Computational Materials Science 64 (2012) 2–6

Contents lists available at SciVerse ScienceDirect

Computational Materials Science

journal homepage: www.elsevier.com/locate/commatsci

Experimental characterization and mechanical modeling of creep induced rafting in superalloys

Bernard Fedelich [a,*], Alexander Epishin [b], Thomas Link [b], Hellmuth Klingelhöffer [a], Georgia Künecke [a], Pedro Dolabella Portella [a]

[a] Federal Institute for Materials Research and Testing (BAM), Berlin, Germany
[b] Technical University Berlin, Institute for Materials Science and Technologies, Berlin, Germany

ARTICLE INFO

Article history:
Received 26 October 2011
Received in revised form 15 May 2012
Accepted 31 May 2012
Available online 4 July 2012

Keywords:
Single crystal
Superalloys
Rafting
Creep
Viscoplasticity
Constitutive law

ABSTRACT

A constitutive model has been developed for the high temperature mechanical behavior of single crystal superalloys, including rafting and its consequences. The flow stress depends on the γ channel width via the Orowan stress. An evolution equation for channel widening during high temperature straining has been derived and calibrated with measurements. Therein, rafting is assumed to be driven by the relaxation of internal stresses. The model is able to represent the mechanical softening at high stresses consecutive to rafting. The model has been applied to simulate rafting during uniaxial creep in several crystal orientations, in notched specimens as well as in cyclically loaded specimens.

1. Introduction

Single crystal nickel-base superalloys are hardened by small intermetallic γ'-precipitates of Ni_3Al-type. The efficiency of this precipitation hardening strongly depends on the morphology and size of the precipitates. Under high temperature creep conditions, which are typical for service in gas turbines, the γ/γ'-microstructure gradually degrades: It becomes rafted, coarsens and eventually inverts topologically. This decreases the efficiency of precipitate hardening and hereby deteriorates the mechanical properties.

Constitutive laws for single crystal superalloys like [1] usually don't take explicitly into account the rafting phenomenon and therefore may overestimate the residual mechanical strength of the material after high temperature creep. To characterize the kinetics of rafting, comprehensive microstructural investigations and mechanical tests have been performed for the superalloy CMSX-4 [2], which is widely used in turbine industry. In parallel, a specific viscoplastic constitutive model has been developed to predict the kinetics of rafting as well as the resulting degradation of the mechanical strength for single crystal superalloys [3]. The later has been designed to predict the deformation behavior of the alloy in its as received condition as well as after high temperature degradation, under monotonous or cyclic loading and for arbitrary oriented crystals.

In the previous model version [3], the rafting process requires an external stress for initiation. However, rafting has also been observed after high temperature load-free annealing [4]. It can be explained by the residual stresses caused by the heterogeneous lattice parameters at the scale of the dendrites. In the present paper, the model has been extended to represent rafting during high temperature exposure without external load, thus also improving the model capabilities in the low stress regime. In addition, verification tests have been simulated to assess the ability of the model to predict rafting with more complex loading conditions.

2. Constitutive model

2.1. Geometrical description of the morphology evolution

The microstructure influence is assumed to mostly depend on the channel width $w(t)$ measured perpendicularly to the rafts, which increases during creep due to two phenomena:

- The homothetic growth of γ'-precipitates, called isotropic coarsening.
- The coalescence of adjacent precipitates, called rafting.

* Corresponding author. Address: BAM, Division 5.2, 12200 Berlin, Germany. Tel.: +49 30 81043104; fax: +49 30 81041527.
E-mail address: bernard.fedelich@bam.de (B. Fedelich).

0927-0256/$ - see front matter © 2012 Elsevier B.V. All rights reserved.
http://dx.doi.org/10.1016/j.commatsci.2012.05.071

In accordance, $w(t)$ varies between two time-dependent limits, which correspond to either the ideal cube or the infinite plate microstructure for a given coarsening degree. A measure of the coarsening degree is the microstructure period in the direction perpendicular to the rafts $\lambda_{[001]}$ (see Fig. 1). Direct measurements of $\lambda_{[001]}$ by Scanning Electron Microscope (SEM) have shown that the coarsening rate is roughly independent of the external stress. Hence, a time and temperature dependent relationship of the form

$$\lambda_{[001]} = \lambda^0_{[001]}\left[1 + D_0\,\exp(-\frac{Q_\lambda}{RT})\,t\right]^a \tag{1}$$

has been assumed, in which the constants $\lambda^0_{[001]}$, D_0 and Q_λ have been fitted with quantitative SEM measurements. For a given volume fraction of the γ'-fraction V', the two limits mentioned above are

$$w_{cube} = \left(1 - \sqrt[3]{V'}\right)\lambda_{[001]} \quad \text{and} \quad w_{raft} = (1 - V')\lambda_{[001]}. \tag{2}$$

Rafting progress can then be described by the dimensionless parameter

$$\xi = \frac{w - w_{cube}}{w_{raft} - w_{cube}}, \tag{3}$$

which varies between 0 (cubes) and 1 (infinite plates).

2.2. Kinematics

In view of the small strain range assumed here, the additive decomposition of the total strain $\boldsymbol{\varepsilon}$ in an elastic $\boldsymbol{\varepsilon}^e$ and a plastic part $\boldsymbol{\varepsilon}^p$ together with the Hooke's law for the Cauchy stress $\boldsymbol{\sigma}$ apply i.e.

$$\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}^e + \boldsymbol{\varepsilon}^p, \quad \boldsymbol{\sigma} = \mathbf{C} : \boldsymbol{\varepsilon}^e, \tag{4}$$

where $\mathbf{C}$ denotes the cubic stiffness tensor. The octahedral and the cubic slip systems will be throughout denoted with the superscript o, respectively c. In particular, the plastic flow rate can be decomposed in the form

$$\dot{\boldsymbol{\varepsilon}}^p = \frac{1}{2}\sum_{g=1}^{12}(\mathbf{n}^o_g \otimes \mathbf{m}^o_g + \mathbf{m}^o_g \otimes \mathbf{n}^o_g)\dot{\gamma}^o_g + \frac{1}{2}\sum_{g=1}^{6}(\mathbf{n}^c_g \otimes \mathbf{m}^c_g + \mathbf{m}^c_g \otimes \mathbf{n}^c_g)\dot{\gamma}^c_g, \tag{5}$$

where $\mathbf{m}^{o,c}_g$ denote the slip directions and $\mathbf{n}^{o,c}_g$ the slip plane normal vectors. The resolved shear stresses on either family of slip systems are $\tau^{o,c}_g = \mathbf{m}^{o,c}_g \cdot \boldsymbol{\sigma} \cdot \mathbf{n}^{o,c}_g$.

2.3. Octahedral systems

For the octahedral systems, the deformation is initiated by glide of dislocation loops in the narrow γ channels. The dislocations can only expand when the local resolved shear stress of a slip system exceeds the Orowan stress

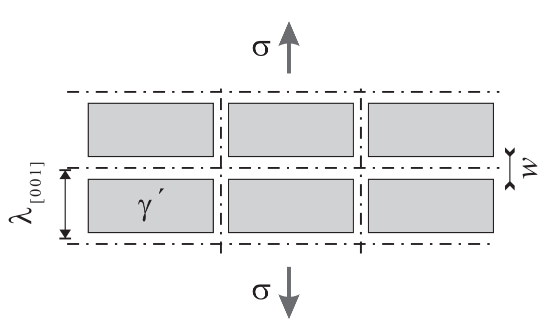

Fig. 1. Real and idealized morphology during uniaxial [0 0 1] high temperature creep.

$$\tau^{Orowan} = \alpha\frac{\mu\,b}{w}, \tag{6}$$

where the current channel width is denoted by w, b is the magnitude of the Burgers vector and μ is the shear modulus. The constant α will be treated as an adjustable parameter. Dislocation glide is assumed to be thermally activated and the flow rule is taken as

$$\dot{\gamma}^o_g = \dot{v}^o_g\,\mathrm{sign}(\tau^o_g - x^o_g), \quad \text{with}$$
$$\dot{v}^o_g = \rho^o_g \sinh\left[\frac{V^o_f}{kT}|\tau^o_g - x^o_g|\left\{1 - \left[1 + \left(\frac{|\tau^o_g - x^o_g|}{\tau^{orowan}}\right)^s\right]^{-1/s}\right\}\right], \tag{7}$$

where x^o_g is the back stress on the slip system g. The Boltzmann constant is denoted by k, V^o_f is an activation volume and T is the absolute temperature. The quantity ρ^o_g is proportional to the dislocation density of the corresponding system. We assume for it a law with saturation, i.e.

$$\rho^o_g = \rho^o_0 + \left(\rho^o_\infty - \rho^o_0\right)[1 - \exp(-\;\; v^o_g/b^o)], \tag{8}$$

where the constant b^o corresponds to the cumulated slip amount at saturation. The degree of smoothness of the elastic–plastic transition is controlled by the exponent s (see [3] for more details). Kinematic hardening is described by a tensor variable denoted by $\mathbf{X}^o$, as resulting from the calculations of the internal stresses in the γ/γ' compound performed in [5]. The back-stresses at the level of the slip system are then obtained by

$$x^o_g = \mathbf{n}^o_g \cdot \mathbf{X}^o \cdot \mathbf{m}^o_g. \tag{9}$$

The internal stress $\mathbf{X}^o$ is proportional to a tensorial strain-like internal variable α^o which varies following the contributions of all slip systems, i.e.

$$\mathbf{X}^o = c^o\alpha^o, \quad \dot{\alpha}^o = \frac{1}{2}\sum_{g=1}^{12}\left(\mathbf{n}^o_g \otimes \mathbf{m}^o_g + \mathbf{m}^o_g \otimes \mathbf{n}^o_g\right)\dot{\alpha}^o_g, \tag{10}$$

where c^o is a numerical constant homogeneous to a stiffness. Conversely, the contribution $\dot{\alpha}^o_g$ of each slip system to the rate of α^o is assumed to take the form

$$\dot{\alpha}^o_g = \dot{\gamma}^o_g - \dot{v}^o_g g^o(x^o_g) - h^o\,(x^o_g). \tag{11}$$

The second and the third terms on the right hand side of (11) correspond to dynamic and static recovery, respectively. Here also, thermally activated processes are assumed, i.e.

$$g^o\,(x) = d^o \sinh\left[\frac{V^o_d x}{kT}\right], \quad h^o(x) = h^o \sinh\left[\frac{V^o_s x}{kT}\right], \tag{12}$$

where V^o_s and V^o_d are activation volumes and d^o and h^o are dimensionless constants.

2.4. Cubic systems

The plastic shear rate for the cubic systems is supposed to follow a similar thermal activation law (without exponent) of the form

$$\dot{\gamma}^c_g = \dot{v}^c_g\,\mathrm{sign}(\tau^c_g - x^c_g), \quad \dot{v}^c_g = \rho^c_g \sinh\left[\frac{V^c_f\left\langle\left|\tau^c_g - x^c_g\right| - r^c_0\right\rangle}{kT}\right]. \tag{13}$$

Here, and in the following, similar notations to the octahedral systems are used. According to the observations on $\langle 1\;1\;1\rangle$ specimens and their interpretation by Discrete Dislocation Simulations [6], cubic slip is actually related to the simultaneous activation of $a/2\langle 0\;1\;\bar{1}\rangle$ dislocations on conjugate octahedral planes. Here, cubic