

# Constitutive modeling of creep behavior in single crystal superalloys: Effects of rafting at high temperatures

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## ABSTRACT

Rafting and creep modeling of single crystal superalloys at high temperatures are important for the safety assessment and life prediction in practice. In this research, a new model has been developed to describe the rafting evolution and incorporated into the Cailletaud single crystal plasticity model to simulate the creep behavior. The driving force of rafting is assumed to be the relaxation of the strain energy, and it is calculated with the local stress state, a superposition of the external and misfit stress tensors. In addition, the isotropic coarsening is introduced by the cube root dependence of the microstructure periodicity on creep time based on Ostwald ripening. Then the influence of rafting on creep deformation is taken into account as the Orowan stress in the single crystal plasticity model. The capability of the proposed model is validated with creep experiments of CMSX-4 at 950 °C and 1050 °C. It is able to predict the rafting direction at complex loading conditions and evaluate the channel width during rafting. For [001] tensile creep tests, good agreement has been shown between the model predictions and experimental results at different temperatures and stress levels. The creep acceleration can be captured with this model and is attributed to the microstructure degradation caused by the precipitate coarsening.

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## 1. Introduction

Nickel-based single crystal superalloys (SX) are widely used for gas turbine blades due to their excellent creep, fatigue and corrosion resistance at high temperatures [1,2]. These outstanding mechanical properties mainly result from the two-phase microstructure consisting of a high volume fraction (close to 70%) of  $\gamma'$  precipitates embedded uniformly in the  $\gamma$  matrix. During the high temperature service above 900 °C, rafting, i.e. the directional coarsening of cuboidal  $\gamma'$  phases into a lamellar structure, usually occurs and has a significant effect on creep deformation of single crystal superalloys [3,4].

Since the early 1990s, a large sum of experimental research has been carried out on the kinetics and characterization of microstructure evolution in single crystal superalloys. It has been found that  $\gamma'$  precipitates tend to link to each other and form rafts in different directions under complex loading conditions. Lukas [5] conducted the tensile and compressive creep tests in the [001] direction and pointed out that a negative lattice misfit resulted into a directional coarsening perpendicular (or parallel) to the

loading axis under tension (or compression). Studies reported by Jacome [6] and Han [7] showed that a single crystal superalloy under [011] tensile creep exhibited a plate-like structure at an angle of 45° to the loading axis. Other researchers [8,9] found that rafting did not occur or highly localized in [111]-oriented creep tests. Apart from uniaxial creep tests, Kamaraj and Serin [10,11] studied the rafting under the multiaxial stress state with double shear tests in [001] and [110] orientations. In addition, the importance of the lattice misfit and stress state has been discussed by Pollock [12], Kamaraj [13], Wu [14] and Mughrabi [15]. Another significant phenomenon discovered by Matan [16] was that there was a threshold strain of 0.1% for rafting at 950 °C. The spontaneous rafting proceeded without the applied stress once the threshold strain had been exceeded. With the metallurgical analysis, the mechanism and kinetics of rafting have been partially explained. However, there are few attempts to correlate the rafting mechanism to the quantitative description of the directional coarsening and a competent model for the spontaneous rafting and characterization of microstructure evolution at complex loading conditions is still in great need.

Constitutive models have been proposed by researchers to evaluate the effect of rafting on creep deformation of single crystal superalloys. Reed [17] suggested a phenomenological model by introducing an attrition coefficient to represent the gradual equilibrium of dislocation network. This model was capable of

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describing the experimental results but the attrition coefficient changed with the temperature and stress level, which limited it for engineering application. Epishin [18] found out that the channel width during rafting could be described by the modified Arrhenius formula in a wide range of temperatures and stress levels. Tinga [19] extended it to a multiaxial stress state later and applied it into the crystal plasticity framework to simulate the tensile and cyclic tests, but the feasibility of the model for creep tests remained to be checked. Fedelich [20] developed a dimensionless parameter to consider effects of directional and isotropic coarsening on the channel widening, respectively. Then it was incorporated into a hyperbolic sine flow rule to simulate the creep deformation. However, the model did not consider the isotropic hardening and dislocation interaction on intersecting slip systems and it failed to describe the creep acceleration at low stress levels. Shastry [21] proposed a modified model by taking the precipitates shearing and rafting into account, but it was verified with experimental results at 1144 K. It was considered that rafting was not significant at that temperature. Recently, Graverend [22] reported a microstructure-sensitive model to investigate the mechanical behavior under complex loading conditions like non-isothermal creep, fatigue and creep-fatigue. For creep tests, it only involved single crystal alloys with a negative lattice misfit under tension. Also, there are few models which have both advantages of a clear physical mechanism and a high accuracy.

Although a lot of research has focused on the rafting kinetics and creep deformation, there is not a sufficient method for rafting characterization under various loading conditions, such as uniaxial loading in different directions, double shear creep and rafting without the external stress. Furthermore, the concurrent creep deformation and microstructure evolution in single crystal superalloys have not been explained clearly. In this research, a new model has been developed to describe the rafting evolution quantitatively based on the physical mechanism of directional coarsening at the multiaxial stress state. It shows a powerful ability of the rafting evaluation and then is incorporated into the Cailletaud single-crystal plasticity model [23] to simulate the creep behavior. Good agreement has been shown between the model predictions and experimental results for CMSX-4 at different temperatures and stress levels.

## 2. Model presentation

### 2.1. Rafting direction criterion

Rafting is the morphological change of  $\gamma'$  precipitates from cuboids to rafts. It has been well known that the rafting direction depends on both the sign of lattice misfit and applied stress [24]. Therefore, a criterion for rafting direction prediction is helpful to understand the microstructure evolution and guide the modeling of material behavior. Since the rafting is usually considered as a result of the atom diffusion caused by the hydrostatic stress or the loss of coherency at the  $\gamma$ - $\gamma'$  interfaces due to the plastic deformation, the internal stress state seems to be a critical factor in the kinetics of rafting, especially the role of the misfit stress. The difference of lattice parameters between  $\gamma$ - and  $\gamma'$ -phase contributes to a misfit stress in the  $\gamma$  channels. The misfit stress tensor  $\sigma_i$  in three types of channels is given by

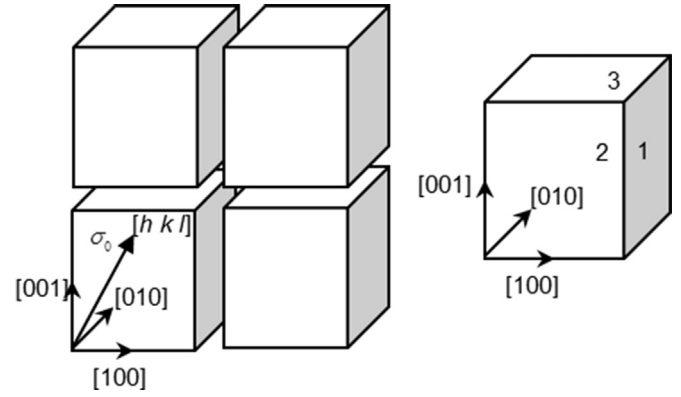


Fig. 1. Schematic representation of the loading direction and three types of channels in single crystal superalloys.

$$\sigma_{i,1} = \begin{bmatrix} \alpha\sigma_i & 0 & 0 \\ 0 & -\sigma_i & 0 \\ 0 & 0 & -\sigma_i \end{bmatrix}, \sigma_{i,2} = \begin{bmatrix} -\sigma_i & 0 & 0 \\ 0 & \alpha\sigma_i & 0 \\ 0 & 0 & -\sigma_i \end{bmatrix}, \sigma_{i,3} = \begin{bmatrix} -\sigma_i & 0 & 0 \\ 0 & -\sigma_i & 0 \\ 0 & 0 & \alpha\sigma_i \end{bmatrix} \quad (1)$$

where the subscript 1, 2 and 3 represent the matrix channels parallel to (100), (010) and (001) planes respectively (Fig. 1);  $\sigma_i$  is the magnitude of the misfit stress as large as 500 MPa and it is positive (or negative) in a single crystal superalloy with a negative (or positive) lattice misfit;  $\alpha$  is a factor indicating that the misfit stress across the channel is lower than that in the channel ( $0 < \alpha < 1$ ). For example, the misfit stress in the [100] direction can be negligible compared with that along [010] and [001] in channel 1. Therefore, the value of  $\alpha$  is chosen as 0.1 in this research.

The external stress tensor  $\sigma_{app}$  in the crystal coordinate system can be used to represent a complex loading condition at high temperatures. When a specimen is loaded in the form of stress tensor denoted as  $\sigma_0$  in the global coordinate system, the stress tensors in crystal and global coordinate systems can be linked by a transformation matrix

$$[\sigma_{app}] = [\mathbf{A}][\sigma_0] \quad (2)$$

Therefore, the internal stress in the  $j$ -type channel is the superposition of the external and misfit stress

$$\sigma_j = \sigma_{app} + \sigma_{i,j} \quad (j = 1, 2, 3) \quad (3)$$

The difference of internal stress states in three types of channels leads to rafting. It has been pointed out that it is easier for dislocations in channels with a larger stress to accumulate and deposit on the  $\gamma$ - $\gamma'$  interface, which will relieve the misfit stress to expand the interface [25]. As a result, rafting will be along the direction of the maximum stress. In solid mechanics, the Mises stress is usually taken as a representation for material yielding, i.e. the beginning of plastic deformation. Herein, the Von-Mises stress is chosen as a characterization parameter for rafting

$$\sigma_s = \sqrt{\frac{1}{2}[(\sigma_x - \sigma_y)^2 + (\sigma_y - \sigma_z)^2 + (\sigma_z - \sigma_x)^2 + 6(\tau_{xy}^2 + \tau_{yz}^2 + \tau_{zx}^2)]} \quad (4)$$

With the method proposed above, the Mises stress in different channels can be obtained under complex loading conditions and the rafting direction can be predicted in consequence.

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