Elastic strain energy induced split during precipitation in alloys

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ABSTRACT

The elastic strain energy induced split during the precipitation of the isostructural transformation in the modeled A—B alloys is simulated by the phase field method. The simulation implies that for the single precipitating particle in the modeded alloy, the particle with initial scale in the range from $80l$ to $320l$ ($l = 12.18$ Å) is to split during aging. For the modeled alloy, the γ' particle is to split at about $5.0 \times 10^3 \tau$ ($\tau = 4.45$ s) after the split incubation period. At the end of split the total interfacial energy obtains a maxima and the total elastic energy holds a minima at about $2.4 \times 10^4 \tau$. The requirement of the four-blocks split may be given by the relationship between the elastic strain energy coefficient, the positive gradient energy coefficient and the solute concentration inhomogeneity. In multi-particles systems, the particles split into other appearances due to the additional interaction energy induced by the non-symmetrical arrangement of the particles, The increment of the interaction elastic energy has little effect on the interfacial energy during precipitation in multi-particles systems.

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1. Introduction

Miyazaki et al. [1], has observed that the precipitating particles of some kinds of alloys, e.g. Ni—Ti, Ni—Al and Ni—Cu—Si, split into clusters of smaller doublet while they are been coarsening. For some other kinds of alloys, e.g. Ni—Si, Ni—Al and Ni—Al—Ti, the precipitating particles even split into octet of cube. These phenomena of precipitating split during coarsening may not be explained by the existent theories, although some theories take the effect of the elastic interaction on the stability of the microstructure and the distribution of the precipitating particles into account [2,3]. Considering the coherent elastic strain energy during the precipitating procedure, the driven force of the phase transformation is not only the relaxation of the interfacial energy but also the relaxation of the total energy, including the elastic strain energy, the interfacial energy and the interaction energy among the particles.

Miyasaki et al. [1,4], implies that the value of interaction energy decreases rapidly along with the increment of the distance between two particles and the decrement of the bulk of the precipitate, and reveals that the value of the interaction energy is the lowest while the volumes of the two particles are identical. In other words, the system of two particles with the some distance and at the same volume may be the most stable. It could be concluded that the split of one particle into two or eight blocks with the same volume has not to overcome the energy barrier. Generalizing the precipitating procedure of the two phases into real alloys, the final disperse distribution of the particles might be obtained and which could be very stable during the successive aging.

In this work, a phase-field model for simulating the split of precipitating particles during aging induced by the misfit elastic strain energy is established, and with which the split phenomenon in the single particle and the multi-particles systems of the modeled A—B alloy is studied.

2. The simulation model

2.1. The kinetic equation

The goal of this work is to simulate the split of precipitating particles in solid transformation of the modeled A—B alloy. The precipitate coarsening kinetics may be given by Cahn—Hilliard

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equation

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

where F is the free energy functional with respect to the solute concentration $c(\boldsymbol{r},t)$ of the system, M is the mobility of atoms.

To accelerate the computation, the modeled A−B alloy with almost the same physical properties as the Ni−Al superalloy but for the distribution of the solute concentration is discussed in this work. It should be noted that for compounds in certain real alloys, e.g. the Ni-based superalloys in which the ordered γ'-Ni$_3$Al(L1$_2$) precipitate separates from the disordered γ-NiAl(fcc) matrix, the structural field parameters $\phi_i(\boldsymbol{r},t)$ may be concerned because of the anti-phase boundary (APB) [5,6].

However, if the APB is ignored for the modeled alloys discussed in this work, and with the assumption that the crystal lattice parameter $a(\boldsymbol{r},t)$ is determined by the distribution of the solute concentration $c(\boldsymbol{r},t)$ in the isostructural transformation, the transition of the crystal structure may be represented by the variation of the solute concentration. So that for the isostructural transformation from fcc-γ to L1$_2$-γ', the redistribution of the concentration during the ordering may reveals the transition of the crystal structures. Fig. 1 is the phase diagram of the modeled alloy where γ-fcc phase is the disordered BA and γ'-L1$_2$ is the ordered B$_3$A. The discussion in the following is applicable for certain real alloys, except for the difference in the phase diagrams. By the way, the temperature effect is hidden in the free energy density function.

Ignoring the structural field parameters, the free energy functional F of the concentration inhomogenous system may be given by

$$F = \int_V \left[f[c(\boldsymbol{r},t)] + \frac{\beta}{2} \left| \nabla c(\boldsymbol{r},t) \right|^2 \right] \mathrm{d}V + E^{el}, \tag{2}$$

where β is the positive gradient energy coefficient corresponding to the solute concentration, E^{el} is the total elastic energy of the system, and $f[c(\boldsymbol{r},t)]$ is the local free energy density with respect to the local concentration.

For convenience in the following discussion, the disordered matrix phase is named as γ, and the precipitate phase which separates out from the matrix is named as γ'. It should be emphasized that the γ and γ' are not the real phases because the split is discussed just theoretically here. The elastic strain energy induced by the misfit between γ and γ' may be obtained from the microstructural elastic theory [7]. There are three contributions to the elastic strain energy, the misfit from various phases, the
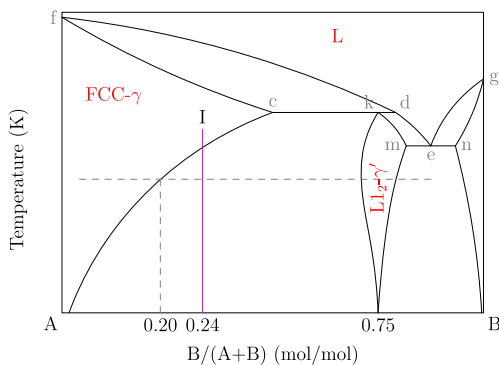

Fig. 1. The phase diagram of the modeled A−B alloy.

inhomogeneity of the elastic constant, and the extra applied strain or stress. With the assumption that the elastic constant $C_{ijkl}(\boldsymbol{r},t)$ are functions of the solute concentration only, the elastic constant may then be expressed by

$$C_{ijkl}(\boldsymbol{r},t) = C^0_{ijkl} + \left[\frac{\partial C_{ijkl}(\boldsymbol{r},t)}{\partial c} \right]_{c=c_0} \Delta c(\boldsymbol{r},t) + \cdots, \tag{3}$$

where C^0_{ijkl} denotes the average elastic constant of the alloy, c_0 is the concentration of the alloy, and $\Delta c(\boldsymbol{r},t) = c(\boldsymbol{r},t) - c_0$ is the inhomogenous part of the local solute concentration. Under the first order approximation, Eq. (3) may be given by

$$C_{ijkl}(\boldsymbol{r},t) = C^0_{ijkl} + \Delta C_{ijkl} \Delta c(\boldsymbol{r},t), \tag{4}$$

where $\Delta C_{ijkl} = (C^p_{ijkl} - C^m_{ijkl})/(c^p - c^m)$. The relationship between the lattice parameter $a(\boldsymbol{r},t)$ and the solute concentration $c(\boldsymbol{r},t)$ is also assumed by

$$a(\boldsymbol{r},t) = a_0 + \left[\frac{\partial a(\boldsymbol{r},t)}{\partial c} \right]_{c=c_0} \Delta c(\boldsymbol{r},t) + \cdots, \tag{5}$$

where a_0 is the crystal lattice parameter of the alloy with the average concentration c_0. With the assumption that the crystal lattice satisfies the Vegard law, Eq. (5) may be simplified as

$$a(\boldsymbol{r},t) = a_0 + \varepsilon^0 a_0 \Delta c(\boldsymbol{r},t), \tag{6}$$

where $\varepsilon^0 = (a^0 - a^0)/a_0(c^p - c^m)$ is the crystal lattice expansion coefficient. Substituting $c(\boldsymbol{r},t)$ by the matrix lattice parameter c^m or the precipitate lattice parameter c^p, Eq. (5) represents the lattice of the matrix or the precipitate respectively. The local stress free strain $\varepsilon^0_{kl}(\boldsymbol{r},t)$, indicating the misfit strain between the matrix and the precipitate, may then be obtained by

$$\varepsilon^0_{ij}(\boldsymbol{r},t) = \frac{a(\boldsymbol{r},t) - a_0}{a_0} = \varepsilon^0 \delta_{ij} \Delta c(\boldsymbol{r},t), \tag{7}$$

in which δ_{ij} is the Kronecker-δ function. The elastic strain may be expressed by

$$\varepsilon^{el}_{ij}(\boldsymbol{r},t) = \varepsilon^a_{ij} + \delta\varepsilon_{ij}(\boldsymbol{r},t) - \varepsilon^0_{ij}(\boldsymbol{r},t), \tag{8}$$

where ε^a_{ij} is the extra applied strain, $\delta\varepsilon_{ij}(\boldsymbol{r},t)$ is the inhomogenous strain which is defined as

$$\delta\varepsilon_{ij} = \frac{1}{2} \left(\frac{\partial u_i}{\partial r_j} + \frac{\partial u_j}{\partial r_i} \right), \tag{9}$$

where $\boldsymbol{u}$ is the local displacement field. By the Hooke law and combined with the mechanical equilibrium condition, the elastic strain energy may be given by Ref. [7].

$$E^{el} = \frac{V}{2} C^0_{ijkl} \varepsilon^a_{ij} \varepsilon^a_{kl} - V\Delta C_{ijkl} \varepsilon^a_{ij} \varepsilon^0_{kl} \overline{(\Delta c)^2} + \frac{1}{2} \int \left[C^0_{ijkl} \varepsilon^0_{ij} \varepsilon^0_{kl} \right.$$
$$\left. - n_i \sigma^*_{ij} \Omega_{kl}(\boldsymbol{n}) \sigma^*_{kl} n_l \right] \left| \Delta c(\boldsymbol{g}) \right|^2 \frac{\mathrm{d}^3 q}{(2\pi)^3}, \tag{10}$$

where $\Delta c(\boldsymbol{g})$ is the Fourier transform of $\Delta c(\boldsymbol{r})$. Under the assumption of no applied strain and homogenous elasticity, which means that $\varepsilon^a_{ij} = 0$ and $\Delta C_{ijkl} = 0$, the total elastic strain energy of the system may then be obtained