Simulations for a New Phase-Field Model for Phase Transitions Driven by Configurational Forces

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Abstract. In this paper, we shall investigate an initial (Neumann-) boundary value problem for a phase-field model proposed about a decade ago by Alber and Zhu to describe structural phase transitions driven by configurational forces, and this model differs from the famous Allen-Cahn model by a non-smooth term of the gradient of an order parameter. Numerical examples show that how the total energy for the Alber-Zhu model evolves with different values of the mobility coefficient and isotropic interfacial energy coefficient. Also a numerical comparison with the Allen-Cahn model shows that solutions to the Alber-Zhu model reach the equilibrium much faster than those to the Allen-Cahn model, moreover, the algorithms are more stable.

1. Introduction
Phase-field approach, emerged in 1980s, is a quite young but very powerful tool, from both theoretical and numerical aspects, to model various processes, such as phase separation, solidification, cavitation, reverse domain coarsening, incompressible fluids, see, e.g., [1, 2], and dispersion phenomenon in the wild populations and riverbed transplant, Ref. [3, 4]. Two well-known models, i.e. the Allen-Cahn and Cahn-Hilliard model are widely employed to study these phenomena which possess a feature of phase changes dominated by diffusion of atoms.

There is another important type of phase transitions which is diffusionless. To model this process, Alber and Zhu proposed two kinds of phase-field models in 2006 and 2007, respectively, which we call them the Alber-Zhu model that is divided into two cases distinguished by whether the parameter is conserved or not. One application of this model is to describe martensitic phase transformation in shape memory alloy, sintering in powder metallurgy. There have been many papers which study this new model, we refer the reader to, e.g., [5-14].

2. Phase-Field Model
We shall introduce the phase-field model in its original version by Alber and Zhu, Then simplify it to a slightly simple one while its essential difficulties remain.

To begin with, we first introduce some notations. Let \( \Omega \) be an open bounded domain in \( \mathbb{R}^3 \) to represent the points of a material body. Using a function \( S(t, x) \in \mathbb{R} \) to describe the material variation in time. For instance, suppose we choose the double-well potential function as \( (1-S^2)^2 \), it allows the value of \( S \) to vary between zero and one, inclusively, which shows that the material is in the matrix phase or second phase, if the number of \( S \) approaches to zero or one. But, in between, if some other number, it will be expressed that there exist the mixed phase between purely new phase in the simulation. The unknown \( T(t, x) \) in equations of (1)-(3) is a symmetric matrix.
\[ -\text{div}_x T(t, x) = b(t, x) \quad (1) \]
\[ T(t, x) = D(\varepsilon(\nabla_x u(t, x)) - \varepsilon S(t, x)) \quad (2) \]
\[ S_i(t, x) = -c(\psi'_\alpha(\varepsilon \nabla_x u(t, x)), S(t, x)) - \nu \Delta_x S(t, x) [\nabla_x S(t, x)] \quad (3) \]
\[ u(t, x) = \gamma(t, x), S_i(t, x) = 0 \quad (t, x) \in [0, \infty) \times \bar{\Omega} \quad (4) \]
\[ S(0, x) = S_0(x) \quad x \in \Omega \quad (5) \]

The \( c \) and \( \nu \) in the equations are the mobility coefficient, isotropic interfacial energy coefficient. The elasticity tensor \( D : \mathbb{S}^3 \rightarrow \mathbb{S}^3 \) is a linear, symmetric, positive definite mapping. Given are the volume force \( b : [0, \infty) \times \Omega \rightarrow \mathbb{R}^3 \).

For the system, we find the following main features.

1. It is an elliptic-parabolic coupled system of partial differential equations subject to Neumann boundary conditions.

2. The first two equations differ a linear system of elasticity by the term of \( \varepsilon \).

3. The parameter is not conserved since the value of \( \int_{\bar{\Omega}} S(t, x) dx \) is changing with time.

To simplify these equations, we make the following assumptions.

1. Ignoring elastic effect in this model and keep only its solid-solid transitions effect.

2. We convert this 3-D boundary value problem into 1-D and still represent by \( S(t, x) \in \mathbb{R} \).

Hence we can reduce our model into its 1D version as follows.

\[ S_i(t, x) = -c(\psi'_\alpha(S) - \nu \Sigma_{\alpha x}) \quad (t, x) \in (0, T_f) \times \Omega \quad (6) \]
\[ S_x = 0 \quad (t, x) \in (0, T_f) \times \bar{\Omega} \quad (7) \]
\[ S(0, x) = S_0(x) \quad x \in \Omega \quad (8) \]

In Section 3, we present some numerical experiments to show the effect between \( c \) and \( \nu \) about equation (6) -- (8) in 2D. In a former paper of mine [17], we proved the existence of weak solutions by using the Aubin-Lions lemma, Banach’s fixed Point Theorem and a series of \( a \) prior estimates and observed numerically the sensitivity of the parameters in the model. However, it only takes a set of data into account, while comparing to the Allen-Cahn model, not fully considering the factors of the system. Here, by varying the double-well potential function and the initial value, we find that the Alber-Zhu model takes less time to reach equilibrium state once again.

3. Simulations

We divide this section into two subsections, one is for the study of the evolution, with the different values of the parameters \( c \), and \( \nu \), of the total energy, and another is devote to the comparison of the results based on the Alber-Zhu model and its counterpart, i.e. the Allen-Cahn model.

3.1. Validation for \( c \) and \( \nu \)

With the help of total energy formula, the finite difference method is used to describe time variation of energy with \( c \) and \( \nu \). Sixteen experiments are performed to study the responses of Alber-Zhu model in figure 1, referencing from [16]. The thickness of interface is different and the mobility coefficient is changeless from top to bottom. It is classified according to four cases. Similarly, given the initial parameters, we study the effect of the mobility coefficient by numerical experiments which are listed in figure 1 from left to right.

Choosing the following parameters: \( \Omega = 100 \times 100 \); mobility coefficient \( c=0.2, 0.299, 0.35 \) or \( c=1.8 \) (from left to right for each rows in figure 1); Isotropic interfacial energy coefficient \( \nu = 2.55e^{-5}, 4e^{-5}, 6e^{-5}, 8e^{-5} \) etc.
6e-5 or $\nu = 4e-4$ (from top to bottom for each columns in figure 1); the double-well potential function $\psi = (S^2 - 1)^2 4^{-1}$.

![Figure 1](image)

**Figure 1.** Time evolution of total energy with various $c$ and $\nu$ in Alber-Zhu model.

Firstly, observing from the row direction, we find that first three lines have reaches equilibrium state without the last line, showing that the simulation are good as hoped for its isotropic interfacial energy coefficient amplified. It is sometimes possible to enlarge the number of isotropic interfacial energy coefficient. However, these “extra” enlarging may extend time to reach the equilibrium state just like the last row in figure 1.

In the fourth column, compared first three lines to the last one, we find that it has a rising course after it declining, because there is no existing for coexistence of two types of martensitic variants. That is to say, it’s far more likely that with the value of $\nu = e-5$, martensitic variants can coexist.

Continuing to monitor the figure 1, we find that the decline of total energy will be increased when the value of $c$ increases. And this experimental evidence supports my result in my former paper [17].

3.2. Comparisons between the Alber-Zhu Model and the Allen-Cahn One

In a phase-field model, a double-well potential function is usually chosen and this function does actually work. Usually, its minimum accords with phase points in the simulation. The initial value takes a key role during the experiment and analysis components of alloys.
In this case, the drawing makes use of blue and red, where blue means that it is Allen-Cahn model. Similarly, red represents Alber-Zhu model. Choosing the following dates to complete a total of 9 experiments: \( \Omega =100 \times 100 \); mobility coefficient \( c=0.2 \); isotropic interfacial energy coefficient \( \nu =2.55 \times 10^{-5} \); initial value \( S_0 =0.05 \cos(8\pi x) \cos(8\pi y)+0.5 \), \( 0.05 \sin(8\pi x) \sin(8\pi y)+0.5 \) or \( S_0=0.1 \text{rand}(1)+0.5 \) (from left to right for each rows in figure2); the double-well potential function \( \psi= (S^2-1)^2 4^{-1} \), \( \psi= (1-S^2) S^2 \) or \( \psi = 0.0039 S^2 2^{-1} - 0.9961 S^4 4^{-1} + 0.9923 S^6 6^{-1} \) (from top to bottom for each columns in figure 2); the certain coefficient of the last double-well potential function is from [15].

![Figure 2](image)

**Figure 2.** Comparison Alber-Zhu model to the Allen-Cahn model with various \( S_0 \) and \( \psi \).

Although the total energy of these two models drops with the time, the trends of it are distinct among different initial value and double-well potential function. From the figures from different columns, we discover the last column that arrive the same dates with its high speed when the initial value is selected as \( S_0 =0.1 \text{rand}(1)+0.5 \).

However, for example, continuous function with different double-well potential functions, two models’ total energy approximation cannot achieve similar results in every time for initial values which are not random. When the \( S_0 \) is given by \( 0.05 \cos(8\pi x) \cos(8\pi y)+0.5 \), the total energy of Allen-Cahn model declines more slowly than that of the Alber-Zhu model, even it is an unfinished process in (d) within a given time to reach its equilibrium state.

The following simulations about the Allen-Cahn model and the Alber-Zhu model from top to bottom for each columns in figure 3 are given through experiments under the given data in figure 2 (g). Four typical “inflection point” are selected and used to draw the evolution. They are \( t^* =200, 400, 800 \) and \( 1000 \) (from left to right for each rows in figure 3). Here, \( t^* \) represents time in level.
Figure 3. Evolution of martensitic phase based on the Allen-Cahn model and the Alber-Zhu model

Observation of figure 2 (g) reveals that the equilibrium has been reached by using the Alber-Zhu model at \( t^* = 800 \), but this is not true by using the Allen-Cahn model. That can be seen in (c) and (g) in figure 3. In addition, we discover the existence of two types of variants in (d) and (h), and this is consistent with figure 2 that the isotropic interfacial energy coefficient \( \nu \) influence the type of variant during the martensitic transformation.

4. References

[1] ALLEN S and CAHN J 1979 A microscopic theory for antiphase boundary motion and its application to antiphase domain coarsening Acta Mater 27(6) pp 1085–1095
[2] LIU C and SHEN J 2003 A phase field model for the mixture of two incompressible fluids and its approximation by a Fourier-spectral method Physica D 179(3–4) pp 211–228
[3] Coheh D and Murray J 1981 A generalize diffusion model for growth and dispersal in a population J. Math. Biology 12(2) pp 237–249
[4] Hazewinkel M, kaashoek J and Leynse B 1985 Pattern formation for a one dimensional evolution equation based on Thoma river basin model (Econometric institute, Erasmus University)
[5] Alber H and Zhu P 2007 Evolution of phase boundaries by configurational forces Arch Ration Mech Anal 185(2) pp 235–286
[6] Alber H and Zhu P 2006 Solutions to a model with nonuniformly parabolic terms for phase evolution driven by configurational forces SIAM J Appl Math 66(2) pp 680–699
[7] Hans D and Zhu P 2007 Solutions to a model for interface motion by interface diffusion[J] Proceed ings of the Royal Society of Edinburgh 138(5) pp 923–955
[8] Alber H and Zhu P 2011 Interface motion by interface diffusion driven by bulk energy: justification of a diffusive interface model[J] Continuum Mechanics & Thermodynamics 23(2) pp 139–176
[9] Zhu P 2012 Regularity of solutions to a model for solid–solid phase transitions driven by configurational forces[J] Journal of Mathematical Analysis & Applications 389(2) pp 1159–1172.
[10] Zhu P 2012 Solvability via viscosity solutions for a model of phase transitions driven by configurational forces[J] Journal of Differential Equations 251(10) pp 2833–2852
[11] Ou Y and Zhu P 2011 Spherically symmetric solutions to a model for phase transitions driven by configurational forces[J] Journal of Mathematical Physics 52(9) pp 345–360
[12] Kawashima S and Zhu P 2011 Traveling waves for models of phase transitions of solids driven by configurational forces[J] Discrete and Continuous Dynamical Systems-Series B (DCDS-B) 15(1) pp 309–323
[13] Alber H and Zhu P 2011 Solutions to a model with Neumann boundary conditions for phase transitions driven by configurational forces[J] Nonlinear Analysis Real World Applications 12(3) pp1797–1809
[14] Sheng W and Zhu P 2018 Viscosity solutions to a model for solid–solid phase transitions driven by material forces[J] Nonlinear Analysis Real World Applications 39 pp 14–32
[15] CUI S, WAN J, RONG Y and ZHANG J 2017 Phase-field simulations of thermomechanical behavior of MnNi shape memory alloys using finite element method Comput Mater Sci 139 pp 285–294
[16] BINER S 2017 Programming phase-field modelling (Switzerland: Springer International Publishing)
[17] Chen M Numerical simulations and existence of weak solutions for a class of phase field models, submitted