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Influence of cooling rate on the formation of bimodal microstructures in nickel-base superalloys during continuous two-step aging

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ABSTRACT

The formation and evolution of bimodal microstructures during the continuous two-step aging in nickel-base single crystal superalloys are simulated through phase-field method. The change of γ′/γ lattice misfit from the first to the secondary aging temperature has been considered in present model. The focus of this study is to explore the influence of cooling rate (after the first aging) on the evolutions of primary and secondary γ′ precipitates. It is demonstrated that the primary γ′ precipitates formed in the first aging become more cubic during the secondary aging. With the cooling rate increasing, the precipitation number and the growth rate of secondary γ′ precipitate are increased during the followed secondary aging. And the size of secondary γ′ precipitate is also the biggest for the case after the high-speed cooling based on the contributions of the greatest chemical driving force and massive coalescences of neighboring secondary γ′ precipitates. Besides, the precipitation of secondary γ′ phase from the γ-channel occurs only when the γ-channel width is greater than a critical value, and in present work, the critical value is about 35 nm, 52.5 nm and 87.5 nm, respectively, for the case after high-speed, medium and low-speed cooling.

1. Introduction

As an important high-temperature structure material, nickel-base single crystal superalloys have excellent high temperature mechanical properties and are widely used as turbine-blade materials in gas turbine of aircraft and power engines [1]. Their excellent mechanical properties are mainly originated from the microstructure which consists of $L1_2$-typed Ni_3Al phase (γ′ precipitate) and face-centered cubic Ni-rich phase (γ matrix). Plenty of experiments have shown that the factors of γ' precipitate, such as shape, size, volume fraction and spatial arrangement, play a critical role in determining the mechanical properties of nickel-base single crystal superalloys during service [1–6]. In particular, the size and volume fraction of different generations of γ' precipitates are influential and therefore have garnered much attention.

It is known that the size and spatial arrangement of γ′ precipitates are strongly affected by the heat treatments [4,7–12]. The treatment procedure generally includes two steps: solution treatment and aging treatment. Bimodal microstructures containing the bigger (primary) and smaller (secondary) γ' precipitates are usually formed during the continuous cooling after the solution treatment. The multiple nucleation occurring at different undercoolings below the γ' solvus should be responsible for this formation of bimodal microstructure [6–8]. For the single crystal superalloys, in general, the aging process is carried out in two steps: the first aging process is to obtain the uniformly dispersed γ' precipitate, and the secondary aging is to adjust the γ' precipitate shape to have a better cubic degree [1]. According to the study of our team, it is known that during the cooling after the first aging, the fine secondary γ' precipitates produce among the γ channels between the primary γ' precipitates when cooling in air [4]. If the sample continuous to aging again at a low temperature, the secondary γ' precipitate will grow up [4]. While for the continuous two-step aging, the secondary γ' precipitates may emerge during the secondary aging but not during the cooling after first aging [11].

In addition, the cooling rate after the solution or aging treatment can affect the precipitation behavior of γ' precipitate. With the increased cooling rate after solution treatment, according to Singh et al. [10], the sizes of primary and secondary γ' precipitates decrease because of the limitations of diffusion time and elements mobility. When the cooling rate is rather fast, a large amount of fine γ' precipitates forms without significant difference in size [8]. Changing the cooling rate after the first aging would also influence the performance of secondary γ' precipitates and this performance is different for different

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alloy systems. In the study of the precipitation of γ' phases during the cooling after first aging worked by Yang [4] and Yu [5], it was shown that the fine secondary γ' phases precipitated in the γ channels during the air cooling while no secondary γ' phases were observed after the furnace cooling. During the secondary aging, the secondary γ' phases generally dissolve and disappear with the aging time increasing. However, there has been relatively little research conducted on the effect of cooling rate on the evolution of multiple generations of γ' precipitate during the continuous two-step aging [11]. While this effect is important to adopt the suit heat treatment to optimize the γ' precipitate, it is therefore necessary to carry out the work in this aspect.

Phase-field method has emerged as a powerful method to simulate the realistic microstructure evolution [13]. For nickel-base single crystal superalloys, the dendrite growth during the directional solidification has been investigated in detail through phase-field method [13–15]. Besides, the growth and coarsening of γ′ precipitate during the aging with or without applied stress [16–18], as well as the rafting of γ′ precipitate during the creep [19–22], have been simulated extensively with this method. In addition, several phase-field simulations have been done to study the formation of multiple generations of γ′ precipitates during continuous cooling [9,10]. The purpose of this paper is to simulate the evolution of bimodal microstructures of γ' precipitates during the continuous two-step aging by the phase-field method. Different cooling rates after the first aging have been set to explore the effect of cooling rate on the formation and evolution of bimodal microstructures. It should be pointed out that in the above mentioned simulations of the multiple γ′ precipitations, the temperature dependent γ′/γ lattice misfit was set as a constant in their modes though the temperature has changed during the cooling. However, it is known that the γ′/γ lattice misfit has significant influence on the γ′ evolution [16]. Thus, the change of γ′/γ lattice misfit from the first aging temperature to secondary aging temperature, as well as the elastic inhomogeneity, has been considered in the present model to make our simulation results more close to the experimental results. In addition, the relationship between secondary γ' precipitate and γ-channel width has been discussed in this paper.

2. Model description

2.1. Phase-field model

The microstructure evolution during the two-step aging is controlled by the phase-field model proposed by Boussinot et al. [11]. A single concentration field $c(\boldsymbol{r}^*,t)$ is used to describe the precipitation and coarsening of γ′ precipitate from γ matrix. The temporal evolution of the field variable is given by the Cahn-Hilliard equation [23]:

$$\frac{\partial c(\boldsymbol{r},t)}{\partial t} = M\nabla^2\frac{\delta F}{\delta c(\boldsymbol{r},t)} + \xi_c(\boldsymbol{r},t) \tag{1}$$

where $\boldsymbol{r}$ and t represent the position coordinates and aging time, respectively. M is the diffusion mobility, F is the total free energy of the system and ξ_c is the fluctuation terms satisfying the fluctuation-dissipation theorem [24]. The total free energy F is the sum of the chemical free energy F_{ch} and elastic energy E_{str} and given by:

$$F = \int_V \left\{ f_{hom}(\boldsymbol{r}) + \frac{\alpha}{2}|\nabla c(\boldsymbol{r},t)|^2 \right\} dV + E_{str} \tag{2}$$

where the integral term represents the chemical free energy. α is the gradient coefficients relied on the γ′/γ interface energy σ:

$$\sigma = \frac{(c_p - c_m)^3\sqrt{\mu\alpha}}{3\sqrt{2}} \tag{3}$$

$f_{hom}(\boldsymbol{r})$ is the homogeneous free energy density and given in a double-well polynomial:

$$f_{hom}(\boldsymbol{r}) = \mu(c(\boldsymbol{r},t) - c_m(T))^2(c(\boldsymbol{r},t) - c_p(T))^2 \tag{4}$$

where T is the Kelvin temperature, c_m and c_p are the equilibrium concentrations of γ and γ' phases, respectively. The Al concentration of γ' precipitates depends on the temperature weakly and thus is assumed constant: $c_p = 0.25$. While the Al concentration of γ matrix is strongly temperature-dependent and is therefore assumed as the function of Kelvin temperature, i.e.

$$c_m = 1.5 \times 10^{-4}T - 0.05095 \tag{5}$$

μ is the free energy scale of the system and defined as:

$$\mu = \frac{kT}{2V_a c_m(T)(1 - c_m(T))(c_p(T) - c_m(T))^2} \tag{6}$$

where k is the Boltzmann constant, V_a is the volume of Al atomic.

The mobility coefficient M is related to the diffusion coefficient of Al atom in γ matrix D by:

$$M = \frac{D}{2\mu(c_p(T) - c_m(T))^2} \tag{7}$$

$$D = D_0\exp(-\Delta U/kT) \tag{8}$$

where $D_0 = 1.45 \times 10^{-4}\,\mathrm{m^2 s^{-1}}$ and $\Delta U = 2.8\,\mathrm{eV}$.

The contribution of elastic energy to the morphological evolution of γ' and γ phases is described by the micro-elasticity theory [25]. For the elastically inhomogeneous system of γ'/γ phases with different elastic moduli, the elastic energy F_{el} is calculated by the following equation:

$$F_{el} = \frac{1}{2}\int_V \lambda_{ijkl}(\boldsymbol{r})\varepsilon_{ij}^{el}(\boldsymbol{r})\varepsilon_{kl}^{el}(\boldsymbol{r})dV \tag{9}$$

where $\lambda_{ijkl}(\boldsymbol{r})$ is the local elastic modulus tensor, $\varepsilon_{ij}^{el}(\boldsymbol{r})$ is the elastic strain. Assumed that $\lambda_{ijkl}(\boldsymbol{r})$ is the function of local concentration, then it can be written as:

$$\lambda_{ijkl}(\boldsymbol{r}) = \overline{\lambda}_{ijkl} + \Delta\lambda_{ijkl}\Delta c(\boldsymbol{r}) \tag{10}$$

where $\overline{\lambda}_{ijkl} = \lambda_{ijkl}^{p}\overline{c(\boldsymbol{r})} + \lambda_{ijkl}^{m}(1 - \overline{c(\boldsymbol{r})})$ is the average elastic modulus, $\Delta\lambda_{ijkl} = \lambda_{ijkl}^{p} - \lambda_{ijkl}^{m}$ is the difference between elastic moduli of γ' (λ_{ijkl}^{p}) and γ (λ_{ijkl}^{m}), and $\Delta c(\boldsymbol{r}) = c(\boldsymbol{r}) - \overline{c(\boldsymbol{r})}$.

For the system without plastic deformation, the total strain $\varepsilon_{ij}(\boldsymbol{r})$ is the sum of elastic strain $\varepsilon_{ij}^{el}(\boldsymbol{r})$ and stress-free transform strain $\varepsilon_{ij}^{o}(\boldsymbol{r})$ introduced by the coherent phase transformation of γ → γ′, thus the elastic strain can be written as:

$$\varepsilon_{ij}^{el}(\boldsymbol{r}) = \varepsilon_{ij}(\boldsymbol{r}) - \varepsilon_{ij}^{o}(\boldsymbol{r}) \tag{11}$$

where $\varepsilon_{ij}^{o}(\boldsymbol{r})$ is associated with the γ'/γ lattice misfit δ by $\varepsilon_{ij}^{o}(\boldsymbol{r}) = \delta\Delta c\delta_{ij}/(c_p - c_m)$.

The lattice misfit, δ, is defined according to

$$\delta = 2 \times \left[\frac{a_{\gamma'} - a_\gamma}{a_{\gamma'} + a_\gamma} \right] \tag{12}$$

where $a\gamma'$ and $a\gamma$ are the lattice parameter of γ' and γ phases, respectively, and the values of them depend on the elemental compositions in each phases. According to the Ref. [1], the lattice parameter of γ phase is approximated through:

$$a_\gamma = 3.524 + 0.110x_{\mathrm{Cr}}^{\gamma} + 0.478x_{\mathrm{Mo}}^{\gamma} + 0.444x_{\mathrm{W}}^{\gamma} + 0.441x_{\mathrm{Re}}^{\gamma} + 0.179x_{\mathrm{Al}}^{\gamma} + 0.422x_{\mathrm{Ti}}^{\gamma} + 0.700x_{\mathrm{Ta}}^{\gamma}\,\text{Å} \tag{13}$$

and the lattice parameter of γ' precipitate is approximated through:

$$a_{\gamma'} = 3.570 - 0.004x_{\mathrm{Cr}}^{\gamma'} + 0.208x_{\mathrm{Mo}}^{\gamma'} + 0.194x_{\mathrm{W}}^{\gamma'} + 0.262x_{\mathrm{Re}}^{\gamma'} + 0.258x_{\mathrm{Ti}}^{\gamma'} + 0.500x_{\mathrm{Ta}}^{\gamma'}\,\text{Å} \tag{14}$$

With the fall of aging temperature, the elemental compositions of γ' and γ phases vary so that the lattice parameter of each phases alters. Then used the Eq. (12), the change of γ'/γ lattice misfit could be calculated. Therefore, the relationship between γ'/γ lattice misfit and temperature is established. Taking the Ni-Al model alloy for example, with the temperature increasing, the γ'/γ lattice misfit is decreased, in