2 \hat{S}(t, y) dy + \frac{1}{\mu} \int_a^d x^2 \int_a^x \hat{b}(t, y) dy dx \right). \end{aligned} \quad (20)$$

Therefore, (14)–(15) can be reduced to the following single equation

$$\frac{\partial}{\partial t} (r^2 \hat{S}) + c \frac{\partial}{\partial r} \left(r^2 (\nu \hat{S}_{rrr} + \mathcal{F}) | \hat{S}_r | \right) = 0, \quad (21)$$

with

$$\mathcal{F} = \frac{\lambda}{\mu} (\lambda \hat{S}_r + \hat{b}) + \left(\frac{2\nu}{r} \hat{S}_r - D\bar{\varepsilon} \cdot \bar{\varepsilon} \hat{S} - \hat{\psi}'(\hat{S}) \right)_r. \quad (22)$$

The boundary and initial conditions become

$$(\nu \hat{S}_{rrr} + \mathcal{F}) | \hat{S}_r | = 0, \quad (t, r) \in [0, T_e] \times \partial\Omega, \quad (23)$$

$$\hat{S}(0, r) = \hat{S}_0(r), \quad r \in \Omega. \quad (24)$$

Consequently, the existence of spherically symmetric solutions to problem (1)–(7) is equivalent to solvability of problem (21)–(24), since \hat{u} can be obtained from formula (20) once \hat{S} is known.

The domain Ω is reduced to an interval: $\Omega = (a, d)$ is a bounded open interval with constants $a < d$. We write $Q_{T_e} := (0, T_e) \times \Omega$, where T_e is a positive constant.

To state the existence result for this problem we need two definitions. For $\mathcal{A} \subset Q_{T_e}$, $g : \mathcal{A} \rightarrow V \subset \mathbb{R}$ and $t \in [0, T_e]$ let

$$\mathcal{A}(t) = \{x \mid (t, x) \in \mathcal{A}\} \quad \text{and} \quad g(t) : \mathcal{A}(t) \rightarrow V, \quad g(t)(x) = g(t, x).$$

Definition 1.1 Let $\mathcal{A} \subset Q_{T_e}$ such that $\mathcal{A}(t)$ is open for almost all $t \in [0, T_e]$, and let $\alpha \in \mathbb{N}_0$. We call $g : \mathcal{A} \rightarrow \mathbb{R}$ the α -th local weak derivative of $S \in L^2(Q_{T_e})$ with respect to x in \mathcal{A} , if for almost all $t \in [0, T_e]$ the function $g(t)$ belongs to $L^{2,\text{loc}}(\mathcal{A}(t))$ and is the local weak derivative of S in the usual sense:

$$g(t) = \partial_x^\alpha S(t)|_{\mathcal{A}(t)}, \quad (25)$$

and if moreover there exists a sequence $\{\mathcal{A}_n\}_n$ of measurable sets $\mathcal{A}_n \subset \mathcal{A}$ with $g|_{\mathcal{A}_n} \in L^2(\mathcal{A}_n)$ for all $n \in \mathbb{N}$, such that

$$\text{meas} \left(\mathcal{A} \setminus \bigcup_{n=1}^{\infty} \mathcal{A}_n \right) = 0.$$

Remark 1. The uniqueness of local weak derivatives in the sense of this definition is obvious because of (25), and it is clear that if \mathcal{A} is open and if S has the local weak derivative $\partial_x^\alpha S$ in the usual sense in \mathcal{A} , then $\partial_x^\alpha S$ is also a local weak derivative in the sense of our definition. So Definition 1.1 generalizes the ordinary definition; this allows us to use the same name and the same notation $\partial_x^\alpha S$ as for ordinary local weak derivatives.

For a function $S \in L^2(0, T_e; H_N^2(\Omega))$, where $H_N^2(\Omega) = \{f \in H^2(\Omega) \mid \frac{\partial}{\partial n} f = 0, \text{ on } \partial\Omega\}$, let

$$\mathcal{A}^S = \{(t, r) \in Q_{T_e} \mid |S_r(t, r)| > 0\}.$$

By the Sobolev embedding theorem we see that $S_r(t)$ is continuous for almost all $t \in (0, T_e)$. This implies that $\mathcal{A}^S(t)$ is open for almost all t .

Definition 1.2 Let $\hat{b} \in L^\infty(0, T_e; L^2(\Omega))$ and $\hat{S}_0 \in L^2(\Omega)$. A function \hat{S} with

$$\hat{S} \in L^2(0, T_e; H^2(\Omega)) \cap L^\infty(Q_{T_e}), \quad \hat{S}_r(t) \in H_0^1(\Omega) \text{ a.e. in } (0, T_e), \quad (26)$$

is a weak solution of the problem (21) – (24), if and only if \hat{S} , with local weak derivative \hat{S}_{rrr} in $\mathcal{A}^{\hat{S}}$ and $|\hat{S}_r| \hat{S}_{rrr} \in L^1(\mathcal{A}^{\hat{S}})$, satisfies that

$$(r^2 \hat{S}, \varphi_t)_{Q_{T_e}} + c \left(\nu r^2 \hat{S}_{rrr} |\hat{S}_r|, \varphi_r \right)_{\mathcal{A}^{\hat{S}}} + c \left(r^2 \mathcal{F} |\hat{S}_r|, \varphi_r \right)_{Q_{T_e}} + (r^2 \hat{S}_0, \varphi(0))_\Omega = 0 \quad (27)$$

holds for all $\varphi \in C_0^\infty((-\infty, T_e) \times \mathbb{R})$.

For the function $\hat{\psi}$, we need the following

Assumptions A. The function $\hat{\psi}(S)$ is a smooth double-well potential, and it has two local minima at S_- and S_+ with $S_- < S_+$, one local maximum at S_* satisfying $S_- < S_* < S_+$; and $\hat{\psi}'(S) > 0$ for $S_- < S < S_*$ and $\hat{\psi}'(S) < 0$ for $S_* < S < S_+$. For simplicity, we assume further that

$$\begin{aligned} \hat{\psi}^{(k)}(S_+) &= 0 \text{ for } 1 \leq k \leq 2m_1 - 1, \hat{\psi}^{(2m_1)}(S_+) > 0, \\ \hat{\psi}^{(k)}(S_-) &= 0 \text{ for } 1 \leq k \leq 2m_2 - 1, \hat{\psi}^{(2m_2)}(S_-) > 0. \end{aligned}$$

and that $\hat{\psi}(S) \sim S^{2\ell_1}$ as $S \rightarrow \infty$, $\hat{\psi}(S) \sim S^{2\ell_2}$ as $S \rightarrow -\infty$, where m_1, m_2, ℓ_1 , and ℓ_2 are positive integers. Let $\ell = \max\{\ell_1, \ell_2\}$. Assume that $\ell > 1$.

Remark 2. One typical example of $\hat{\psi}$ which satisfies assumptions A is $\hat{\psi}(S) = (S(1-S))^2$, with $S_+ = 1$, $S_- = 0$, $\ell = \ell_1 = \ell_2 = 2$ and $m_1 = m_2 = 1$.

We are now in a position to state the main result of this paper.

Theorem 1.3 *Assume that the double-well potential $\hat{\psi}$ satisfies assumptions A. Then to all $\hat{S}_0 \in H^1(\Omega)$ and $\hat{b} \in L^2(Q_{T_e})$ with $\hat{b}_t \in L^2(Q_{T_e})$ there exists a weak solution \hat{S} to (21)–(24), which in addition to (26) satisfies (20) and*

$$\hat{S} \in L^\infty(0, T_e; H^1(\Omega)), \quad \hat{S}_t \in L^{\frac{4}{3}}(0, T_e; W^{-1, \frac{4}{3}}(\Omega)), \quad (28)$$

$$|\hat{S}_r| \hat{S}_{rrr} \in L^{\frac{4}{3}}(Q_{T_e}), \quad (29)$$

where we defined $|\hat{S}_r| \hat{S}_{rrr} = 0$ on $Q_{T_e} \setminus \mathcal{A}^{\hat{S}}$.

The main difficulties of the proof of this theorem are caused by the term $|S_r|$ which results in that eq. (21) is degenerate and its coefficients are non-smooth. The coefficient of the principal term in (21) contains $|S_r|$, so this principal term can only be defined over a domain $\mathcal{A}^{\hat{S}}$ which may be not open. This leads to the difficulty of definition of weak derivatives \hat{S}_{rrr} .

Related results are Alber and Zhu [1] – [6], Kawashima and Zhu [12], and those for the degenerate Cahn-Hilliard equation and for the equation of thin film $S_t = -\operatorname{div}_x(m(S)\nabla_x \Delta_x S)$, where $m(S)$ vanishes at zero. We refer to [9, 11] and the references therein. However, the mathematical properties of (3) containing the term $|\nabla_x S|$ differ essentially from the ones of these equations.

2. Sketch of the proof of the main result

The proof of Theorem 1.3 consists of the following three steps. For simplicity, we drop the upper-script $\hat{\cdot}$, i.e. change \hat{S}, \dots back to S, \dots .

Step 1. Construction of approximate solutions

To construct approximate solutions to (21)–(24) we prove that there exist weak solutions to the following initial-boundary value problem

$$(r^2 S)_t + c (r^2 (\nu S_{rrr} + \mathcal{F}_\kappa) |S_r|_\kappa)_r = 0 \quad \text{in } Q_{T_e}, \quad (1)$$

$$S_r = 0 \quad \text{on } [0, T_e] \times \partial\Omega, \quad (2)$$

$$(\mathcal{F}_\kappa + \nu S_{rrr}) |S_r|_\kappa = 0 \quad \text{on } [0, T_e] \times \partial\Omega, \quad (3)$$

$$S|_{t=0} = S_0 \quad \text{in } \Omega, \quad (4)$$

where κ is a fixed positive constant, $|y|_\kappa$ is defined by $|y|_\kappa = \sqrt{|y|^2 + \kappa^2}$, and \mathcal{F}_κ is the smoothed \mathcal{F} in which b is replaced by its smooth approximation b^κ .

Eq. (1) is quasi-linear, uniformly parabolic over a domain that S_r is bounded. However it is not easy to prove the existence of classical solution to problem (1)–(4), whence we consider the weak solutions to this problem. By definition, $S \in L^2(0, T_e; H^1(\Omega))$ with $S_{rrr} \in L^2(Q_{T_e})$ is a weak solution of (1)–(4) if and only if for all $\varphi \in C_0^\infty((-\infty, T_e) \times \mathbb{R})$

$$-(r^2 S, \varphi_t)_{Q_{T_e}} = (r^2 S_0, \varphi(0))_\Omega + c(r^2(\nu S_{rrr} + \mathcal{F}_\kappa)|S_r|_\kappa, \varphi_r)_{Q_{T_e}}. \quad (5)$$

Step 2. Main a-priori estimates

Lemma 2.1 *There is a constant C , independent of κ , such that for any $t \in [0, T_e]$*

$$\|S_r^\kappa\|_{H^1(\Omega)}^2 + \int_{Q_t} (|S_r^\kappa|_\kappa + \kappa)|S_{rrr}^\kappa|^2 d(\tau, y) \leq C, \quad (6)$$

$$\| |S_r^\kappa|_\kappa S_{rrr}^\kappa \|_{L^{\frac{4}{3}}(Q_t)} \leq C. \quad (7)$$

Step 3. Limits

To investigate the limits of approximate solutions constructed in Step 1, we need the Egorov theorem.

Theorem 2.2 (Egorov) *Let (Γ, Σ, μ) be a measure space with $\mu(\Gamma) < \infty$, let f, f^1, f^2, f^3, \dots be real valued, measurable functions on Γ , and assume that $f^j(x) \rightarrow f(x)$ as $j \rightarrow \infty$ for almost every $x \in \Gamma$.*

Then, for every $\varepsilon > 0$ there is a subset $M_\varepsilon \subset \Gamma$ with $\mu(M_\varepsilon) > \mu(\Gamma) - \varepsilon$ such that $f^j(x)$ converges to $f(x)$ uniformly on M_ε . That is, for every $\delta > 0$ there is an N_δ such that when $j > N_\delta$ we have that for every $x \in M_\varepsilon$

$$|f^j(x) - f(x)| < \delta.$$

With the help of this theorem we can get the local weak derivative S_{rrr} as follows. Decompose the set $\hat{\mathcal{A}}_n = \{(t, r) \in Q_{T_e} \mid |S_r(t, r)| > \frac{1}{n}\}$ into a set \mathcal{A}_n (on which the sequence S_r^κ converges uniformly to S_r and thus satisfies $|S_r^\kappa| \geq \frac{1}{2n}$ for sufficiently small κ) and the set $\hat{\mathcal{A}}_n \setminus \mathcal{A}_n$ (which has small measure). Using the uniform estimate $\int_{Q_{T_e}} (|S_r^\kappa|_\kappa + \kappa)|S_{rrr}^\kappa|^2 d(\tau, r) \leq C$, we can then show that S_{rrr}^κ converges in $L^2(\mathcal{A}_n)$ to S_{rrr} . Finally, we apply the fact that \mathcal{A}^S differs from $\bigcup_{n=1}^\infty \mathcal{A}_n$ only by a set of measure zero. We then have the following key lemma.

Lemma 2.3 *The limit function S has the local weak L^2 -derivative S_{rrr} on \mathcal{A}^S in the sense of Definition 1.1. Moreover, there exists a subsequence S^κ such that $|S_r^\kappa|_\kappa S_{rrr}^\kappa \rightharpoonup \chi$, weakly in $L^{\frac{4}{3}}(Q_{T_e})$, where the function $\chi = \chi(t, r)$ in $L^{\frac{4}{3}}(Q_{T_e})$ is given by $\chi = 0$, if $S_r = 0$, and $\chi = |S_r|S_{rrr}$, if $S_r \neq 0$.*

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