Commun. Comput. Phys.
doi: 10.4208/cicp.110310.090911a

Vol. **11**, No. 5, pp. 1697-1717
May 2012

Parareal in Time Simulation of Morphological Transformation in Cubic Alloys with Spatially Dependent Composition

Li-Ping He* and Minxin He

Department of Mathematics, Shanghai Jiaotong University, Shanghai 200240, China.

Received 11 March 2010; Accepted (in revised version) 9 September 2011

Communicated by Longqing Chen

Available online 12 January 2012

Abstract. In this paper, a reduced morphological transformation model with spatially dependent composition and elastic modulus is considered. The parareal in time algorithm introduced by Lions et al. is developed for longer-time simulation. The fine solver is based on a second-order scheme in reciprocal space, and the coarse solver is based on a multi-model backward Euler scheme, which is fast and less expensive. Numerical simulations concerning the composition with a random noise and a discontinuous curve are performed. Some microstructure characteristics at very low temperature are obtained by a variable temperature technique.

AMS subject classifications: 52B10, 65D18, 68U05, 68U07

Key words: Morphological transformation, multi-model scheme, parareal in time simulation.

1 Introduction

Many time-stepping methods have been developed for phase field models. Several explicit and implicit finite element schemes of the Cahn-Hilliard model were studied with mathematical rigor by Barrett et al. [3], Feng and Prohl [15], Elliott et al. [9–12]. Wang and Khachaturyan [35] considered Euler method for the three-dimensional field model of martensitic transformations. The semi-implicit Fourier spectral method for the Cahn-Hilliard model was proposed by Chen and Shen [5]. The large time-stepping semi-implicit methods for epitaxial growth models were proposed by Xu and Tang [40], and the Gauss-Seidel projection finite difference method of micromagnetics model was developed by Wang et al. [38]. For the phase field crystal model, Cheng [6] proposed an efficient algorithm, while Wu et al. [39] developed the stable difference nonlinear-multigrid

*Corresponding author. *Email addresses:* lphe@sjtu.edu.cn (L.-P. He), sophiaminxinhe@gmail.com (M. He)

method. In resent studies, see, e.g., [13,14,34], the unconditionally stable algorithms were developed for the Cahn-Hilliard equation. These algorithms allow for an increasing time step in Cahn-Hilliard systems as time proceeds.

In this paper, we consider the strain-induced morphological transformation model of cubic alloys, in which the composition and elastic modulus are spatially dependent. This model was proposed by Wang et al. [36] and developed by [27,28,30–33,37,41–44] where it is assumed that the composition and elastic modulus are positive constant. The advantages of such a model is the effects of coherent elastic strains on the kinetics of morphological transformations in solid state precipitation without any a prior assumptions on the possible morphologies that could develop, and an nonstructural decomposition of a cubic disordered phases in a binary alloy is then carried out. But we meet several difficulties in simulations. For instance, how to deal with the model if the composition includes a random noise or a discontinuous curve. As we only obtain an explicit representation of the model in reciprocal space (we can not derive its explicit one in physical space), solving the nonlinear equation at each time step becomes much more expensive. To overcome the difficulties mentioned above, we shall consider the reduction method for the morphological transformation model and numerical techniques. The possible contributions of this work are (i) the reduced morphological transformation model in dimensionless form is derived; (ii) the multi-model backward Euler scheme is developed, which is fast and inexpensive; (iii) a variable temperature model with numerical techniques are given; in particular, numerical simulations concerning the microstructure characteristic at very low temperature are performed; and (iv) the parareal in time algorithm is achieved for longer-term simulation.

This paper is organized as follows: In Section 2 the Önsager equation with spatially dependent composition and elastic modulus is shown. Section 3 derives the reduced morphological transformation model. Section 4 develops the multi-model method and variable temperature technique, and the offline-online procedures are discussed. Moreover, numerical simulations concerning the composition with a random noise and a discontinuous curve are reported. Section 5 is devoted to the parareal in time algorithm. Finally, we give some conclusions in Section 6.

2 Kinetic equation with spatially dependent composition

2.1 The Önsager equation

Let $c(\boldsymbol{r})$ be the atomic fraction of solute atoms, K_B be the Boltzmann's constant, T be the absolute temperature, $\lambda(\boldsymbol{r}-\boldsymbol{r}')$ be a matrix of kinetic coefficients related to probabilities of elementary diffusional jumps from lattice site $\boldsymbol{r}$ to $\boldsymbol{r}'$ of a Bravais lattice during a time unit, and $\mathcal{F}_{\text{ree}}$ be the total free energy including the strain energy contribution. Then it is well know that the crystal lattice site diffusion in a binary substitution alloy is determined by a diffusible relaxation of the nonequilibrium single site occupation probability of a solute atom at crystal lattice site $\boldsymbol{r}$ and at time t, which is denoted by $\eta(\boldsymbol{r},t)$ and satisfies the