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Study of γ' rafting under different stress states – A phase-field simulation considering viscoplasticity

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ABSTRACT

The γ'/γ evolution in nickel superalloys under different stress states and stress values at 1223 K was simulated through the phase-field method to study the 45°-type rafting mechanism and the influence of orientation deviation on the γ'/γ evolution. The simulation results demonstrate that for the shear stress case, 45°-type rafting appears under the external shear stress of 137 MPa. In 45°-type rafting, the equivalent stress inhomogeneity in the γ channel induces a directional diffusion of γ'-forming elements into the low-equivalent-stress areas which are distributed along the diagonal directions. Based on the simulations, a model for the 45°-type rafting mechanism has been proposed. In addition, the influence of orientation deviation on γ'/γ evolution originates from the introduction of shear stress components. With increasing external stress, the shear stress component is increased, which causes the rafting direction to approach the 45° direction. Furthermore, the existence of orientation deviation accelerates the process of γ' rafting.

1. Introduction

Nickel-based single-crystal superalloys are among the most important high-temperature structural materials for manufacturing turbine blades used in both aeronautical and stationary gas turbines; single-crystal blades with the [001] crystallographic orientation ([001] single-crystal blades) are of particular importance [1]. During the service of the turbine engine, [001] single-crystal blades are subjected to combinations of high temperatures and stresses, mainly uniaxial tension produced by centrifugal force. Under such conditions, the initial cubic γ' precipitates tend to coarsen directionally in the phenomenon known as γ' rafting, which profoundly affects the mechanical performance of the superalloys [2–4]. Therefore, extensive efforts have been devoted to studying γ' rafting under tension or compression, by means of experiments [5–9], theoretical studies [10,11] and numerical simulations [12–19].

However, during service, the [001] single-crystal blade endures not only uniaxial tension but also biaxial stress produced by thermal gradients in cooled regions, flowing gas on the blade and local stress concentration [20]. Therefore, multiple states of stress, such as tension, compression, and shear, are applied to the single-crystal blades. In engineering applications, the [001] crystal orientation of the [001] single-crystal blade is not strictly aligned to the axis of the casting, but usually deviates within an angle of 15° (i.e. $\theta < 15°$) [1]. This angle is generally called the orientation deviation angle and is shown in Fig. 1a. When the uniaxial tension σ_Z is applied along the axis of a single-crystal blade, it can be decomposed into two components with the $\langle 001 \rangle$ directions regarded as Cartesian axes (i.e. a $Y'OZ'$ coordinate system): a normal stress component along the [001] orientation (i.e. $\sigma_{Z'}$) and a shear stress component within the (001) plane (i.e. $\sigma_{Z'Y'}$), as shown in Fig. 1b. Therefore, during service, both tensile and shear stresses are applied on the [001] single-crystal blades because of orientation deviation. Thus, the effect of shear stress on single-crystal blades during service should also be investigated.

As mentioned above, much work has dedicated to the studies of

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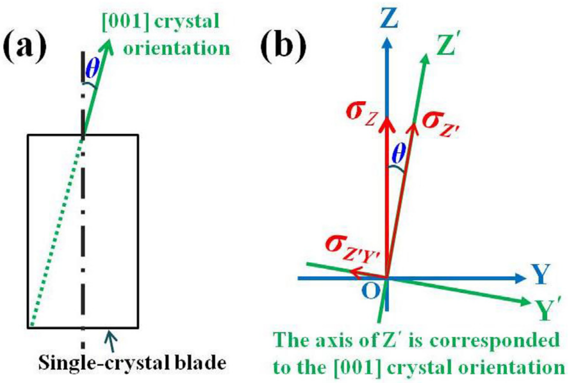

Fig. 1. Schematics of (a) orientation deviation and (b) force analyze of a [001] single-crystal blade when applied with uniaxial tension σ_Z. θ is the orientation deviation angle.

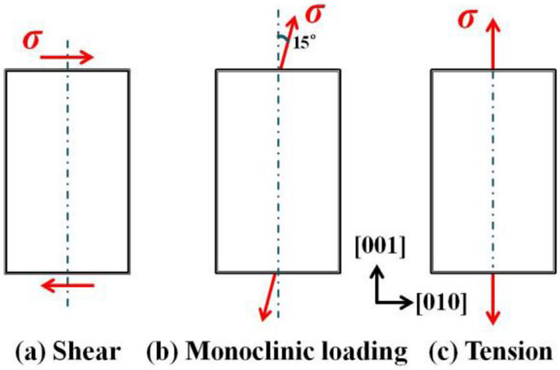

Fig. 2. Schematics of stress loadings on the [001] single-crystal sample. The [001] crystal orientation is parallel to the axis of sample.

γ' rafting during tensile or compressive creep tests, while the influence of shear stress on γ' rafting characteristics has been infrequently reported. Based on a double shear creep test technique [21], Kamaraj et al. [20] observed that γ' rafting occurred at an angle of 45° relative to the direction of shear stress in the CMSX–6 superalloy. In the present study, this rafting is called 45°-type rafting. Furthermore, Touratier et al. [22] found that 45°-type rafting appeared at very high cumulated strain values. In addition, it has been reported that after high-temperature creep deformation, the γ' precipitates in the necked zone generally raft along the direction reoriented 45° (or less) away from the tensile axis [22,23]. It is well known that both tensile and shear stresses appear in the necked zone. The mechanism controlling such 45°-type rafting has not yet been clearly elucidated, thus it requires further studies.

With the development of computational simulations, the phase-field method (PFM) has emerged as a powerful tool to simulate phase transformations and to explore the mechanism of microstructural evolutions [13–17,19,24,25]. By coupling the plastic strain field with the phase-field model [13,14,17,19,25], the γ-channel plasticity during high-temperature creep can be considered in simulation. The 45°-type γ' rafting is accompanied by a high plastic strain accumulation. Thus, the coupled phase-field model enables the simulation of γ'/γ evolution under shear conditions.

In this study, we use a coupled phase-field model [25] proposed earlier to simulate the γ'/γ evolution during creep. Three kinds of stress states, i.e., shear, monoclinic loading, and tension, are applied to the [001] single-crystal sample. Here, the [001] crystal orientation is strictly aligned to the axis of the [001] single-crystal sample. The schematic of the loading on the sample is shown in Fig. 2. The shear stress is applied within the plane normal to the [001] direction, the monoclinic loading is applied along the direction 15° away from the [001] direction, and the tensile stress is applied along the [001] direction. The monoclinic loading of the strict [001] single-crystal sample is equivalent to the tension applied to the [001] single-crystal sample with an orientation deviation angle of 15°. The simulation results for the tension case are used for comparison with the monoclinic loading case. The aim of the present study is to investigate 45°-type rafting mechanism and the influence of orientation deviation on γ'/γ evolution.

2. Model description

2.1. Ginzburg–Landau free energy

A set of field variables is used to describe the microstructural evolution in the PFM. The concentration field $c(\mathbf{r})$ describes the morphologies of the γ' and γ phases and the three long-range ordered (LRO) parameter fields $\eta_i(\mathbf{r})$ $(i = 1,2,3)$ describe the ordering of the γ' phase [26]. Four ordered γ' precipitates are characterized by the following LRO parameters: $(\eta_1,\eta_2,\eta_3) = (1,1,1)\eta_o$, $(\bar{1},\bar{1},1)\eta_o$, $(\bar{1},1,\bar{1})\eta_o$, $(1,\bar{1},\bar{1})\eta_o$.

It is known that microstructural evolution is driven by the decrease of total energy. The total free energy F of γ'/γ evolution during creep consists of the non-equilibrium free chemical energy F_{ch}, elastic energy F_{el} and plastic energy F_{pl} and can be expressed as a function of all field variables. As usual, F_{ch} can be approximated by a standard Ginzburg–Landau function [13,26]:

$$F_{ch} = \int_V \left[f(c,\eta_i) + \frac{\alpha}{2}|\nabla c|^2 + \frac{\beta}{2}\sum_{i=1}^{3}|\nabla \eta_i|^2 \right] dV \tag{1}$$

where V is the volume of studied system, $f(c,\eta_i)$ is the local free energy density of a homogeneous system, and α and β are the constant gradient coefficients, implying an isotropic interfacial energy. $f(c,\eta_i)$ is presented in a Landau polynomial form:

$$\begin{aligned} f(c,\eta_i) = \Delta f \Bigg[& \frac{1}{2}(c - c_m)^2 + \frac{B}{6}(c_2 - c)\sum_{i=1}^{3}\eta_i^2 - \frac{C}{3}\eta_1\eta_2\eta_3 \\ & + \frac{D}{12}\sum_{i=1}^{3}\eta_i^4 \Bigg] \end{aligned} \tag{2}$$

where c_m and c_p are the equilibrium concentrations of the γ matrix and γ' precipitate, respectively, and c_2 is an arbitrary constant chosen between c_m and c_p; here, $c_2 = 0.18$. B, C, and D are constants related to c_2, c_m, c_p and the equilibrium LRO parameter η_o through [13]:

$$\begin{aligned} B &= 2(c_p - c_m)\big/\eta_0^2 \\ C &= 6(c_p - c_m)(c_2 - c_m)\big/\eta_0^3 \\ D &= 2(c_p - c_m)(c_p + 2c_2 - 3c_m)\big/\eta_0^4 \end{aligned} \tag{3}$$

2.2. Elastic energy

The contribution of elastic energy to the γ'/γ evolution is described by micro-elasticity theory [27]. For an elastically inhomogeneous system, the elastic energy F_{el} is calculated using the general equation [12]: