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Phase field simulation of precipitates morphology with dislocations under applied stress

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ABSTRACT

A phase field dynamic model was developed and used to investigate the effects of dislocations and applied strain on the precipitation behavior and microstructure evolution of model binary alloys. The simulations show that the local microstructure depends not only on the relative magnitude of the dislocation stress and the stress induced by the applied strain, but also on the composition and magnitude of the stress. Its also shown that the applied strain makes the phase decomposition quickly. The results suggest that the microstructure of an alloy and its evolution may be controlled by finding suitable combination between dislocation, applied strain and composition, and the theoretical calculations are helpful in predicting what those combinations should be.

1. Introduction

Applied stress and dislocation stress affect the morphology of alloy during the solid-state phase transformation. An applied stress can introduce an additional lattice mismatch strain when the elastic constants of the matrix and the precipitates are different; it also induces the coupling elastic strain energy during the structure transformation. The applied stress can also modify the morphologies of the precipitate particles, e.g. their size, shape, volume fraction, orientation with respect to the matrix, and phase transformation kinetics, thus affecting the mechanical and physical properties of a material [1–7]. On the other hand, the dislocation stress field can change the velocity of migrating atoms and the direction in the diffusion phase transformation, influencing in this way the local precipitates morphology and the phase transformation velocity [8–11], which in turn results in a change of the local microstructure. In addition to the applied stress and dislocation stress, the coherency elastic stress arising from the crystal lattice mismatch between the matrix and the precipitates is also important, and it affects the solid-state transformation as well [12,13]. For predicting and controlling the properties and morphology of materials it is thus crucial to understand how the applied stress, dislocations and coherency stress affect the microstructures' evolution during a solid-state phase transformation [14–17].

Numerous experimental and theoretical studies have been devoted to investigate this issue [1–13]. For example, Miyazakr et al. [3] investigated the morphological changes of γ' particles in Ni–15 at.%Al alloy single crystals due to annealing at 1023 K under tensile and compressive loads in a [0 0 1] cube direction. They found that both rods and plates of γ' are aligned parallel to the tensile axis [0 0 1] and perpendicular to the compressive axis [0 0 1]. On the other hand, Fährmann et al. [7] studied the effect of pre-strain and the development of rafting during aging. They found that the pre-strain paths modify the initial structure of γ/γ' interfaces and that the local state of stress contributes the driving force for rafting. Theoretical studies that employed the phase field simulation technique have been used to investigate the effects of applied stress and dislocation stress on a solid-phase transformation [4–11]. For example, Li and Chen [4] investigated the shape evolution and splitting pattern of coherent particles under applied stresses. They found that the elongation direction of the precipitates was influenced by the applied strain direction, the relative magnitude of the elastic constant of the precipitates and matrix, and the sign of the lattice mismatch. Gururajan and Abinandanan [5] studied the precipitates rafting under the uniaxial stress, and their results showed that the purely elastic stress-driven rafting is possible, the rafting is more pronounced for the soft precipitates, and the sign of the applied stress is the same as that of the misfit. Finel et al. [6] analyzed the microstructure evolution in the presence of a lattice misfit and with inhomogeneous elastic constants; they found that the external load

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along an axis makes the microstructure anisotropic, and that the situation qualitatively differs depending on the sign of the applied stress.

The dislocation effects on the precipitation behavior and morphology have been studied by Hu and Chen [10] with Mura's [18] dislocation eigenstrain in Fourier space with periodic boundary condition. Thus, they found that coherent nucleation may become barrierless under the influence of the local elastic field of a dislocation. Li et al. [11] investigated the effects of dislocations on the Fe–Cr alloy spinodal decomposition using Stroh's [19,20] dislocation formula, and their results showed that dislocations facilitate the phase decomposition and that special morphologies appeared induced by the tilt grain boundary. Finally, He [21] and Chen [22] studied the spinodal morphology of thin film with periodic dislocations; their results showed that the dislocations change the local microstructure pattern.

All the studies above have focused on the effect that either applied stress or dislocations stress introduce in a solid-state transformation. The combined effect of applied elastic strain and dislocations on the morphology is not very clearly yet, and that is an interested question. In this paper, we will study this combined effect by investigating the precipitation behavior and microstructure of model binary alloys with dislocations under applied strain. The effects of the relative magnitude of applied stress and dislocation stress on the local morphology and phase transformation velocity were also investigated.

2. Methodology

In this section we describe the model that has been used to investigate how dislocation and applied stress affect the morphology of alloy during a solid-state transformation.

2.1. The phase field model

The microstructure evolution of a binary alloy, *A*–*B*, during precipitation can be described by the solute composition $c(\mathbf{x}, t)$ at any point $\mathbf{x}$ at time t, and it is governed by the Cahn–Hilliard diffusion equation [23,24]

$$\frac{\partial c}{\partial t} = \nabla \cdot \left[M \cdot \nabla \left(\frac{\delta F}{\delta c} \right) \right], \tag{1}$$

where M is the chemical mobility and c is the atom fraction of the element B. F in the equation above is the total free energy of the simulated system, and it is given by the expression

$$F = \int_V \left[f(c) + \frac{1}{2} k (\nabla c)^2 + E_{el} \right] dV, \tag{2}$$

where $f(c)$ is the local chemical free energy density per unit volume, $1/2k(\nabla c)^2$ represents the concentration gradient energy per unit volume, and E_{el} is the elastic energy density per unit volume.

The chemical free energy density per unit volume of *A*–*B* for the regular solution approximation is given by

$$f(c) = \frac{(1-c)G_A^0 + cG_B^0 + \Omega c(1-c) + RT[c \ln c + (1-c)\ln(1-c)]}{V_m}, \tag{3}$$

where G_A^0 and G_B^0 are the standard molar Gibbs free energies of pure *A* and *B*, respectively, Ω is the interaction parameter, chosen as $\Omega = 18$ kJ/mol, R is gas constant, T is the absolute temperature, and V_m denotes the molar volume of the alloy. $G_A^0 = G_B^0 = 0$ was adopted as the reference energy level for the Gibbs free energy.

The concentration gradient coefficient is expressed as [25,26]

$$k = \frac{1}{V_m} \frac{1}{6} r_0{}^2 \Omega, \tag{4}$$

where r_0 is the interatomic distance at stress-free state and changes with composition by simply obeying Vergard's law. The mobility M is assumed to be a constant for simplicity.

The phase field equation results from substituting Eq. (2) into Eq. (1), and the final result is given by the expression

$$\frac{\partial c}{\partial t} = M \nabla^2 \left[\frac{\delta f(c)}{\delta c} - k \nabla^2 c + \frac{\delta E_{el}}{\delta c} \right]. \tag{5}$$

2.2. Elastic stress

The elastic energy in Eq. (5) includes the energy induced by the eigenstrain, applied and dislocation strain. To introduce the applied strain into the total elastic energy, the inhomogeneous elastic modulus tensor is considered, i.e. the elastic modulus of precipitates and the matrix are different. The local elastic modulus tensor can be represented as follows:

$$C_{ijkl} = C_{ijkl}^0 + \Delta C_{ijkl} \Delta c, \tag{6}$$

where $\Delta c = c - c_0$, c_0 is the average composition at the zero stress reference, $C_{ijkl}^0 = \lambda C_{ijkl}^{\mathrm{P}} + (1-\lambda) C_{ijkl}^{\mathrm{M}}$ is the average modulus with λ the volume fraction of the precipitates, and C_{ijkl}^{M} and C_{ijkl}^{P} are the elastic modulus tensors of the matrix phase and precipitates, respectively, $\Delta C_{ijkl} = C_{ijkl}^{\mathrm{P}} - C_{ijkl}^{\mathrm{M}}$.

The elastic strain of the system including the applied strain and dislocation can be given as

$$\varepsilon_{ij}^{el} = \varepsilon_{ij}^{a} + \varepsilon_{ij} - \varepsilon_{ij}^{0} - \varepsilon_{ij}^{d}, \tag{7}$$

where ε_{ij}^{a} is the applied strain, ε_{ij} is the internal strain, ε_{ij}^{0} is the eigenstrain caused by the compositional inhomogeneity and is given by

$$\varepsilon_{ij}^{0} = \varepsilon_0 \delta_{ij} \Delta c, \tag{8}$$

where $\varepsilon_0 = 1/a(da/dc)$ is the composition expansion coefficient of the lattice parameter and δ_{ij} is the Kronecker-delta function. The dislocation eigenstrain ε_{ij}^{d} in Eq. (7) for an edge dislocation with Burgers vector $\mathbf{b} = (b_1, 0, 0)$ can be expressed as [18]

$$\varepsilon_{21}^{d} = \frac{1}{2} b_1 \delta(x_2) H(-x_1), \tag{9}$$

where $\delta(x_2)$ is Dirac's delta function and $H(-x_1)$ is the Heaviside step function, they each has the property

$$\delta(x - x_0) = \begin{cases} 0 & (x \neq x_0) \\ +\infty & (x = x_0) \end{cases}, \tag{10}$$

$$H(-x_1) = \begin{cases} 1 & x_1 < 0 \\ 0 & x_1 > 0 \end{cases}. \tag{11}$$

The other components of the eigenstrain ε_{ij}^{d} are zero. In the calculation, the Burgers vector of the dislocation is expressed by the Gaussian function given in the literature [10].

Then the local elastic stress can be given by Hook's law,

$$\sigma_{ij}^{el} = (C_{ijkl}^0 + \Delta C_{ijkl} \Delta c)(\varepsilon_{ij}^{a} + \varepsilon_{ij} - \varepsilon_{ij}^{0} - \varepsilon_{ij}^{d}). \tag{12}$$

By using the relationship of displacement u_i and internal strain ε_{kl},

$$\varepsilon_{kl} = \frac{1}{2} \left\{ \frac{\partial u_k}{\partial x_l} + \frac{\partial u_l}{\partial x_k} \right\}, \tag{13}$$

where u_i is used to denote the ith component of the displacement. The internal strain can be obtained by solving the mechanical equilibrium equation

$$\frac{\partial \sigma_{ij}^{el}}{\partial x_j} = 0. \tag{14}$$