



The split of dendritic precipitates with interfacial anisotropy in solid transformations in alloys



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ABSTRACT

The dendritic precipitates may be obtained during isothermal treatment at the MSC temperature for a long time in solid transformations in the modeled alloy. The split of dendrite may occur while the temperature declines successively from the MSC point during quenching. The dendritic morphology is determined by the intensity of the interfacial anisotropy, and the split is related to the competition between the interfacial energy and the misfit strain energy. The doublet and octocube are possible while the dendritic particle is small, but if dendritic particle is large, the octodendrite may be obtained. The split of dendritic particles during aging is induced by the MSC effect which may be expressed by the MSC function which is determined by three parameters, the MSC rate β , the MSC delay t_0 and the initial value of the MSC function α . The phase transformations during isothermal treatment at MSC point are spontaneous and equilibrium processes, however, phase transformations from MSC to the lower temperature during quenching are the spontaneous but non-equilibrium processes.

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1. Introduction

Yoo et al. [1] have discussed the morphology of precipitates in phase transformations without applied stress or applied strain in two kinds of commercial Ni-base alloys by dilatometry. In their work, the morphology evolution of precipitates is related to the heat treatment. The different cooling rates during quenching result in the different morphologies. It may be concluded from Grosdidier's work [2] that the morphology evolution of the γ' particle in Ni-base alloys is correlated to aging temperature. From Liu's work [3], the critical size of precipitates for splitting is at least $40l$ ($l = 1.22$ nm), which implies a problem that how the misfit strain energy behaves while the radius of the particle is less than $40l$. How the particle grows to $40l$ without misfit strain energy is very important.

Kamara et al. [4] discover that the crystal lattice parameters of a certain phase is related to the temperature, and the crystal lattice

parameters of different phases obey different rules. As examples, Kamara et al. have studied four kinds of Ni-base alloys. It implies that the temperature dependent crystal lattice parameters of γ' and γ may intersect at some temperature in some Ni-base alloys. If the temperature dependent crystal lattice parameters of γ' and γ intersect at some point, the misfit strain might be zero at the intersection. The calculations with the molecular dynamics method [5] and the first-principles method [6,7] have confirmed that the misfit strain of some Ni-base alloys may be zero at some temperature. If Ni-base alloys are isothermally treated at the intersection for a long time, the precipitates may grow only controlled by the interfacial energy but not by the misfit strain energy. The intersection of the temperature dependent lattice parameters is called the misfit strain conversion (MSC) temperature. If the MSC point exists, it may be concluded that the misfit strain is zero at MSC temperature, and the misfit strain energy varies successively along with the decline of the aging temperature during quenching.

Because the growth of the precipitates is only controlled by the interfacial energy when the alloy is isothermally treated at the MSC temperature, the precipitates may grow into dendritic morphology. The purpose of this work is to simulate the growth of the dendritic morphology and the split of dendritic particles considering the MSC effect.

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2. The temperature dependent elastic strain energy

2.1. The temperature dependent elastic strain

For the isostructural phase transformation from pseudo f.c.c. (γ) to L1₂ (γ'), the transition of the crystal lattices may be expressed by the redistribution of the concentration during ordering [3,8,9]. 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' . The temperature independent elastic strain energy induced by the misfit between γ and γ' may be obtained from the theory of microstructural elastic field derived by A. G. Khachaturyan [10,11]. There are three contributions to the misfit strain energy, the misfit from different phases, the inhomogeneity of the elastic constant, and the extra applied strain or stress.

The temperature dependent crystal lattice parameter $a(c, T)$, which is related to the solute concentration $c(\mathbf{r}, t)$ and the local temperature $T(\mathbf{r}, t)$, is assumed by

$$da(c, T) = \left[\frac{\partial a(c, T)}{\partial c} \right]_{c_0, T} dc(\mathbf{r}, t) + \left[\frac{\partial a(c, T)}{\partial T} \right]_{c, T_0} dT(\mathbf{r}, t), \quad (1)$$

With the assumption that the crystal lattice parameter of the alloy satisfies the Vegard's law, Eq. (1) is simplified by

$$a(c, T) = a(c_0, T_0) + \varepsilon_0^c(T)a(c_0, T_0)dc + \varepsilon_0^T(c)a(c_0, T_0)dT, \quad (2)$$

where $a(c_0, T_0)$ is the crystal lattice parameter of the alloy with respect to the average concentration c_0 at referential temperature T_0 , $T(\mathbf{r}, t)$ is the temperature of the alloy at position \mathbf{r} , $\Delta c(\mathbf{r}, t) = c(\mathbf{r}, t) - c_0(\mathbf{r}, t)$ is the inhomogeneous part of the local solute concentration,

$$\varepsilon_0^c(T) = \frac{a(c_p, T) - a(c_m, T)}{a(c_m, T)[c_p(T) - c_m(T)]}, \quad (3)$$

is the temperature dependent eigen misfit strain which is induced by the difference of the crystal lattices between the matrix and precipitates at temperature T . In the isostructural phase transformations, the misfit strain is induced by the inhomogeneity of the solute concentration $c(\mathbf{r}, t)$ at temperature T [3]. $\varepsilon_0^T(c)$ is the thermal expansion coefficient due to the variation of the temperature of certain phase which is specified by certain concentration $c(\mathbf{r}, t)$, and it is defined by

$$\varepsilon_0^T(c) = \left(\frac{1}{a} \frac{\partial a}{\partial T} \right)_{T_0}. \quad (4)$$

The local stress free strain $\varepsilon_{ij}^0(c, T)$ between the matrix and the precipitate may then be given by

$$\varepsilon_{ij}^0(c, T) = \varepsilon_{ij}^c(T)\Delta c(\mathbf{r}, t) + \varepsilon_{ij}^T(c)\Delta T(\mathbf{r}, t), \quad (5)$$

where

$$\varepsilon_{ij}^c(T) = \varepsilon_0^c(T)\delta_{ij} \quad \text{and} \quad \varepsilon_{ij}^T(c) = \varepsilon_0^T(c)\delta_{ij}, \quad (6)$$

in which δ_{ij} is the kronecker- δ function. The total elastic strain may be obtained

$$\varepsilon_{ij}^{el}(\mathbf{r}, T) = \bar{\varepsilon}_{ij}^a + \delta\varepsilon_{ij}(\mathbf{r}, T) - \varepsilon_{ij}^0(c, T), \quad (7)$$

where $\bar{\varepsilon}_{ij}^a = \bar{\varepsilon}_{ij} + \varepsilon_{ij}^a$, in which $\bar{\varepsilon}_{ij}$ defined by

$$\int_V \delta\varepsilon_{ij}(\mathbf{r}, T)d^3r = 0 \quad (8)$$

is the homogeneous part of the total strain, ε_{ij}^a the applied strain, and $\delta\varepsilon_{ij}(\mathbf{r}, T)$ the inhomogeneous part of the total strain which is defined by

$$\delta\varepsilon_{ij}(\mathbf{r}, T) = \frac{1}{2} \left[\frac{\partial u_i(\mathbf{r}, T)}{\partial r_j} + \frac{\partial u_j(\mathbf{r}, T)}{\partial r_i} \right], \quad (9)$$

where $\mathbf{u}(\mathbf{r}, T)$ is the local displacement field.

2.2. The temperature dependent elastic constant

With the assumption that the elastic constants $C_{ijkl}(c, T)$ are functions of the solute concentration $c(\mathbf{r}, t)$ and the temperature $T(\mathbf{r}, t)$, the elastic constants may then be given by

$$dC_{ijkl}(c, T) = \left[\frac{\partial C_{ijkl}(c, T)}{\partial c} \right]_{c_0, T} dc + \left[\frac{\partial C_{ijkl}(c, T)}{\partial T} \right]_{c, T_0} dT \quad (10)$$

Under the first order approximation of the inhomogeneity of solute concentration $\Delta c(\mathbf{r}, t)$ and the inhomogeneity of temperature $\Delta T(\mathbf{r}, t)$, Eq. (10) may be given by

$$C_{ijkl}(c, T) = C_{ijkl}(c_0, T_0) + \Delta C_{ijkl}^c(T)\Delta c(\mathbf{r}, t) + \Delta C_{ijkl}^T(c)\Delta T(\mathbf{r}, t) \quad (11)$$

where $C_{ijkl}(c_0, T_0)$ denotes the average elastic constants of the alloy at concentration c_0 and temperature T_0 ,

$$\Delta C_{ijkl}^c(T) = \frac{C_{ijkl}^p(T) - C_{ijkl}^m(T)}{c^p(T) - c^m(T)} \quad (12)$$

is the inhomogeneous part of the elastic constants induced by the local concentration inhomogeneity, and

$$\Delta C_{ijkl}^T(c) = \left[\frac{\partial C_{ijkl}(c, T)}{\partial T} \right]_{c, T_0} \quad (13)$$

is the rate of the elastic constant to the change of the temperature.

2.3. The temperature dependent elastic strain energy

The temperature dependent total elastic energy may be expressed as

$$E^{el}(T) = \frac{1}{2} \int_V C_{ijkl}(c, T)\varepsilon_{ij}^{el}(\mathbf{r}, T)\varepsilon_{kl}^{el}(\mathbf{r}, T)d^3r. \quad (14)$$

With the assumption that the distribution of temperature is homogeneous all over the aging system, the temperature satisfies

$$\frac{\partial T(\mathbf{r}, t)}{\partial r_j} = 0. \quad (15)$$

Substituting Eq. (7) and Eq. (11) into Eq. (14), and considering the homogeneous temperature condition Eq. (15) the total elastic energy E^{el} may be given by Refs. [9,10]

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