A visco-plastic damage model for high temperature creep of single-crystal superalloys

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Abstract

The micromechanics of the high temperature creep and damage accumulation in single crystal nickel base superalloys is important for the design of turbine blades and vanes in advanced commercial and military gas turbines. We have developed a robust predictive tool to relate single crystal macroscopic behaviour and fracture initiation to micromechanical events. A crystallographic-based model for non-isothermal high temperature cyclic deformation has been fully coupled with the damage kinetics. The model significantly improves the quality of material deformation predictions on cyclic and thermal-cyclic loading.
Keywords: super-alloys, single crystal, constitutive modeling, dislocation kinetics.

1 Introduction

Historically, secondary creep effects with associated modelling techniques (Larson-Miller, etc.) were used in engineering calculations. However, during the thermal-mechanical loading of high temperature single crystal turbine parts, all three creep stages: primary, secondary and tertiary, manifest themselves and none of them can be neglected. A creep law is especially important in the case of non-homogeneous thermal loading which results in intensive stress redistribution and relaxation.

Several damage mechanisms, namely multiplication of mobile dislocations, void and micro-crack growth and the scale effects caused by dislocation extrusions/intrusions and necking, have been considered. Our damage model bridges the gap between dislocation dynamics and continuum mechanics scales. Damage accumulation causes tertiary creep and shear localization around local concentrators, which is essential for airfoil life prediction.

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The constitutive model has been implemented in the commercial finite element software ANSYS as a material user routine to predict creep anisotropy and yield thermal dependence. The model is calibrated against stress-strain and crystallographic texture predictions against test data up to 25% strain. The developed non-isothermal, crystal–viscoplastic, damage mechanics model is used for creep, cyclic ratcheting and thermal mechanical fatigue (TMF) analysis.

2 Viscoplastic model

We have used standard viscoplastic power law creep with a back stress [1] to represent the response of the material. The constitutive law for the inelastic strain, $\gamma_i^{\,p}$, along slip plane i will be written as

$$\dot{\gamma}_i^{\,p} = \dot{\gamma}_0 \left(\frac{\rho_m}{\rho_0} \right) \left| \frac{\tau_i - \omega_i}{s_i^*} \right|^n \operatorname{sgn}\left(\frac{\tau_i - \omega_i}{s_i^*} \right), \tag{1}$$

where $\dot{\gamma}_0$ is a time constant, ρ_m is the mobile dislocation density, ρ_0 is a arbitrary reference dislocation density, τ_i is the slip plane resolved shear stress, s_i^* is the isotropic yield stress, ω_i is the slip plane back stress, and $(\dot{\ })$ is the rate of change with respect to time. The isotropic yield stress, s_i^*, is assumed to be a constant throughout this discussion but is actually a variable with its own evolution equation. The back stress will be taken to evolve according to [1,2]:

$$\dot{\omega}_i = \lambda_0 \left| \dot{\gamma}_i^{\,p} \right| \left(\omega_\infty \sqrt{\frac{\rho_p}{\rho_p^{ss}}} \operatorname{sgn}\left(\dot{\gamma}_i^{\,p} \right) - \omega_i \right) \tag{2}$$

where λ_0 is a time constant, ω_∞ is the steady state back stress, ρ_p is the pinned dislocation density, and ρ_p^{ss} is the value of the steady state pinned dislocation density. The total slip shear strain, γ_i, includes the elastic part and can be written, for a single active slip plane, as

$$\gamma_i = \frac{\tau_i}{G} + \gamma_i^{\,p} \tag{3}$$

where G is the shear modulus for along the slip plane.

The initial conditions will be taken as

$$\omega_i = 0 \quad \gamma_i^{\,p} = 0 \quad at\ t = 0 \tag{4}$$

3 Dislocation kinetics model

The mobile and the pinned dislocations will also evolve over time. We have chosen to represent the evolution as two body interactions, and have assumed that the entropy production, $\dot{s}$, is given by [3]:

$$\dot{s} = C\sum_{i=1}^{n_{slip}}\left(\frac{\tau_i - \omega_i}{s^*}\right)\dot{\gamma}_i^{\,p} \geq 0\,, \tag{5}$$

where the parameter C is a constant, and n_{slip} is the number of slip systems.

Note that from equation (1) that $\dot{\gamma}_i^{\,p}$ is already a linear function of the mobile dislocation density and, hence, if the dislocation evolution equations vary linearly with the inelastic strain rate then to represent two body interactions they must also be proportional to linear combination of the mobile and pinned dislocation densities. Based on these constraints, we have chosen the evolution equation for the mobile dislocation density to be

$$\dot{\rho}_m = \alpha\sum_{i=1}^{n_{slip}}\left(\frac{\tau_i - \omega_i}{s^*}\right)\dot{\gamma}_i^{\,p}\left(\frac{\varepsilon^2\rho_m^{ss} + \rho_p^{ss} - \rho_p - \varepsilon^2\rho_m}{\rho_0}\right) \tag{6}$$

where α is a time constant, ρ_m^{ss}, is the saturated mobile dislocation density, ρ_p^{ss}, is the saturated pinned dislocation density, and ε^2 is a positive constant. Equation (6) includes the annihilation of mobile dislocations and also includes their conversion to pinned dislocations. For the pinned dislocation density we have taken the evolution equation to be

$$\dot{\rho}_p = \beta\sum_{i=1}^{n_{slip}}\left(\frac{\tau_i - \omega_i}{s^*}\right)\dot{\gamma}_i^{\,p}\left(\frac{\rho_p^{ss} - \rho_p}{\rho_0}\right) \tag{7}$$

where β is a time constant. The pinned dislocations grow at a rate that is proportional to the mobile dislocation density because of the presence of the plastic strain rate term. Throughout this paper, for the initial conditions we have taken

$$\rho_m = \rho_0 \quad \rho_p = 0 \quad at\ t = 0 \tag{8}$$

Of course, they can be generalized if the need arises.

4 Damage parameters

There are several mechanisms leading to the macrocracking or high temperature rupture. We define damage parameters (up to five in the extended model) reflecting each of these mechanisms. Not all of them are equally important at all conditions. In this paper we focus on damage associated with mobile dislocations multiplication d_d and briefly review effects caused by evolution of porosity

d_v and microcracking d_c on the elastic moduli. We also considered damage effects related to the interactions of dislocation loops with the free surfaces. This damage was defined through the change in the shear modulus as $G = (1 - d_s)G_0$. In this discussion we will illustrate the development of the creep and void damage models, but the illustrations of the effects of damage will include only the changes in shear modulus. The presented damage model is based on a "damage rate conservation" assumption stating that all damage mechanisms are interconnected and caused by entropy generation as follows:

$$\sum_{\substack{damage \\ mechanisms}} \dot{d}_i \sim \dot{s}. \tag{9}$$

We define damage caused by the increase of the dislocation density as

$$d_d = 1 - \frac{\rho_0}{\rho_m} \tag{10}$$

The increase of d_d from zero to unity causes the fast raise of $\dot{\gamma}^p$ (see eq. (1)). In turn it leads to the tertiary creep or even elimination of the secondary creep stage called sigmoidal creep. This dislocation driven mechanism does not directly affect crystallographic structure or material elastic properties. Two other major damage mechanisms are void development and microcracking. Both change the part stiffness, and can be defined through the variation of elastic parameters as follows:

$$\begin{aligned} &\frac{E}{1+\nu} = (1 - d_c)\frac{E_0}{1+\nu_0}; \\ &\frac{E}{3(1-2\nu)} = (1 - d_v)\frac{E_0}{3(1-2\nu_0)} = K = (1 - d_v)K_0 \end{aligned} \tag{11}$$

where E_0 and υ_0 are the original Young's modulus and Poisson ratio; K_0, is the original bulk modulus. Thus, having d_c and d_v calculated we are able to adjust the materials elastic response during the loading. It can be shown that E and K decrease with the increase of damage parameters. The quantity d_v changes with the pore volume fraction, v, and was found from a model based on the bulk modulus variation for a sphere with central hole. Variation of effective moduli with cracking is a well known problem (e.g., [4]). Finally, relations for the damage parameters for materials with cracks and voids have the following form:

$$d_c(f) = \frac{\ln(\sec(\frac{\pi}{2}f))}{\frac{1}{8}f + \ln(\sec(\frac{\pi}{2}f))}; \qquad d_v(\upsilon) = \frac{\left(1 - 2\nu_0 + \frac{1+\nu_0}{2}\right)\upsilon}{1 - 2\nu_0 + \frac{1+\nu_0}{2}\upsilon} \tag{12}$$

where f is crack volume fraction. To complete the damage model, the evolution equations are needed. It is assumed that the coalescence of voids is the source of the micro-cracks and the pile-up of mobile dislocations causes void nucleation.

From these considerations and the damage "conservation rule" (9) the damage kinetics equations can be written in the following simplified form:

$$\dot{d}_d = C_1 \sum_{i=1}^{n_{slip}} \left(\frac{\tau_i - \omega_i}{s^*} \right) \dot{\gamma}_i^{\,p} (1 - d_d)^2; \tag{13}$$

Void growth obeys the Wilkinson-Ashby equation and creep crack growth is linearly proportional to the C^*-parameter where $C^* \sim f\dot{\varepsilon}^c$. Crack nucleation rate is proportional to the probability of the event that at least three pores coalesce along a line. The probability of pore occurrence in the fixed volume is governed by Poisson stochastic process [5]. Pore coalescence occurs when a pore appears to be inside a sphere of two average pore radii from the center of another pore. The number of crack nucleation sites is proportional to probability of the occurrence of such an event, which, in turn, is $N_c \sim \frac{1}{2}\upsilon\Gamma(8\upsilon,3)$ where $\Gamma()$ – is incomplete Gamma function. The microcrack fraction nucleation rate is equal to $\frac{1}{3} f \dfrac{\dot{N}_c}{N_c}$; therefore the final evolution relationship for the voids and cracks fractions has the form:

$$\begin{aligned} \dot{d}_v &= \frac{\partial d_v}{\partial \upsilon}\dot{\upsilon}; \quad \dot{d}_c = \frac{\partial d_c}{\partial f}\dot{f} \\ \dot{\upsilon} &= \underbrace{C_2 \frac{\upsilon(1-\upsilon)}{(1-\upsilon^{1/n})^n}\sigma_{kk}^n}_{\text{void growth}} + \underbrace{C_4 \frac{\dot{d}_d}{(1-d_d)^2}}_{\text{void nucleation rate}}; \\ \dot{f} &= \underbrace{C_3 f \dot{\varepsilon}_e^c}_{\substack{\text{creep crack} \\ \text{growth}}} + \underbrace{\tfrac{1}{3} f \frac{\dot{\upsilon}}{\upsilon}\left(1 + \frac{8\upsilon\Gamma'(8\upsilon,3)}{\Gamma(8\upsilon,3)}\right)}_{\substack{\text{crack nucleation} \\ \text{rate}}} \end{aligned} \tag{14}$$

where C_1 - C_4 are temperature dependant parameters and n – is the creep exponent.

The last damage parameter, d_{TW}, was defined through the change in the bulk modulus as

$$\overline{G} = (1 - d_{TW})G_0 \tag{15}$$

where G_0, is the original shear modulus and will be referred to as the thin-walled debit [6] d_{TW}, and was based on the intersection of dislocation loops with the surface. Consider a flat dislocation loop of radius R with the normal to the plane of the loop at an angle θ with respect to the length of a uniaxial stress test specimen. It can be shown that the average density of dislocation loops intercepting the surface, N_1, for a specimen of thickness H is

$$N_I = 4\rho_m \frac{\langle R \rangle}{H} \cos\theta \tag{16}$$

where $\langle R \rangle$ is the average dislocation loop radius. For many dislocations intercepting the surface, the average number moving the surface right, μ, can be found from the binomial distribution as

$$\mu = \frac{N_I}{2} \tag{17}$$

while the standard deviation, σ, satisfies

$$\sigma^2 = \frac{N_I WL}{4} \tag{18}$$

where W and L are the width and length of a surface. If each dislocation has Burger's vector b, then average absolute distance, $\overline{S}$ each surface moved from the mean is

$$\overline{S} = \frac{b}{2\pi}\sqrt{N_I WL} \tag{19}$$

We can approximate the change in the shear modulus by considering a panel with shear applied at the top and held at the bottom. The bottom has a length equal to the original thickness, H, and the top has length $H - \overline{S}$. The average modulus, $\overline{G}$, can then be found from

$$\overline{G} = G_0 \frac{\overline{S}/H}{\ln\left(\dfrac{1}{1-\overline{S}/H}\right)}. \tag{20}$$

The damage, d_{TW}, becomes

$$d_{TW} = 1 - \left(\overline{G}/G_0\right) \tag{21}$$

5 Typical response

A typical creep response, that includes many of the effects that we can represent, can be illustrated using the parameters and initial conditions shown in Table 1. The dislocation density evolution is shown in Figure 1. Initially the mobile dislocation density grows slowly, then rises as the pinned the dislocation density levels out, and finally grows exponentially toward the steady state value.

In Figure 2 each of the individual damage parameters initially grows rapidly, with the damage parameters controlling the shear modulus and isotropic yield stress accelerating at around 16000 seconds.

Figure 3 shows the total strain as a function of time. Clearly all three modes are present including a short primary creep interval, a fairly long secondary creep region and a steep tertiary creep region.

The primary creep region is controlled by the rapidity with which the back stress and the pinned dislocations reach steady state. For Figure 3 the primary creep region is short. The tertiary creep region is very steep and is controlled the

damage evolution rates and the rate of mobile dislocation generation. The steady part can be lengthened or shortened by changing the rates of the primary and tertiary creep response. Clearly, the initial conditions, such as the initial pinned and mobile dislocation density and the initial back stress will also control the length each the primary, secondary and tertiary creep regions.

Table 1: Material parameters and initial conditions.

Parameters:			
α	2.00E+07	$\dot{\gamma}_0$	0.00001
β	2.00E+10	λ	1.00E+03
G/s_0	100	ρ_p^{ss}	2.00E+10
n	3	ρ_0	5.00E+06
$\cos\theta$	0.57735027	ρ_m^{ss}	1.00E-04
ω_∞ / s_0	0.25		2.00E+15
H	0.15	WL	6.00
b	2.00E-08	<R>/H	50.00

Initial Conditions:			
ρ_m	5.00E+06	γ^p	0
ρ_p	0.00E+00	ω	0
ρ	5.00E+06	τ/s_0	0.3

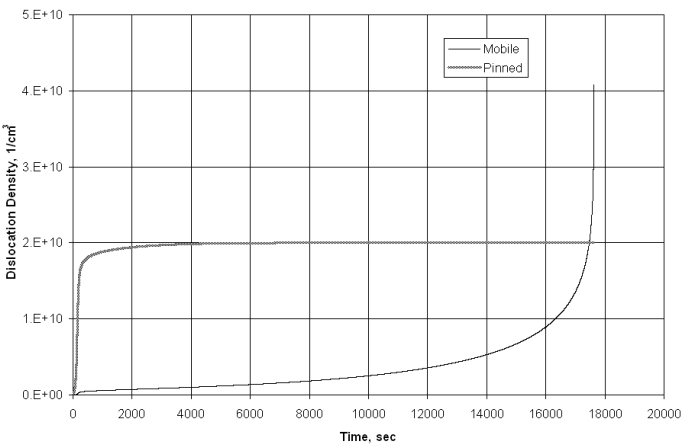

Figure 1: Dislocation density for data in Table 1.

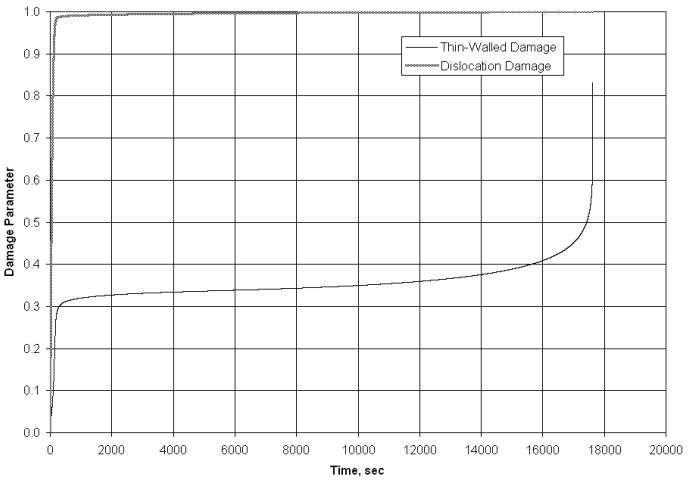

Figure 2: Damage parameters for data in Table 1.

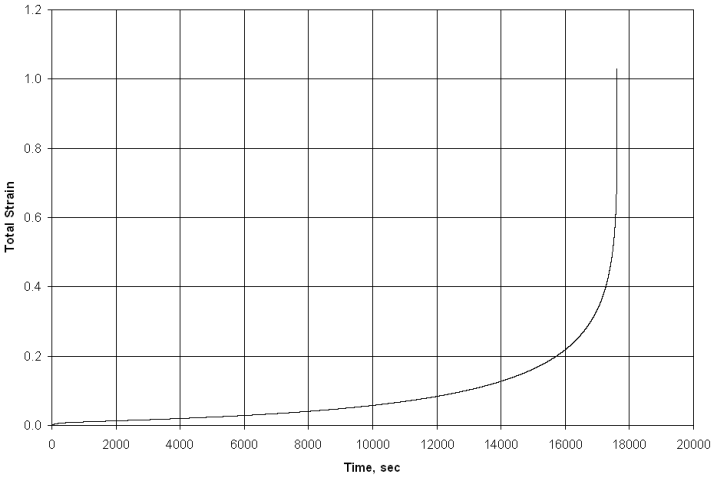

Figure 3: Total strain for data in Table 1.

6 Conclusions

We have studied creep behaviour of single crystal Ni-based superalloys using a dislocation–based viscoplastic model. The model is focused on analysis of high temperature deformation and is coupled with damage kinetics allowing the prediction of tertiary creep and failure initiation at high temperature. We were able to predict generic creep response including primary, secondary and tertiary stages as well as sigmoidal creep. Varying the model damage parameters we

obtained different tertiary creep responses allowing sensitivity study and model parameters calibration. It is important to note that model internal state variables have clear physical meanings and were chosen in rational matter. Macroscopic parameters, such as back stress ω, creep strain rate $\dot{\gamma}^{p}$ and others depend on densities of mobile and pinned dislocations and their kinetics. Damage nucleation and accumulation is defined by entropy generation and is described by dislocation density, pore and micro-crack volume fractions. All introduced damage parameters are interconnected: crack nucleation is defined by pore coalescence and pore nucleation which is in turn defined by the increase in dislocation density. The simple mesoscopic model presented sheds light on the formulation and calibration of crystal – viscoplastic, damage mechanics constitutive model and allows estimates for the role of different damage mechanisms in creep and creep – fatigue modeling of single crystal materials.

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