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Solutions to a model with Neumann boundary conditions for phase transitions driven by configurational forces

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ABSTRACT

We study an initial boundary value problem of a model describing the evolution in time of diffusive phase interfaces in solid materials, in which martensitic phase transformations driven by configurational forces take place. The model was proposed earlier by the authors and consists of the partial differential equations of linear elasticity coupled to a nonlinear, degenerate parabolic equation of second order for an order parameter. In a previous paper global existence of weak solutions in one space dimension was proved under Dirichlet boundary conditions for the order parameter. Here we show that global solutions also exist for Neumann boundary conditions. Again, the method of proof is only valid in one space dimension.

1. Introduction

In [1] we have investigated a system of partial differential equations modeling the evolution of a phase interface in solid bodies and proved that in the case of one space dimension an initial boundary value problem to this system has global solutions.

This system has been derived in [2,3] from a sharp interface model for martensitic phase transformations in a solid body. The sharp interface model consists of the equations of linear elasticity theory coupled with an equation posed on the interface, which determines the normal speed of the interface. To find the phase field model, the interface condition was transformed in a first step by rigorous mathematical arguments into a Hamilton–Jacobi transport equation for a smooth order parameter. In a second step a regularizing term was inserted into the Hamilton–Jacobi equation to avoid that the order parameter develops singularities after a finite time. This regularizing term, which consists of the Laplace operator with a small positive parameter ν, was inserted such that the second law of thermodynamics holds. For details of this procedure, for mathematical investigations of phase field models in both cases that the order parameter is conserved and non-conserved, and for the background in continuum mechanics we refer to [4,2,5–14].

This derivation suggests that solutions of this system of partial differential equations converge to solutions of the original sharp interface model for $\nu \to 0$. The usage of the new system of partial differential equations as a phase field model for martensitic transformations depends on this asymptotic behavior. Yet, it is not obvious whether this convergence really holds. To verify it, we construct in [6] an asymptotic solution for the system of partial differential equation, which indeed converges to a solution of the sharp interface model for $\nu \to 0$.

The asymptotic behavior of the new phase field model differs in an essential way from the asymptotic behavior of the standard model, which consists of the equations of linear elasticity theory coupled with the Allen–Cahn equation. The

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asymptotic behavior of this standard model is studied in [15] by formal methods. The result given there shows that in the limit sharp interface model the driving force of the interface motion contains a term with the mean curvature of the interface, which cannot be avoided. On the other hand, the limit model of the new phase field model does not contain such a curvature term. It is possible to make the constant multiplying the mean curvature term in the limit model of the Allen–Cahn model small by choosing a parameter in the Allen–Cahn model appropriately, but in [6] it is shown by analytical considerations and numerical examples, that in this case the numerical solution of the Allen–Cahn model becomes very ineffective, and that when the same physical problem is simulated with the new phase field model the computing time is smaller by a large factor.

This property makes the new phase field model interesting and justifies further investigation. It would be important to prove rigorously that solutions converge to solutions of the sharp interface model for $\nu \to 0$; the result in [6] is formal, since the asymptotic solutions constructed there satisfy the new phase field model only up to an error term in the right-hand side of the equations. For a rigorous proof it is necessary to show that the error in the solution caused by this error term in the right-hand side tends to zero for $\nu \to \infty$. Such a proof needs an existence result for the phase field model. In this paper we do not estimate this error term, but we continue the investigation of the existence theory, which we started in [1]. There we proved that an initial-boundary value problem to the new phase field model in one space dimension has solutions, if the displacement field and the order parameter both satisfy Dirichlet boundary conditions. Here we show that solutions exist for the one-dimensional problem when the order parameter satisfies homogeneous Neumann boundary conditions.

We next formulate the initial-boundary value problem in one space dimension and the main result of the paper. For the original form of the phase field model in three space dimensions we refer the reader to [1].

Let $\Omega = (a, d)$ be a bounded open interval, which represents the material points of a solid bar. T_e is a positive constant, which can be chosen arbitrarily large. We write $Q_{T_e} = (0, T_e) \times \Omega$ and define

$$(v, \varphi) = \int_Z v(y)\varphi(y)\mathrm{d}y,$$

where $Z = \Omega$ or $Z = Q_{T_e}$. If v is a function defined on Q_{T_e}, we denote the mapping $x \mapsto v(t, x)$ by $v(t)$. If no confusion is possible we sometimes drop the argument t and write $v = v(t)$. The crystallographic structure of the material can vary in space and time. We assume that two different structures, called phases, are possible. The different phases are characterized by the order parameter $S(t, x) \in \mathbb{R}$. A value of $S(t, x)$ near to zero indicates that the material is in the matrix phase at the point $x \in \Omega$ at time t, a value near to one indicates that the material is in the second phase. The 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 $T(t, x) \in \mathcal{S}^3$, where $\mathcal{S}^3$ denotes the set of symmetric 3×3-matrices. If we denote the first column of the matrix $T(t, x)$ by $T_1(t, x)$ and set

$$\varepsilon(u_x) = \frac{1}{2}\left((u_x, 0, 0) + (u_x, 0, 0)^T\right) \in \mathcal{S}^3,$$

then the unknowns must satisfy the quasistatic equations

$$-T_{1x} = b, \tag{1.1}$$

$$T = D(\varepsilon(u_x) - \bar{\varepsilon}S), \tag{1.2}$$

$$S_t = -c\left(\psi_S\big(\varepsilon(u_x), S\big) - \nu S_{xx}\right)|S_x| \tag{1.3}$$

for $(t, x) \in Q_{T_e}$. Since the Eqs. (1.1) and (1.2) are linear, the inhomogeneous Dirichlet boundary condition for u can be reduced in the standard way to the homogeneous condition. For simplicity we thus assume that u satisfies homogeneous Dirichlet boundary conditions. The initial and boundary conditions therefore are

$$u(t, x) = 0, \quad (t, x) \in [0, T_e] \times \partial\Omega, \tag{1.4}$$

$$S_x(t, x) = 0, \quad (t, x) \in [0, T_e] \times \partial\Omega, \tag{1.5}$$

$$S(0, x) = S_0(x), \quad x \in \Omega. \tag{1.6}$$

Here $\bar{\varepsilon} \in \mathcal{S}^3$ is a given matrix, the misfit strain, and $D : \mathcal{S}^3 \to \mathcal{S}^3$ is a linear, symmetric, positive definite mapping, the elasticity tensor. In the free energy

$$\psi^*(\varepsilon, S, \nabla_x S) = \psi(\varepsilon, S) + \frac{\nu}{2}|\nabla_x S|^2, \tag{1.7}$$

where

$$\psi(\varepsilon, S) = \psi(\varepsilon(\nabla_x u), S) = \frac{1}{2}\Big(D(\varepsilon - \bar{\varepsilon}S)\Big) \cdot (\varepsilon - \bar{\varepsilon}S) + \hat{\psi}(S), \tag{1.8}$$

we choose for $\hat{\psi} \in C^2(\mathbb{R}, [0, \infty))$ a double well potential with minima at $S = 0$ and $S = 1$. The scalar product of two matrices is $A \cdot B = \sum a_{ij}b_{ij}$. Also,

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