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Elastic instability condition of the raft structure during creep deformation in nickel-base superalloys

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Abstract

A condition for destabilizing the raft structure has been deduced from elastic energy calculations with the concept of "effective eigenstrain", where the effect of creep deformation is included in addition to the lattice mismatch. The calculations indicate that the 001 raft structure is stabilized by a small amount of creep deformation but becomes unstable when the creep strain in the γ phase exceeds the magnitude required to fully relax the lattice mismatch. The excess creep strain is required to produce an internal elastic field that suppresses further creep deformation, and has to be introduced in the primary creep stage. Via the instability of the 001 raft structure, the raft structure gradually turns into a wavy one in the second creep stage before its collapse.

Keywords: Nickel alloys; Dynamic phenomena; Continuum mechanics

1. Introduction

Nickel-base single-crystal superalloys, which are currently used in turbine blades of aero engines or gas turbines, are key materials in modern high-temperature engineering. These alloys are hardened by cuboidal $L1_2$-ordered γ' precipitates which are coherently formed in the face-centered cubic (fcc) disordered γ matrix and form a simple cubic array with its axes parallel to the axes of the underlying cubic crystal structures. When superalloys are subjected to a creep test at high-temperatures under a relatively low tensile stress along the [001] direction, γ' cuboids are coarsened normal to the stress direction to form the "raft structure" (the raft structure in this case is termed "normal raft" or "001 raft"). The excellent creep strength of superalloys originates from the microstructure containing such a raft structure in which the lateral γ/γ' interfaces block the dislocation motion [1–3]. If the raft structure remains, the creep rate is small. At the later stage of creep deformation, however, the raft structure unfortunately collapses (pinching-off of the γ phase), accompanied by the acceleration of creep deformation (see Fig. 1). Hence, understanding the mechanisms behind the collapse of the raft structure is important for further extension of the lifetime of newly developed superalloys. Although the formation mechanism has extensively been discussed [4–14], the collapse mechanism is still a thoroughly open question. According to Fig. 1, the interfaces of γ/γ' lamellae tilt and/or wave from the initial plane of (001) precursory of its collapsing as reported by Epishin et al. [15]. This implies to us that origin of the local tilting of γ/γ' interfaces is an important factor in understanding the collapse mechanism. In this report, the instability condition of the 001 raft structure that leads the structure to collapse is deduced from elastic energy calculations with valiations of the crystallographic direction of the γ/γ' interface of the raft structure. In the calculations, we introduce the concept of "effective eigenstrain" where the effect of creep deformation is included in addition to the lattice mismatch.

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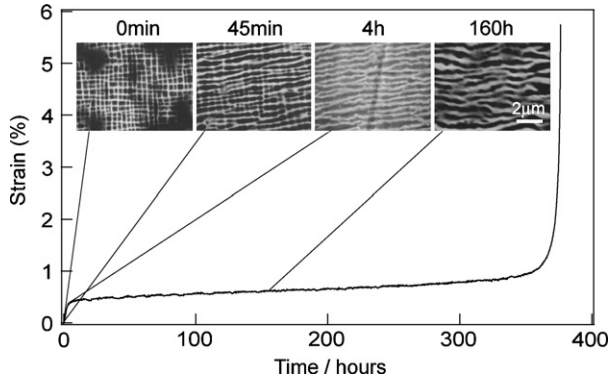

Fig. 1. Typical creep curve of nickel-base superalloy. The alloy is TMS-26 and the condition of creep deformation is tensile stress of 137 MPa at 1373 K. Inset SEM micrographs show the microstructural change through creep deformation.

2. Method of the calculation

Microstructural evolution and stability of the microstructure are governed by the total free energy. The total mechanical energy, i.e. Gibbs' free energy of the system, U, is expressed as

$$U = U_{\text{int}} + U_{\text{ext}} + U_{\text{pot}} \tag{1}$$

where U_{int}, U_{ext} and U_{pot} are the internal elastic energy, elastic energy caused by an application of an external stress, and the potential energy of an external stress, respectively. We assume the elastic constants of the γ and γ' phases are equal to each other in the following calculations. On the assumption, only U_{int} is affected by the morphology of the microstructure. From experimental results and theoretical calculations [13,16,17], creep dislocations in modern superalloys move only in the γ channels spreading perpendicular to the applied stress and cannot pass through the γ channels parallel to the applied stress or γ' precipitates under a typical tensile creep condition, for example, at 1373 K under 137 MPa. Furthermore, creep dislocations are almost homogeneously induced in the lateral γ channels [18,19]. As a consequence, only (or mainly) the γ phase is plastically deformed homogeneously by the movement of creep dislocations. With this knowledge, the "effective eigenstrain" of the γ phase with respect to the γ' phase is expressed by the summation of the lattice constant mismatch between the γ and γ' phases, ε_0, and the plastic strain by creep deformation of the γ phase, ε_{p}. The former is defined as $\varepsilon_0 = (a_\gamma - a_{\gamma'})/a_\gamma$, where a denotes the lattice parameter. If we inpose the restriction on the tensile stress direction to be exact [0 0 1], all eight of $\langle 1\,0\,1\rangle\{1\,1\,1\}$ slip systems are expected to operate equivalently; the plastic deformation can be treated as a simple tetragonal distortion. The effective eigenstrain in a matrix form is expressed as

$$\varepsilon^*_{\text{eff}} = \begin{pmatrix} \varepsilon_0 - \frac{a_\gamma}{a_{\gamma'}}\frac{\varepsilon_{\text{p}}}{2} & 0 & 0 \\ 0 & \varepsilon_0 - \frac{a_\gamma}{a_{\gamma'}}\frac{\varepsilon_{\text{p}}}{2} & 0 \\ 0 & 0 & \varepsilon_0 + \frac{a_\gamma}{a_{\gamma'}}\varepsilon_{\text{p}} \end{pmatrix} \tag{2}$$

where the value of the factor $a_\gamma/a_{\gamma'}$ is very close to unity, and the factor can be negligible. By using this effective eigenstrain, one can estimate the variation of the internal stress/strain fields and the internal elastic energy with creep deformation.

The calculation of the internal elastic energy due to internal elastic-strain fields, U_{int}, has been carried out by means of the Fourier-transformation method proposed by Khachaturyan [20]. The elastic-strain at a position $\boldsymbol{r}$, $\varepsilon(\boldsymbol{r})$, is calculated as

$$\varepsilon_{mn}(\mathbf{r}) = \frac{1}{2}\int_{-\infty}^{\infty} \left\{ C_{ijkl}\bar{\xi}_1 (G^{-1}_{im}\bar{\xi}_n + G^{-1}_{in}\bar{\xi}_m)\hat{\varepsilon}^*_{kl}(\xi) - \hat{\varepsilon}^*_{mn}(\xi) \right\} \times \exp(\mathrm{i}\xi\cdot\mathbf{r})\mathrm{d}\xi \tag{3}$$

where C_{ijkl} is elastic stiffness constants,$\hat{\varepsilon}^*_{kl}(\xi)$ is the Fourier-transformation of eigenstrain $\hat{\varepsilon}^*_{kl}(\mathbf{r})$ and G_{im} is given by

$$G_{im} = C_{ipmq}\bar{\xi}_p\bar{\xi}_q \tag{4}$$

where $\bar{\xi}$ is the unit vector of ξ. A model of the raft structure used for the computation is illustrated in Fig. 2a. A cubic block containing the γ and γ' lamellarae is set as the lamellar plane normal-tilted from the crystallographic [0 0 1] direction. The model is composed of $64 \times 64 \times 64$ elements; the periodic boundary condition is automatically imposed and the stress normal to the surface (boundary) of the model crystal is set to be zero (i.e., no external force is applied to the surface).

The elastic energy caused by the application of the external stress, U_{ext}, and the potential energy of an external stress, U_{pot}, are calculated as

$$U_{\text{ext}} = \frac{\sigma^2_{\text{ext}}}{2E} \quad \text{and} \quad U_{\text{pot}} = f_\gamma \varepsilon^*_{33}\sigma_{\text{ext}} - \frac{\sigma^2_{\text{ext}}}{E} \tag{5}$$

where E is Young's modulus along the [1 0 0] direction, σ_{ext} is the applied external stress along the [0 0 1] direction and f_γ is the volume fraction of the γ phase.

The material parameters are used with reference to the experimental creep curve of the TMS-26 alloy in Fig. 1. The lattice mismatch, ε_0, is set to be 0.2%, and the elastic constants used in the calculations are $C_{11} = 210$, $C_{12} = 150$ and $C_{44} = 95$ GPa, which were experimentally measured at 1273 K [21]. The volume fraction of the γ phase, f_γ, is set to be 7/16, referring to the value experimentally determined from SEM micrographs in Fig. 1.

3. Results

Fig. 2b–f shows equi-energy contours of the internal elastic energies U_{int} calculated as a function of crystallographic orientation of the lamellae normal. The creep strain in the γ phase, ε_{p}, is set to be (b) 0%, (c) 0.2%, (d) 0.4%, (e) 0.6% and (f) 0.8%, respectively. For $\varepsilon_{\text{p}} = 0\%$, the minimum of the internal elastic energy shown in Fig. 2b is achieved when the lamellae normal is parallel to the [0 0 1] and [1 0 0] directions. As seen in Fig. 2c–d, the energy at the [0 0 1] direction decreases with the increase