Phase field simulation of the collapse of the rafted structure in Ni-based superalloys

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Abstract. Microstructural evolution in single crystal Ni-based superalloys is investigated by the phase field simulation. During creep, the morphology of the γ' phase changed from the cuboidal shape to the rafted one, and the rafted structure was collapsed in the late stage of creep. The simulation on the microstructural evolution is based on thermodynamic information, diffusion equation, elastic anisotropy and a homogeneous lattice misfit. It is found that caused by external stress result in the morphological change of the γ' phase to the rafted structure, and this rafted structure is collapsed by inhomogeneous lattice misfit. These morphological changes can be explained by the change in stable morphology of the γ' phase.

Introduction

Single crystal (SC) Ni-based superalloys have superior resistance to high temperature and are used for turbin blades in gas turbins, aircraft engines, etc. Microstructures of these alloys consist of the γ and γ' phases. The creep property of the SC alloys is related closely to their microstructural stability depending on atomic diffusion. The cuboidal γ' phase precipitated in the γ matrix coarsenes and arranges along the <100> crystallographic directions during aging. In the early stage of creep, the γ' phase becomes plate shape being normal to the stress direction so-called rafted structure. In the late stage of creep in a practical SC Ni-based supperalloy, CMSX-4, the rafted structure is found to collapse [1], but the mechanism is not clean. Since the creep strength of the superalloys originates from the stability of the rafted structure [2], it is important to reveal the phenomenon in the morphological evolution.

Recently, the phase field method has been applied for simulating microstructural evolution in SC Ni-based superalloys [3-8]. The phase field approach describes spatial and temporal evolution of the field by solving the evolution equations. The microstructural evolution can be simulated under the condition of reducing the total free energy of the system, which includes chemical free energy, interfacial energy and elastic strain energy. The purpose of this study is to make clean the main factors in the collapse of the rafted structure in SC Ni-based superalloys, by using a series of phase field simulations.

Calculation method

In the phase field model of Ni-based superalloys consisting of the γ and γ' phases, we estimate the total free energy by the following equation,

$$G_{sys} = \int_{\mathbf{r}} \left[G_{chem}(f, \phi_i) + E_{grad}(\phi_i) + E_{str}(\phi_i) \right] d\mathbf{r}, \tag{1}$$

where G_{sys} is the total free energy of the system, G_{chem} is the chemical free energy, E_{grad} is the gradient energy and E_{str} is the elastic strain energy. In this model, the volume fraction of the γ' phase, f ($\mathbf{r}$, t), and four long-range order parameters, ϕ_i ($\mathbf{r}$, t) (i=1,2,3,4) [4], which are used to describe the four types of order domains of the γ' phase, are adopted as field variables. f ($\mathbf{r}$, t)=0 means the γ phase and f ($\mathbf{r}$, t)=1 means the γ' phase. The chemical free energy density is expressed as

$$G_{chem} = G^{\gamma}_{chem}(f_m, T)\{1 - h(\phi_i)\} + G^{\gamma'}_{chem}(f_p, T) h(\phi_i) + W_{12} g(\phi_i), \tag{2}$$

where W_{12} is the double-well potential height [7][8]. The function $h(\phi_i)$ and $g(\phi_i)$ are defined as [8]

$$h(\phi_i) = \sum_{i=1}^{4} \left[\phi_i^3 (10 - 15\phi_i + 6\phi_i^2 \right], \tag{3}$$

$$g(\phi_i) = \sum_{i=1}^{4} \left[\phi_i^2 (1 - \phi_i)^2 \right] + \theta \sum_{i=1}^{4} \sum_{j \neq i}^{4} \phi_i^2 \phi_j^2 . \tag{4}$$

These functions are introduced to distinguish the two-phase. The parameter θ expresses the antiphase boundary. In Eq.(2), G^{γ}_{chem} and $G^{\gamma'}_{chem}$ are the chemical free energy of the γ matrix and the γ' precipitate, and are approximated using parabolic functions

$$G^{\gamma}_{chem} = \frac{1}{2} W_1 f^2, \tag{5}$$

$$G^{\gamma'}_{chem} = \frac{1}{2} W_2 (1 - f)^2, \tag{6}$$

where W_1 and W_2 are the coefficients determined by the Gibbs energy calculation based on the sub-lattice model using the thermodynamic database. In the KKS model [9], the interface region is regarded as a mixture of the γ and γ' phases with different volume fractions of the γ' phase. The volume function f is expressed as

$$f = f^{\gamma}\{1 - h(\phi_i)\} + f^{\gamma'} h(\phi_i), \tag{7}$$

where f^{γ} and $f^{\gamma'}$ are the volume functions of the γ and γ' phases, respectively, which constitute the local interface. The gradient energy is estimated from the artificial order parameters as

$$E_{grad} = \frac{1}{2} \kappa_{\phi} \sum_{i=1}^{4} (\nabla \phi_i)^2, \tag{8}$$

where κ_{ϕ} is the gradient energy coefficient of the order parameter[10]. The parameter, W_{12}, in Eq.(2) and κ_{ϕ} in Eq.(8) are related to both the interfacial energy density, γ_s, and the interface width, 2λ, as[9]

$$\gamma_s = \frac{\sqrt{W_{12} \kappa_{\phi}}}{3\sqrt{2}}, \tag{9}$$

$$2\lambda = \alpha\sqrt{\frac{2\kappa_\phi}{W_{12}}}, \tag{10}$$

where α is a constant which depends on the definition of the interface thickness. The elastic strain energy based on Khachaturyan's microelasticity theory [11] is calculated as

$$E_{str} = \frac{1}{2}C_{ijkl}(\mathbf{r})\left\{\bar{\varepsilon}_{ij} + \delta\varepsilon_{ij}^{c}(\mathbf{r}) - \varepsilon_{ij}^{0}(\mathbf{r})\right\}\left\{\bar{\varepsilon}_{kl} + \delta\varepsilon_{kl}^{c}(\mathbf{r}) - \varepsilon_{kl}^{0}(\mathbf{r})\right\} - \sigma_{ij}^{A}\bar{\varepsilon}_{ij}, \tag{11}$$

where σ_{ij}^{A} and $\bar{\varepsilon}_{ij}$ represent the external stress and the macroscopic strain, respectively. The heterogeneous strain, $\delta\varepsilon_{kl}(\mathbf{r})$, is expressed by usual elasticity relation as

$$\delta\varepsilon_{kl}(r) = \frac{1}{2}\left\{\frac{\partial u_k(\mathbf{r})}{\partial r_l} + \frac{\partial u_l(\mathbf{r})}{\partial r_k}\right\}, \tag{12}$$

where $u_i(\mathbf{r})$ represents the ith displacement component. The eigenstrain is expressed as

$$\varepsilon_{ij}^{0}(r,t) = \varepsilon^{00}\delta_{ij}h(\phi) + \varepsilon_{ij}^{p}, \tag{13}$$

where δ_{ij} is the Kronecher delta function and ε^{00} is the lattice misfit as

$$\varepsilon^{00} = \frac{a_{\gamma'} - a_{\gamma}}{a_{\gamma}}, \tag{14}$$

where $a_{\gamma'}$ and a_{γ} are the lattice parameters of the γ and γ' phase. In Eq.(13), ε^{p}_{ij} represents the plastic strain introduced in the simulation of creep condition. Because the elastic strain energy is considered using the inhomogeneity in elastic constant, an iterative calculation is used for solving the equation [5]. The microstructural evolution can be expressed by calculation under the condition of reducing the total free energy of the system in Eq.(1). Actually, the temporal evolution of the field, the volume fraction and the order parameter, are given by solving the Cahn-Hilliard and Allen-Cahn equations,

$$\frac{\partial f(\mathbf{r},t)}{\partial t} = M\nabla^2\frac{\delta G_{sys}}{\delta f(\mathbf{r},t)}, \tag{15}$$

$$\frac{\partial \phi_i(\mathbf{r},t)}{\partial t} = -L\frac{\delta G_{sys}}{\delta \phi_i(\mathbf{r},t)}, \tag{16}$$

where M is the diffusion mobility and L is the structural relaxation coefficient.

Results and Discussion

2D phase field simulation at 1273K was performed by solving Eqs.(15) and (16) numerically using the conventional difference method under the periodic boundary conditions. The coefficients in the chemical free energy given by Eqs.(5) and (6) are determined as $W_1 = 1.75\times10^3$ J·mol^{-1} and $W_2 = 2.05\times10^3$ J·mol^{-1} on the basis of the Gibbs energy calculation using the thermodynamic database [12]. By fitting to the interfacial energy density, γ_s=14.2 mJ·m^{-2}, in Ni-Al binary alloys [13], the double-well potential height and the gradient energy coefficient are set to be W_{12} and κ_ϕ. Elastic constants of the CMSX-4 alloy at 1273K is used according to the value in [14]. The volume fraction of the γ' phase is

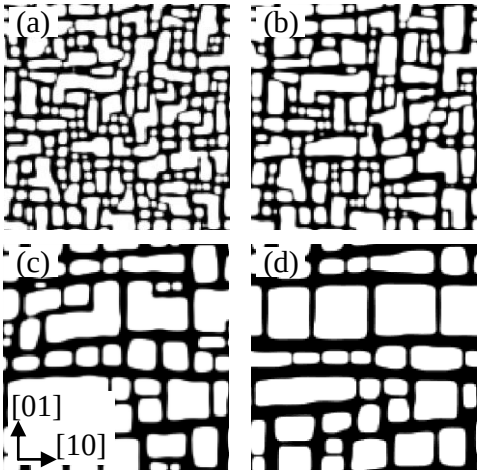

Fig.1 The temporal evolution of the γ' phase at 1273K. (*a*)*t*=50000, (*b*)*t*=100000, (*c*)*t*=500000 and (*d*) *t*=3000000.

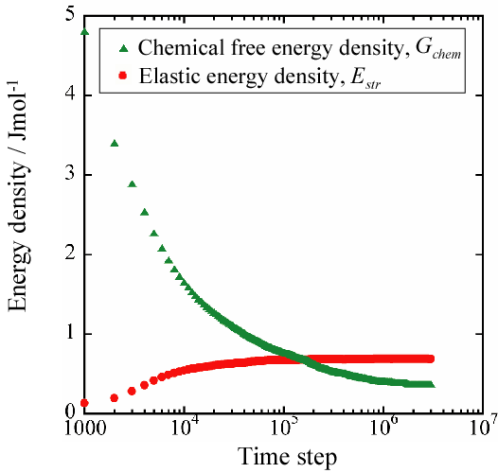

Fig.2 The variation of the chemical free energy and elastic strain energy during coarsening simulation as function of time step.

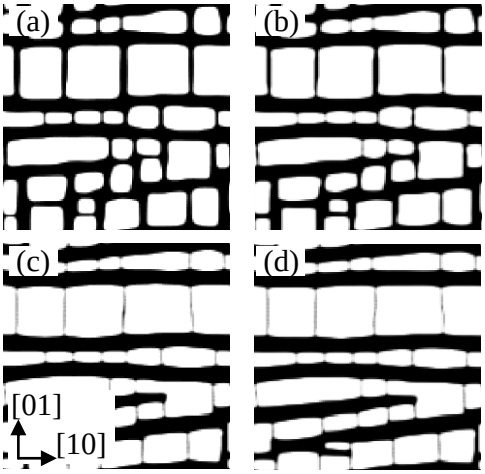

Fig.3 The temporal evolution of the γ' phase at 1273K under 160MPa tension along [01]. (*a*) *t*=3000000, (*b*) *t*=3020000, (*c*) *t*=3080000 and (*d*)*t*=3140000.

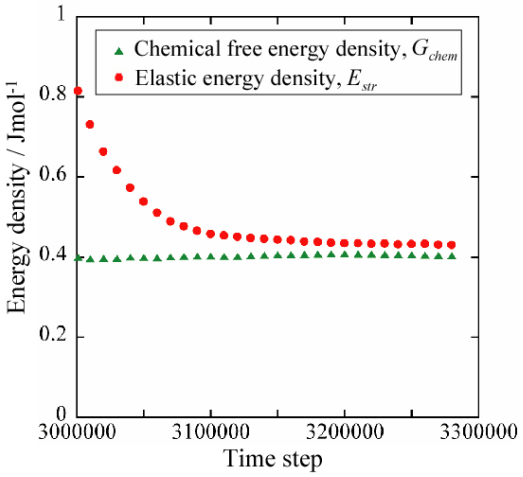

Fig.4 The variation of the chemical free energy and elastic strain energy during rafting simulation as function of time step.

set to be 60% and the lattice misfit is ε^{00}= -0.003. First simulation is started from the supersaturated solid solution with a random noise of the field variables (f,ϕ_l). Fig.1 shows the result showing the coarsening of the γ' phase. The γ' phase is expressed as white area and the γ phase is black area in Fig.1. It is found that the γ' phase change to cuboidal shape and arranges along <10> crystallographic direction of the γ matrix with simulation time. This variation is due to elastic anisotropy. Fig.2 shows the variation of elastic strain energy and chemical free energy with simulation time. It is also found that the chemical free energy is severely reduced during the coarsening of the γ' phase. Secondly, creep condition is simulated by introducing external tensile stress of 160MPa along [01] direction to the microstructure of Fig.1 (d). Assuming that only the γ matrix is uniformly deformed, the plastic strain is calculated as

$$\varepsilon_{ij}^{p} = \begin{pmatrix} \varepsilon_p & 0 \\ 0 & -2\varepsilon_p \end{pmatrix}, \tag{17}$$

where ε_p represents the plastic strain of the matrix and the value, ε_p=0.0075, is obtained as average value of the plastic strain generated by the channel dislocation [13]. Fig.3 shows the result of the

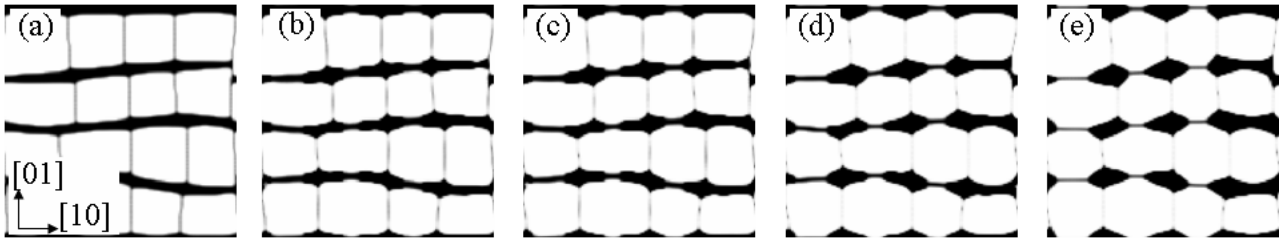

Fig.5 Simulation of the collapse of the rafted structure at 1273K under 160MPa tension along [01]. (*a*) *t*=0, (*b*) *t*=50000, (*c*) *t*=100000, (*d*) *t*=200000 and (*e*) *t*=500000. All time expressed here are dimensionless time steps.

simulation under the creep condition.It is observed that the cuboidal γ' phase coarsens toward the direction normal to the external stress, that is, the rafted structure is formed. This morphological evolution relieves the elastic strain energy accumulated by the anisotropy of the plastic strain. Fig.4 shows the variation of elastic strain energy and chemical free energy during creep simulation. The chemical free energy scarcely changes, meanwhile, the elastic strain energy decreases with rafting. In addition, the simulation of the collapse process of the rafted structure is carried out by changing the lattice misfit from ε^{00}=-0.003 to ε^{00}=-0.001 locally at arbitrary place. Fig.5 (a) shows the initial microstructure constructed by image analysis of a SEM micrograph taken from SC Ni-based superalloy with the rafted structure. The volume fraction of the γ' phase is set to be 70%. As shown in Fig.5 (b)-(d), it is found that the γ' phase coarsens toward not only the rafting direction ([10]) but also locally the direction parallel to the applied stress ([01]) direction. As a result, the γ phase is isolated, which is consistent with the morphological change observed in CMSX-4. This fact indicates that the change in lattice misfit is related to the change in the γ/γ' coherency. Thus, ε^{00}=-0.001 corresponds to the semicoherent interface which relax elastic strain energy. On the other hand, the region where the γ' phase coarsened toward [01] direction is the coherent interface with ε^{00}=-0.003. Therefore, in this simulation on the late stage of creep, it can be said that the morphology of Ni-based superalloys changes due to the decrease of the elastic strain energy caused by inhomogeneous lattice misfit, resulting in a collapse of the rafted structure.

Summary

Phase field simulations of Ni-based superalloys carried out so as to investigate the microstructure variation from the coarsening of the γ' precipitate to the collapse of the rafted structure. In the simulation for aging heat treatment, the morphology of the γ' phase coarsens and changes to cuboidal structure. It is found from the simulation under creep condition that the rafted structure is formed by homogeneous plastic strain in the γ phase for relieving the elastic strain energy. Furthermore, it is found that the inhomogeneous lattice misfit produces the local coarsening toward [01] direction of the γ' phase resulting in the collapse of the rafted structure.

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