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Phase-field modeling the effect of misfit on the precipitation of the second-phase particles and grain coarsening

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ABSTRACT

A modified phase-field model has been used to study the precipitation of the second-phase particles and the coarsening of grains under the influence of lattice mismatch. The elastic strain energy caused by misfit is taken into account, and the force equilibrium equation is solved using the iterative-perturbation method. The simulations show that the morphology of the second-phase particles is significantly influenced by the misfit, and the elastic stress blocks the precipitation of the particles. With the increase of the elastic modulus, the process of grain coarsening changes, and the morphology of the second-phase particle gradually transforms from globular to square and rod. The interactions between solute concentration and the misfit are cooperative, which together control the size of grains.

1. Introduction

Microstructures of most structural materials are consisted of grains and coherent precipitates. To some extent, grain refining is important for improving both the intensity and toughness of materials [1–3]. Various refining measures such as deformation, deep cooling, or others have been implemented to control the grain size, which depends on material processing and service. Dispersive second-phase particles, as an effective means of improving mechanical properties in heat treatment, play an important role on restraining the growth of grains by pinning grain boundaries. In particular, the effect of grain size on mechanical properties has been extensively concerned in recent years [4]. Up to now, there has been amount of simulation technologies to investigate the influence of the second-phase particles on pinning grain boundary. Each variant may have its own misfit because the lattice parameters of precipitated second-phase differ from that of matrix [5]. The elastic displacements of atoms from their equilibrium lattice positions were induced by the lattice mismatch between the product and the matrix. In addition, the magnitude of elastic strain energy generated in coherent microstructures depends on the level of lattice mismatch and the elastic properties of each phase, as well as the shape and spatial distributions of coherent domains [6].

The elastic stress has a significant influence on microstructures. Effects of particle shape changes, particle alignment along specific crystallographic directions and particle splitting, etc. have been attributed to the elastic stress which is caused by misfit. In the last few years, there have been several approaches [5–9] to introduce elastic in-homogeneity into the phase-field models. Zhu et al. [10] have studied the effect of elastic in-homogeneity in microstructure evolution in the phase separation and coarsening systems. Hu and Chen [6] studied the microstructure evolution in elastically inhomogeneous and anisotropic systems using an iterative-perturbation method based on Fourier transformation. And based on the estimation of strain energy of an elastically inhomogeneous solid, Wang et al. [11,12] used a phase-field micro-elasticity theory to research elastically inhomogeneous solids. Bhattacharyya et al. [13] discussed the stress effect on grain boundary migration by using a modified phase field model. However, until now, the effect of elastic strain energy on the precipitation of the second-phase particles and the grain coarsening has not yet been investigated.

In present work, the effect of elastic stress caused by misfit on the evolution of microstructures is explored. A modified phase-field model is employed to simulate grain growth kinetics with the presence of the second-phase particles. A new free energy

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function which is different from the existing simulations [14–25], is constructed. And the new free energy function contains the elastic interaction between grains and second-phase particles. Moreover, the force equilibrium equation is solved using the Fourier spectral iterative-perturbation method. The coherency strain is characterized using the phase-field parameter based on the lowest system free energy principle and the diffusive-interface phase field model, which overcomes the defect of the artificial second-phase particles set beforehand. The outline of the phase-field formulas is initially presented in the work, followed by the results and discussion. At last the conclusions are summarized.

2. Theoretical modeling

2.1. Energy

The total free energy (F) of a given system is written as Eq. (1), and which is consist of chemical energy (F_{ch}) and elastic energy (F_{el}):

$$F = F_{ch} + F_{el} \tag{1}$$

The F_{ch} of the inhomogeneous system is expressed as a function of the field variables:

$$F_{ch} = \int \left[f_0(\eta_1(r), \ldots, \eta_p(r), C(r)) + \frac{\kappa_i}{2}\sum_{i=1}^{p}(\nabla\eta_i(r))^2 + \frac{\kappa_C}{2}(\nabla C(r))^2 \right] d^3r \tag{2}$$

where $f_0(\eta_1(r), \ldots, \eta_p(r), C(r))$ is the bulk free energy density, and κ_C, κ_i are the related to gradient energy coefficients respectively. The interface energy is determined by the gradient term. f_0 is approximated using the following expansion:

$$f_0 = f_1(C) + \sum_{i=1}^{p} f_2(C, \eta_i) + \sum_{i=1}^{p}\sum_{j\neq i}^{p} f_3(\eta_i, \eta_j) \tag{3}$$

where $f_1(C)$ is the function of composition C, $f_2(C, \eta_i)$ is a coupled function of composition C as follows:

$$f_1(C) = -(A/2)(C - C_m)^2 + (B/4)(C - C_m)^4 + (D_\alpha/2)(C - C_\alpha)^4 + (D_\beta/2)(C - C_\beta)^4$$

$$f_2(C, \eta_i) = -(\gamma/2)\left[(C - C_\alpha)^2 + (C - C_\beta)^2\right](\eta_i)^2 + (\delta/4)(\eta_i)^4$$

$$f_3(\eta_i, \eta_j) = (\varepsilon_{ij}/2)(\eta_i)^2(\eta_j)^2 \tag{4}$$

where C_α and C_β are the equilibrium solute concentrations in α and β phase respectively, $C_m = (C_\alpha + C_\beta)/2$, and A, B, D_α, D_β, γ, δ and ε_{ij} are dimensionless parameters. The expression of the bulk free energy density f_0 confirms that grains with different orientations can produce grain boundary, while grains with the same orientation will merge.

Following Hu and Chen [6], we implement an iterative-perturbation method coupled with Fourier spectral implementation to get the analytically approximation solution. By using the displacement field with a first-order approximation, the system elastic energy F_{el} can be expressed as:

$$F_{el} = \frac{1}{2}\int_{-\infty}^{+\infty}\left[\bar{C}_{ijkl}\varepsilon_0\delta_{ij}\varepsilon_0\delta_{kl} - n_j\sigma^0_{ij}\Omega_{kl}(\boldsymbol{n})\sigma^0_{kl}n_l\right]|\Delta\tilde{C}(\boldsymbol{k})|^2\frac{dk}{(2\pi)^3} \tag{5}$$

where $\sigma^0_{kl} = \bar{C}_{ijkl}\varepsilon_0\delta_{ij}$, $\Omega_{kl}(\boldsymbol{n})\Omega_{kl}{}^{-1}(\boldsymbol{n}) = I$, $\Omega_{kl}{}^{-1}(\boldsymbol{n}) = C_{ijkl}n_jn_l$, and $\Omega_{kl}(\boldsymbol{n})$ is the normalized inverse Green tensor, $\boldsymbol{k}$ is the Fourier wave vector, and $\boldsymbol{n} = \boldsymbol{k}/|k|$ is the unit vector in reciprocal space.

2.2. Kinetics

The temporal evolution of the field variables is governed by two equations: the Cahn–Allen equation for the (non-conserved) order parameter field $\boldsymbol{\eta}_i(r,t)$ and the Cahn–Hilliard equation for the (conserved) composition field $C(r,t)$ [6]. When elastic energy contribution is taken into account, the modified Cahn–Allen equation is expressed as:

$$\frac{\partial\boldsymbol{\eta}_i(r,t)}{\partial t} = -L\frac{\delta F}{\delta\boldsymbol{\eta}_i(r,t)} = -L(\mu_{ch\eta} + \mu_{el\eta})$$

$$\frac{\partial C(r,t)}{\partial t} = \nabla\left\{D\nabla\left[\frac{\delta F}{\delta C(r,t)}\right]\right\} = \nabla\{D\nabla[\mu_{chC} + \mu_{elC}]\} \tag{6}$$

where L is the relaxation coefficient and D is the diffusion constant and

$$\mu_{ch\eta} = \frac{\delta F_{ch}}{\delta\eta} = \frac{\partial f_0}{\partial\eta} - 2k_\eta\nabla^2\eta$$

$$\mu_{chC} = \frac{\delta F_{ch}}{\delta C} = \frac{\partial f_0}{\partial C} - k_C\nabla^2 C$$

$$\mu_{el\eta} = \frac{\delta F_{el}}{\delta\eta} = \frac{\delta F_{el}}{\delta\eta^2}\cdot\frac{\delta\eta^2}{\delta\eta} = 2\eta\frac{\delta F_{el}}{\delta\eta^2}$$

$$\mu_{elC} = \frac{\delta F_{el}}{\delta C} = \left\{\left[\bar{C}_{ijkl}\varepsilon_0\delta_{ij}\varepsilon_0\delta_{kl} - n_j\sigma^0_{ij}\Omega_{kl}(\boldsymbol{n})\sigma^0_{kl}n_l\right]\tilde{C}(\boldsymbol{k})\right\}_r \tag{7}$$

It can be seen that the addition of elastic energy leads to the reduction of the equilibrium values of order parameters within each phase, which in turn affects the elastic energy density. This problem is similar to the model of effect of stress on grain boundary migration developed by Bhattacharyya et al. [13]. Here, the parallel way is applied to solve the problem. It can be alleviated if we make F_{el} depend on a function $H(C)$ instead of $C(r)$ such that the value of the function is always maintained at the equilibrium state. Then Eq. (5) can be expressed as:

$$F_{el} = \frac{1}{2}\int_{-\infty}^{+\infty}\left[\bar{C}_{ijkl}\varepsilon_0\delta_{ij}\varepsilon_0\delta_{kl} - n_j\sigma^0_{ij}\Omega_{kl}(\boldsymbol{n})\sigma^0_{kl}n_l\right]|\tilde{H}(C)|^2\frac{dk}{(2\pi)^3} \tag{8}$$

$H(C)$ was defined as follows: $H(C) = C - C_\alpha$, when $C = C_\alpha$; $H(C) = C - C_\beta$, when $C = C_\beta$; $H(C) = C - C_0$ when $C = C_0$; $H'(C) = 0$, when at the triple junction. Therefore, $H'(C)$ can be expressed as:

$$H'(C) = (C - C_\alpha)(C_\beta - C)(C - C_0) \tag{9}$$

Then the elastic potential equation is changed as:

$$\mu_{elC} = \frac{\partial F_{el}}{\partial C} = \left\{\left[\bar{C}_{ijkl}\varepsilon_0\delta_{ij}\varepsilon_0\delta_{kl} - n_j\sigma^0_{ij}\Omega_{kl}(\boldsymbol{n})\sigma^0_{kl}n_l\right]H'(\tilde{C}(\boldsymbol{k}))\right\}_r \tag{10}$$

The modified governing equation for phase-field model is used to study the elastic strain effect on the precipitate of the second phase particles and the grain coarsening.

3. Simulated results and discussion

A finite difference scheme was used to solve the time-dependent Cahn–Allen Eq. (6), and periodic boundary conditions were employed in the simulations. Because the first-order approximation was used to simulate the elastic energy, less than 10% difference of the elastic constants between the precipitate and grains can be introduced by setting of elastic constants, which is similar with practical two-phase alloys. By assuming that the alloys are cubic phase, the nondimensional elastic constants are $C_{11} = 200$, $C_{12} = 150$, $C_{44} = 100$, $C^*_{11} = 220$, $C^*_{12} = 165$, $C^*_{44} = 110$. The simulation is performed in a square lattice consisting of 512×512 unit cells,