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VISCOSITY SOLUTIONS TO A NEW PHASE-FIELD MODEL FOR MARTENSITIC PHASE TRANSFORMATIONS

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Abstract: We investigate a new phase-field model which describes martensitic phase transitions, driven by material forces, in solid materials, e.g., shape memory alloys. This model is a nonlinear degenerate parabolic equation of second order, its principal part is not in divergence form in multi-dimensional case. We prove the existence of viscosity solutions to an initial-boundary value problem for this model.

Keywords: phase-field model, martensitic phase transitions, viscosity solution, initial-boundary value problem

MSC: 35D40, 35K65

1. Introduction

The result presented in this talk is mainly from a recent work [8] by the author and his coworker.

Martensitic transformations are displacive, diffusionless and are responsible for the formation of some microstructures, like martensite which is a key microstructure of some materials and thus determines properties of those materials, for example, shape memory effect [16, 17] of shape memory alloys. Martensite can grow at temperatures close to absolute zero and at speeds in excess of 1000ms^{-1}. Thus it is very difficult to obtain, by observing this process directly, useful information to understand its mechanism, instead mathematical modeling is a powerful tool, for instance, phase-field method has been proved extremely powerful to both theoretical and numerical analysis of phenomena in materials science (see e.g., [9, 10, 20]).

To understand this type of rapidly changing processes, the author and his coworker proposed in [2, 4] a new phase-field model, which consists of a linear elasticity system and a nonlinear degenerate parabolic equation of second order. In this talk we neglect the elasticity effect of solids and formulate a little simpler model. To formulate an initial-boundary value problem for this model, we first introduce some notations. Let Ω be an open bounded domain in $\mathbb{R}^3$ with smooth boundary $\partial\Omega$. It represents the points of a material body. Define $Q_t := (0,t) \times \Omega$. Then the model reads

$$S_t = -c\left(\hat{\psi}'(S) - \nu\Delta_x S\right)|\nabla_x S| \tag{1}$$

which is satisfied in Q_T with $T > 0$. Here, S is an order parameter taking the values between 0 and 1, and $S \approx 0$ and $S \approx 1$ indicate that the material is in phases γ and γ', respectively. ∇_x and Δ_x are, respectively, the gradient and Laplace operators, and S_t denotes the partial derivative of S with respect to t, and

$$|\nabla_x S| = \Big(\sum_{i=1}^{3} |\partial_{x_i} S|^2\Big)^{\frac{1}{2}}.$$

$\hat{\psi}'(S)$ is the derivative of the function $\hat{\psi}(S)$ which is taken as a double-well potential so that $\hat{\psi}(S)$ has at least two local minima, say $S = 0$ and $S = 1$, and a maximum in-between. It holds that $\hat{\psi}\,'(0) = \hat{\psi}\,'(1) = 0$. c, ν are positive constants.

To derive the model, we choose a free energy $\Psi(t) = \int_\Omega \psi(S, \nabla_x S)dx$ with the density

$$\psi(S, \nabla_x S) = \hat{\psi}(S) + \frac{\nu}{2}|\nabla_x S|^2.$$

Straightforward computations show that if equation (1) is satisfied, then the validness of the second law of thermodynamics is guaranteed (cf. Alber and Zhu [2, 3]).

We add, respectively, the following Dirichlet boundary and initial conditions

$$S|_{[0,T]\times\partial\Omega} = 0, \tag{2}$$
$$S|_{\{t=0\}\times\bar{\Omega}} = S_0. \tag{3}$$

Thus we complete the formulation of the initial-boundary value problem.

Let us now compare this model with the Allen-Cahn model which has been widely accepted as a model for phase separation driven by mean curvature, and comprises of

$$S_t = -c\,(\hat{\psi}'(S) - \nu\Delta_x S). \tag{4}$$

This differs from (1) by the gradient term $|\nabla_x S|$. We conclude that:

(i) Equation (1) is degenerate, non-uniformly parabolic with non-smooth coefficients; while (4) is uniformly parabolic with smooth coefficients.

(ii) Our model implies that after a part of a material changes to, say, phase 1 over an open sub-region, then we have $\nabla_x S = 0$ which together with Eq. (1) implies $S_t = 0$, thus S keeps the same value which means the material is kept in phase 1 over that sub-region. This is confirmed by observation. However in the Allen-Cahn model there is no such property, namely, the material is still changing after it achieves its equilibrium over an open sub-domain because even if $\nabla_x S = 0$ over an open sub-region one cannot obtain from (4) that $S_t = 0$ over that sub-domain. Thus, the Allen-Cahn model is suitable for phase separation.

We shall prove the existence of viscosity solutions to problem (1)–(3). The principle part, i.e. $c\nu|\nabla_x S|\Delta_x S$, of this model is not in divergence form, and the order parameter equation is degenerate. Thus to investigate the validity of problem (1)–(3), we employ the notion of viscosity solution. Introduce Hamiltonian H by

$$H(S, q, r) = -c\,(\hat{\psi}'(S) - \nu\, r)|q|, \quad q \in \mathbb{R}^3,\ r \in \mathbb{R}. \tag{5}$$

Definition 1.1 *A function S which belongs to the space $C(\bar{Q}_T)$, is called a viscosity solution to problem* (1)*–*(3) *if S satisfies both $i)$ and $ii)$ below:*

i) S is a sub-viscosity solution to (1)*–*(3)*, i.e. for any function $\phi(t, x)$ in $C^{2,1}(\bar{Q}_T)$, if $S - \phi$ attains its local maximum at (τ, y), then*

$$\phi_t(\tau, y) \le H(S(\tau, y), \nabla_x\phi(\tau, y), \Delta_x\phi(\tau, y)), \tag{6}$$

and there holds that $S(t, x) \le 0$ for all $(t, x) \in [0, T] \times \partial\Omega$, and that $S(0, x) \le S_0(x)$ for all $x \in \Omega$;

ii) S is a super-viscosity solution to (1)*–*(3)*, i.e. for any function $\phi(t, x)$ in $C^{2,1}(\bar{Q}_T)$, if $S - \phi$ achieves its local minimum at (τ, y), then*

$$\phi_t(\tau, y) \ge H(S(\tau, y), \nabla_x\phi(\tau, y), \Delta_x\phi(\tau, y)), \tag{7}$$

and there holds that $S(t, x) \ge 0$ for all $(t, x) \in [0, T] \times \partial\Omega$, and that $S(0, x) \ge S_0(x)$ for all $x \in \Omega$.

Now we may state the main result.

Theorem 1.1 *Let T be a given positive constant. Suppose that $\partial\Omega \in C^{2+\beta}$ for some real positive number $\beta \in (0, 1)$, and that $S_0 \in W_0^{1,\infty}(\Omega)$ satisfies $0 \le S_0(x) \le 1$ for almost every $x \in \bar{\Omega}$. Furthermore, we assume that the potential $\hat{\psi}$ is C^2-continuous.*

Then there exists a viscosity solution S to problem (1) *–* (3) *in the sense of Definition 1.1, such that $0 \le S(t, x) \le 1$ for almost every $(t, x) \in \bar{Q}_T$.*

$$S \in C(\bar{Q}_T) \cap L^\infty(0, T; W_0^{1,\infty}(\Omega)),\ \ S_t \in L^2(Q_T). \tag{8}$$

The main difficulties in the proof of Theorem 1.1 are as follows: First, the equation of S is nonlinear, and its principal part cannot be rewritten in the divergence form, moreover, we shall find that *a priori* estimates of the highest derivative of approximate solutions depend on a term which is a function of the gradient of the order parameter, and plays a role of weight. This term is not uniformly bounded from below with respect to a small parameter, thus it leads to that standard lemmas of compactness do not apply to our problem. So we apply the concept of viscosity solutions. Second, equation (1) is non-uniform, degenerate and its coefficients are not smooth.

Our strategies for overcoming these difficulties are in order. We make a suitable smooth approximation of the non-smooth term, then the equation becomes a uniformly parabolic one with smooth coefficients. We first derive the energy estimates, and also the uniform L^∞-bound of the gradient of S with the help of a technique from the book by Ladyzenskaya et al. [15]. The main idea behind the technique is to show that the measure of the set $\mathcal{A}_K(t) = \{x \in \Omega \mid z(t,x) > K\}$ is zero for sufficiently large K, where z is a nonlinear function in $\nabla_x v$ and v is defined by $S = \phi(v)$ with ϕ being a smooth nonlinear function. However we find it is not able to do this in one step, instead we must divide $\mathcal{A}_K(t) = \{x \in \Omega \mid z(t,x) > K\}$ into $\cup_{i=1}^{\infty} \mathcal{A}_{K,i}(t) = \{x \in \Omega \mid K + i - 1 < z(t,x) \leq K + i\}$ and prove the measure of each subset is zero when K is sufficiently large. After modifying that technique in this way, we can make use of the good term to each subset and establish the L^∞-bound of the gradient of S. Then we employ these estimates to obtain the compactness of the approximate solutions.

We recall some literature related closely to our results. For the viscosity solutions, we refer to Crandall and Lions [12], Crandall, Ishii and Lions [11]. For the model investigated in this talk, the study from various aspects has been carried out, see Alber and Zhu [2, 3, 4, 5, 6, 7], Kawashima and Zhu [14], Ou and Zhu [18], Zhu [21, 22, 23]. Acharya et al. in [1], and Hildebrand et al. in [13] study a model which is closely related to ours.

Notations. Let m, n be nonnegative integers, and $p, q \geq 1$. α denotes a real number in $(0,1)$. Let $L^p(\Omega)$, $W^{m,p}(\Omega)$ are standard Lebesgue and Sobolev spaces, and $H^m(\Omega) = W^{m,2}(\Omega)$. We denote by $C^{m+\alpha}(\overline{\Omega})$ the space of $m-$times differentiable functions on $\overline{\Omega}$, whose $m-$th derivative is Hölder continuous with exponent α. The space $C^{\alpha,\alpha/2}(\overline{Q}_T)$ consists of all functions on $\overline{Q}_T$, which are Hölder continuous in the parabolic distance $\mathrm{d}((t,x),(s,y)) := \sqrt{|t-s| + |x-y|^2}$. $C^{m,n}(\overline{Q}_T)$ and $C^{m+\alpha,n+\alpha/2}(\overline{Q}_T)$ are the spaces of functions, whose x-derivatives up to order m and t-derivatives up to order n belong to $C(\overline{Q}_T)$ or to $C^{\alpha,\alpha/2}(\overline{Q}_T)$, respectively.

2. Existence of solutions

2.1. Approximate solutions

To construct approximate solutions, we formulate an approximate problem to the original problem (1)–(3). To this end, for $\kappa > 0$, we smooth the term $|\nabla_x S|$ as follows

$$|\nabla_x S|_\kappa = \sqrt{|\nabla_x S|^2 + \kappa^2},$$

and choose a sequence $S_0^\kappa \in C_0^\infty(\Omega)$ such that

$$\|S_0^\kappa - S_0\|_{H^1(\Omega)} \to 0$$

as $\kappa \to 0$ since $C_0^\infty(\Omega)$ is dense in $H_0^1(\Omega)$.

Then we can approximate the initial-boundary value problem (1)–(3) by the following problem

$$S_t = c\nu|\nabla_x S|_\kappa \Delta_x S - c\hat{\psi}'(S)(|\nabla_x S|_\kappa - \kappa), \tag{9}$$

and the boundary and initial conditions become

$$\begin{aligned} S|_{[0,T]\times\partial\Omega} &= 0, & (10)\\ S|_{\{0\}\times\bar{\Omega}} &= S_0^\kappa. & (11)\end{aligned}$$

For the sake of simplicity, we use the following notations. Define

$$\begin{aligned} a_{ij} &= a_{ij}(\nabla_x S) = c\nu|\nabla_x S|_\kappa \delta_{ij}, \text{ and} & (12)\\ a &= a(S, \nabla_x S) = c\hat{\psi}'(S)(|\nabla_x S|_\kappa - \kappa) & (13)\end{aligned}$$

where δ_{ij} is the Kronecker delta, $i, j = 1, 2, 3$. Straightforward computations show that

$$\begin{aligned} \frac{c\sqrt{2}\,\nu}{2}(\kappa + |p|)\xi^2 &\leq a_{ij}\xi_i\xi_j \leq c\nu(\kappa + |p|)\xi^2, & (14)\\ \left|\frac{\partial a_{ij}}{\partial p_k}\right| &\leq c\nu, & (15)\\ |a(S,p)| &\leq \mu_1(|S|)P(|p|)(\kappa + |p|)^3, & (16)\\ -\frac{\partial a(S,p)}{\partial S} &\leq \mu_2(|S|)P(|p|)(\kappa + |p|)^3, & (17)\\ \left|\frac{\partial a(S,p)}{\partial p_k}\right| &\leq \mu_3(|S|)P(|p|)(\kappa + |p|)^2. & (18)\end{aligned}$$

where $P(|p|) = (\kappa + |p|)^{-2}$.

Recalling an existence theorem from [15, p. 558], we check that all conditions of this theorem are satisfied for any given $\kappa > 0$, thus we can formulate the following theorem.

Theorem 2.1 *Let $T > 0$. Assume that $\partial\Omega \in C^{2+\beta}$ with some $\beta \in (0, 1)$. For any given κ, the coefficient functions $a_{ij}(p)$ and $a(S, p)$ are continuously differentiable with respect to their arguments S, p, and (14) – (18) are satisfied. Suppose that the following compatibility conditions are satisfied*

$$\begin{aligned} S_0|_{\partial\Omega} &= 0, & (19)\\ \nu|\nabla_x S_0(x)|_\kappa \Delta_x S_0(x) - \hat{\psi}'(S_0(x))(|\nabla_x S_0(x)|_\kappa - \kappa) &= 0 & (20)\end{aligned}$$

for all $x \in \partial\Omega$.

Then there exists a solution $S \in C^{2+\alpha,1+\alpha/2}(\bar{Q}_T)$ of problem (9) – (11). This solution has derivatives $S_{tx_i} \in L^2(Q_T)$, $i = 1, 2, 3$.

2.2. A priori estimates

We list in this subsection *a priori* estimates which are uniform in $\kappa \in (0,1]$, for the approximate solutions. For simplicity we denote $\|f\| = \|f\|_{L^2(\Omega)}$. C is a universal constant which is independent of κ and may vary from line to line.

This subsection is devoted to uniform bound of S and to the energy estimates.

Lemma 2.1 *There hold for almost every $t \in [0,T]$*

$$\|S^\kappa\|_{L^2(0,T;W^{1,\infty}(\Omega))} \leq C, \tag{21}$$

$$\int_0^t \int_\Omega (|\nabla_x S^\kappa|_\kappa |\Delta_x S^\kappa|^2 + |S_t^\kappa|^2)\mathrm{d}\tau \mathrm{d}x \leq C. \tag{22}$$

2.3. Weak solutions to the phase-field model

In this subsection we shall make use of the *a priori* estimates to investigate the limits of the approximate solutions by using the following lemma of compactness.

Lemma 2.2 (Aubin-Lions) *Let B_0, B, B_1 be Banach spaces satisfying that B_0, B_1 are reflexive and*

$$B_0 \subset\subset B \subset B_1.$$

Here, by $\subset\subset$ we denote the compact imbedding. Define

$$W = \left\{ f \mid f \in L^{p_0}(0,T;B_0), f' = \frac{df}{dt} \in L^{p_1}(0,T;B_1) \right\}$$

with T being a given positive number and $1 < p_0, p_1 < +\infty$.

Then the embedding of W into $L^{p_0}(0,T;B)$ is compact.

Proof of Theorem 1.1. We choose

$$B_0 = W^{1,\infty}(\Omega), B = C(\bar{\Omega}), B_1 = L^2(\Omega),$$

and $p_0 = p, p_1 = 2$ (where p is an arbitrary positive number greater than 1), then we infer from Lemma 2.2 that S^κ is a compact sequence in $C(\bar{Q}_T)$. Then by the standard argument for passing to limits in the theory of viscosity solutions, we complete the proof of Theorem 1.1.

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