Phase-field Modeling of the Influence of Elastic Field on the Nucleation and Microstructure Evolution in Precipitation

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Abstract

A phase-field method was employed to study the influence of elastic field on the nucleation and microstructure evolution. Two kinds of nucleation process were considered: one using fixed nucleation probability and the other calculated from the classical nucleation theory. In the latter case, the simulated results show that the anisotropic elastic strain field yields significant effects on the behavior of nucleation. With a large lattice misfit between the matrixes and the precipitates, the nucleation process does not appear fully random but displays some spatial correlation and has a preference for the elastic soft direction. However, with a small lattice misfit, this bias does not look quite clear. On the contrary, in the case of fixed nucleation probability, the elastic field has no influence on the nucleation process. The lattice mismatch also exerts influences on the microstructure morphology: with lattice mismatch becoming larger, the microstructure proves to align along the elastic soft direction.

Keywords: elastic field; nucleation; phase-field method; precipitation

1 Introduction

It is well known that the strength properties of materials are determined by microstructures, and microstructure patterns are affected by processes of nucleation, therefore, by controlling processes of nucleation, a desired microstructure may well be obtained.

The phase-field method used as a powerful tool for microstructure simulation has attracted more and more attention from material researchers in recent years. Moreover, the phase-field method is quite useful for studying not only microstructure evolution but also nucleation processes, especially precipitation. Wang et al. and Li et al.[1-4] studied the process of nucleation by adding a noise term to imitate the effects of thermal fluctuation. If the amplitude is too small, it will take quite a long time to form nuclei, however, if the noise term of a larger amplitude is added, the profiles of concentration and order parameters may be influenced. This means that the method of adding noise terms in the governing equations can only be used in the early stage of nucleation, and once enough nuclei are obtained after a short time, we have to shut off the noise terms. By this way, even the driving force allows nucleation to start again, it will never occur. To overcome the shortcoming, the method proposed by Simmons et al.[5] was adopted. For simplicity a fixed probability can also be used, which assumes that all the nodes in the computation field have the same ability to nucleate. However, if the anisotropic strain field exists near the microstructure, things will change. In this case, some positions must exist with low potential barrier to nucleation while others

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with high one due to strain-induced energy.

The objective of the present paper is to investigate the behavior of nucleation in the anisotropic elastic field with small and large lattice mismatch between matrix and precipitate phases for the purposes of evaluating the effects of the elastic field on the nucleation processes.

2 Model Description

2.1 Nucleation model

From the classical nucleation theory, the nucleation rate is[6]

$$J = \omega C_0 \exp\left(-\frac{\Delta G_{\mathrm{m}}}{k_{\mathrm{B}} T}\right) \exp\left(-\frac{\Delta G^*}{k_{\mathrm{B}} T}\right) \qquad (1)$$

where C_0 is the number of atoms per unit volume, ΔG_{m} is the activation energy for atomic migration per atom, ω is the frequency factor, k_{B} is the Boltzmann constant, T is the absolute temperature, and $\Delta G^* = \pi \sigma^2 / \Delta G_{\mathrm{V}}$ is the energy barrier to form a two-dimension stable spherical nucleus, σ is the interfacial energy, ΔG_{V} is the total bulk free energy which includes the elastic energy contribution $\Delta G_{\mathrm{el}} = G_{\mathrm{el}}(\phi'(r)) - G_{\mathrm{el}}(\phi(r))$, $G_{\mathrm{el}}(\phi'(r))$ and $G_{\mathrm{el}}(\phi(r))$, $\phi'(r)$ and $\phi(r)$ are the elastic energy and long-range order parameters after and before the occurrence of a nucleus respectively[7]. The probability for nucleation can be obtained by calculating J. When the probability is greater than a uniform random variable, nucleation occurs (For details, please refer to Refs.[7,8]).

2.2 Elastic energy model

In a homogenous cubic system proposed by Shen et al.[8], the elastic strain energy can be simply written in a reciprocal space as below

$$E_{\mathrm{el}} = \frac{1}{2} \int' \frac{\mathrm{d}\boldsymbol{g}}{(2\pi)^3} B(\boldsymbol{n}) \hat{\phi}(\boldsymbol{g}) \hat{\phi}^*(\boldsymbol{g}) \qquad (2)$$

where $B(\boldsymbol{n}) = C_{ijkl} \varepsilon_{\mathrm{T}ij} \varepsilon_{\mathrm{T}kl} - n_i C_{ijkl} \Omega_{jk}(\boldsymbol{n}) \varepsilon_{\mathrm{T}ij} \varepsilon_{\mathrm{T}kl} n_j$, $\Omega_{jk}^{-1}(\boldsymbol{n}) = (C_{ijkl} n_i n_l)$, $\boldsymbol{g}$ is the wave vector, $\boldsymbol{n} = \boldsymbol{g}/|\boldsymbol{g}|$, C_{ijkl} is the elastic constant, $\varepsilon_{\mathrm{T}ij}$ is the stress-free strain, $\hat{\phi}(\boldsymbol{g})$ is the Fourier transformation of order parameter $\phi(r)$ in real space. The exclusion of prime($'$) in the symbol of integral means $\boldsymbol{g} = \boldsymbol{0}$, and the star denotes complex conjugate.

2.3 Phase-field model

In this paper, we use the same thermodynamics description as that put forward by Kim et al.[9,10] for the interfacial domain, and the interfacial domain is described as a mixture of matrix and precipitate phases with the same chemical potentials in place of the same compositions.

In the present simulation, one composition field $c(r)$ and one artificial order parameter field $\phi(r)$ are used. Due to the varied volumes of precipitation occupied originally by the matrix, misfit strain energy usually arises in the process of precipitation. So the total free energy of the system is

$$F = \int_V \left[f(c,\phi) + \frac{\varepsilon^2}{2}(\nabla\phi)^2 + f_{\mathrm{el}} \right] \mathrm{d}V \qquad (3)$$

where $f(c,\phi)$ is the local free energy density, f_{el} is the elastic energy density, ε^2 is the gradient energy coefficient, $c = h(\phi)c_{\mathrm{p}} + [1-h(\phi)]c_{\mathrm{m}}$, $\dfrac{\partial f_{\mathrm{p}}}{\partial c_{\mathrm{p}}} = \dfrac{\partial f_{\mathrm{m}}}{\partial c_{\mathrm{m}}}$, c_{m} and c_{p} are the compositions of matrix and precipitate phases respectively. The local free energy density is written as follows

$$f(c,\phi) = h(\phi) f_{\mathrm{p}}(c_{\mathrm{p}}) + (1-h(\phi)) \cdot \\ f_{\mathrm{m}}(c_{\mathrm{m}}) + Wg(\phi) \qquad (4)$$

where $f_{\mathrm{p}}(c_{\mathrm{p}})$ and $f_{\mathrm{m}}(c_{\mathrm{m}})$ are the free energy densities of the precipitate and the matrix phases respectively, W is the double-well height, $g(\phi)$ and $h(\phi)$ are selected from $g(\phi) = \phi(1-\phi)$ and $h(\phi) = \phi^2(3-2\phi)$. Given interfacial energy σ and interface width 2λ, ε and W can be obtained by $\varepsilon = \dfrac{4\sqrt{W}\lambda}{\pi}$, $W = \dfrac{2\sigma}{\lambda}$.

Microstructural evolution is governed by two non-linear equations: the Cahn-Hilliard equation which is used for the composition field and the Ginzburg-Laudau equation for the long-range order parameter field,

$$\frac{\partial\phi}{\partial t} = -M_\phi \frac{\delta F}{\delta\phi} \qquad (5)$$

$$\frac{\partial c}{\partial t} = \nabla M_c \nabla\left(\frac{\delta F}{\delta c}\right) \qquad (6)$$

where M_ϕ and M_c are corresponding mobilities, t is the time.

3 Results and Discussions

3.1 Parameters and conditions

The simulation is performed on a two-dimensional computation domain. The kinetic equations are discretized by 256×256 uniform lattices and the periodic boundary condition is used. The Gibbs free energy of precipitate and matrix phases is taken from the thermodynamic database. The main parameters used in this simulation are listed as follows: interfacial energy $\sigma = 0.02$ J/m^2, elastic constants $C_{11} = 231$ GPa, $C_{12} = 149$ GPa, $C_{44} = 117$ GPa[8]. By variation of the lattice misfit ε, its effect on the process of nucleation was investigated.

3.2 Simulated microstructure morphology

With the model described above, simulation is performed and some interesting results are obtained. From Fig.1, when the nucleation probability is fixed, all the nodes in the computation domain have the same opportunity to nucleate, and the nuclei appear at random despite the large lattice misfit.

In the case of the probability for nucleation calculated from the classical nucleation theory, the nucleation will occur in a nearly random manner when the anisotropy of the elastic field is not obvious as is the case with small mismatch (shown by Fig.2). Because an almost equal probability for nucleation exists all over the computation domain, the preferable nucleation is not clear. However, from Fig.3, in the presence of anisotropic elastic field with large misfit between the matrix and the precipitate phases the nucleation processes do not take place randomly any more. Since the pre-existing particles form some elastic strain field due to the misfit between matrix and precipitate phases, the new-born particles may be affected by the elastic strain energy. Due to elastic interaction, nucleation occurs preferably in the elastic soft directions, that is, ⟨10⟩ and ⟨01⟩ crystallography directions. However, it does not mean that nucleation can not occur in any other directions although less probably. In fact, the preferential nucleation phenomenon shown above is based on the high activation energy and the large misfit which hardly induce nucleation. Since the particles nucleated earlier have enough time to develop an elastic strain field, the later-born nuclei will grow in a well-developed elastic strain field circumstance, and in the elastic soft direction
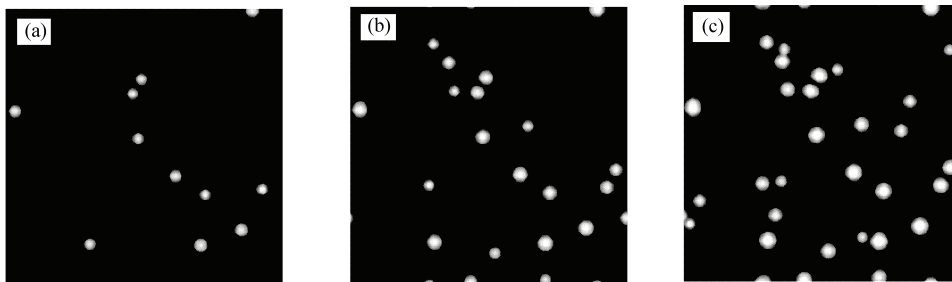

Fig.1　Simulated morphology of nucleation with misfit=0.019 6 (fixed nucleation probability is assumed). (a) n=50; (b) n=150; (c) n=250 (iteration times).
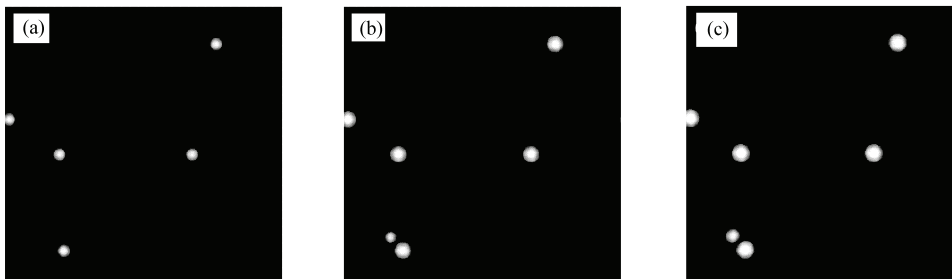

Fig.2　Simulated morphology of nucleation with misfit=0.004 9 (preferable nucleation is not obvious). (a) n=50; (b) n=150; (c) n=250 (iteration times).
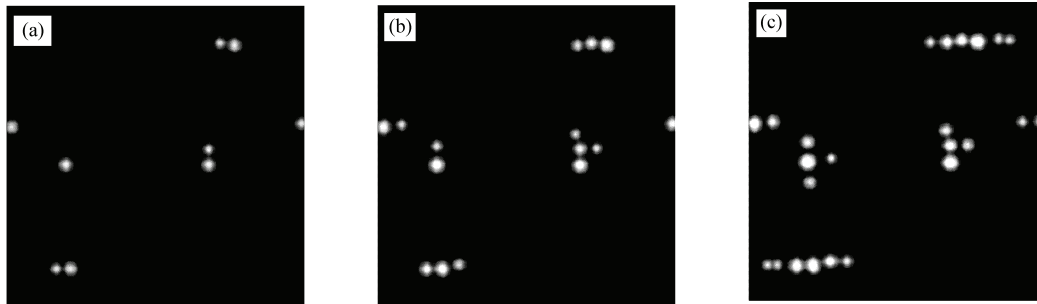
Fig.3   Simulated morphology of nucleation with misfit=0.019 6 (nucleus occurs preferably in the elastic soft direction).
        (a) n=50; (b) n=150; (c) n=250 (iteration times).

the activation energy is low due to the anisotropic elastic strain field. Thus, the nucleus will "choose" a preferable position to appear.

From Fig.4, it can be seen that the microstructure morphology is heavily affected by the mismatch. If the mismatch is small, elastic field has a slight effect on it at earlier time, and the precipitates are nearly spherical. However, if the mismatch is very large, the precipitates will align along the elastic soft direction.
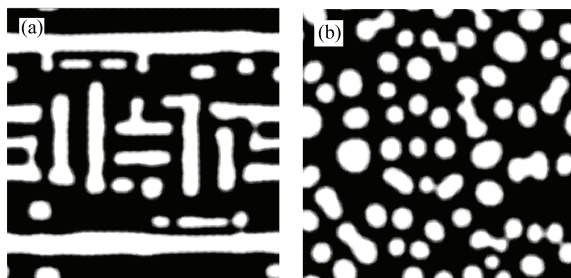

Fig.4   Microstructure pattern with different elastic condition at n=4 000(iteration times). (a)misfit=0.019 6; (b) misfit=0.004 9.

4 Conclutions

In this paper, the phase field method was used to simulate the processes of nucleation and the evolution of the microstructure in the presence of anisotropic elastic strain field. The following conclusions might well be summed up.

(1) When the nucleation probability calculated from the classical nucleation theory is used to get the preferred nucleation, the misfit between matrix and precipitate phases must be large, whereas too small lattice misfit will make the elastic fields have few effects on nucleation processes.

(2) When a fixed nucleation probability is used, no matter how large the lattice misfit is, no prefer-

ential nucleation in the elastic soft direction will appear.

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