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DISLOCATION DYNAMIC MODELING IN HIGH TEMPERATURE SINGLE CRYSTAL VISCOPLASTICITY (PREPRINT)

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Pratt & Whitney

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We have developed a crystallographic–based viscoplastic model for nonisothermal high temperature deformation and coupled it with damage kinetics. Several damage mechanisms, namely the multiplication of mobile dislocations, void growth and including scale effects, caused by dislocation extrusions/intrusions, have been considered. We applied two body interaction concepts from chemical kinetics to include in our constitutive relations the generation and interaction of pinned and mobile dislocations. The relative importance of each of the damage modes at different temperatures and stress levels has been deduced by comparing strain-stress and crystallographic texture predictions calibration against test data and has shown that the dislocation density growth.

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DISLOCATION DYNAMIC MODELING IN HIGH TEMPERATURE SINGLE CRYSTAL VISCOPLASTICITY

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ABSTRACT We have developed a crystallographic–based viscoplastic model for non-isothermal high temperature deformation and coupled it with damage kinetics. Several damage mechanisms, namely the multiplication of mobile dislocations, void growth and including scale effects, caused by dislocation extrusions/intrusions, have been considered. We applied two body interaction concepts from chemical kinetics to include in our constitutive relations the generation and interaction of pinned and mobile dislocations. The relative importance of each of the damage modes at different temperatures and stress levels has been deduced by comparing strain-stress and crystallographic texture predictions calibration against test data and has shown that the dislocation density growth may be important in characterizing primary creep.

INTRODUCTION: An understanding of the micromechanics of 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. Our models must not only predict the creep response of materials in gas turbines they must also be able to model virgin material since most experimental data has been obtained from "as received" materials and "as received" materials have considerably smaller dislocation densities than pre-strained/pre-exposed materials. This can drastically change the primary creep response. The Orowan equation, where strain rate is proportional to the dislocation density, is commonly used to describe the mechanical response of materials. But clearly if the dislocation density increases then the strain will also increase and the equations must include an additional term proportional to rate of growth of dislocation density. We believe that including dislocation density growth rate in our model may predict the observed experimental differences between "as received" materials and pre-strained materials.

PROCEDURES, RESULTS, AND DISCUSSION: We have used a standard viscoplastic power law creep with a back stress to represent the response of the material. The constitutive law for the inelastic strain rate, $\dot{\gamma}_i^{\,p}$ along slip plane i is proportional to the mobile dislocation density, ρ_m, and is written as (Staroslesky et al, 2006) $\dot{\gamma}_i^{\,p} = \dot{\gamma}_0 \left(\rho_m / \rho_0\right) \left|\left(\tau_i - \omega_i\right) / s_i^*\right|^n \operatorname{sgn}\left(\left(\tau_i - \omega_i\right) / s_i^*\right)$, where $\dot{\gamma}_0$ is a time constant, 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. Both s_i^* and ω_i have evolution equations of their own. We obtain relations for mobile and pinned dislocations along each slip system as:

$$\dot{\rho}_m^\alpha = \mathrm{M}\left(\frac{\frac{\tau^\alpha}{1-v} - \omega^\alpha}{s^\alpha}\right)\dot{\gamma}_{in}{}^\alpha\left(\frac{\varepsilon^2\rho_m^{ss} + \rho_p^{ss} - \rho_p^\alpha - \varepsilon^2\rho_m^\alpha}{\rho_0} - Cv^{2/3}\right)(1-v),\ \dot{\rho}_p = \Pi\left(\frac{\frac{\tau^\alpha}{1-v} - \omega^\alpha}{s^\alpha}\right)\dot{\gamma}_{in}{}^\alpha\left(\frac{\rho_p^{ss} - \rho_p^\alpha}{\rho_0}\right)(1-v)$$

where M and Π represents specific time constants, different for the octahedral and cube slip systems, 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, v is the pore volume fraction and has an evolution equation associated with it. Please see Staroselsky, et al (2006) for a more complete discussion of the model. The Orowan (1940) equation is commonly used to describe the mechanical response of materials and is referenced widely [e.g. see Thompson, 2006].

The Orowan equation is generally written for edge dislocations with a dislocation density, ρ, as $\dot{\gamma} = \rho b v$, where γ is the shear strain, v is the dislocation velocity, b is the Burgers' vector, and $(\dot{\ }) = \partial(\ )/\partial t$. However if the dislocation density increases then the strain will also increase and the equation should include a $\dot{\rho}$. For example, we could write $\dot{\gamma} = \rho b\dot{L} + \dot{\rho} bL$. The quantity L is some characteristic dimension which will make the strain rate the total derivative of a function. An equation containing $\dot{\rho}$ is not a new idea, and has been proposed independently by others [e.g., see Gupta, et al, 1974]. The characteristic distance *L* is the key parameter that must be developed. Our proposal is to assign to *L* the distance between pinned dislocations similar to Thompson (2006) where the author has proposed using the average dislocation displacement.

For example consider the singular components of the strain for edge and screw dislocations describe the state of strain in a material. For an edge dislocation in the x-y plane (i.e., the dislocation line is parallel to the z-axis), and the discontinuous slip along the x-axis, the singular part of the displacements in cylindrical coordinates (Nabarro, 1987) are, $\vec{u} = b/2\pi\{\theta, \ln(r/b), 0\}$, where the vector components are along the r, θ, z are the directions respectively. For a screw dislocation in the x-y plane the singular part of the cylindrical displacements (Nabarro, 1987) are $\vec{u} = b/2\pi\{0, 0, \theta\}$. For the edge dislocation the small strain components can be evaluated, and then the maximum shear strain can be readily shown to be $\varepsilon_{\max} = b/2\pi r$ in cylindrical coordinates. Similarly for a screw dislocation the maximum shear strain is $\varepsilon_{\max} = b/4\pi r$. Recall that the maximum engineering shear strain, $\gamma_{\max} = 2\varepsilon_{\max}$, For dislocations that are distributed throughout an area with density, ρ, the strain tensor becomes for both edge and screw dislocations can be written as $\varepsilon_{ij} = \int_S \rho b f_{ij}\left(\vec{r}-\vec{R}\right) dS$,

where S is the area over which the dislocations are distributed, and we have assumed that the rate of change of the integrand over time, t, is slow enough for a steady state in the strains to exist. The dislocation density can include both edge, ρ_e, and screw dislocation densities, ρ_s, where $\rho = \rho_e + \frac{1}{2}\rho_s$. The strain rate can be found by differentiating with respect to time, then $\dot{\varepsilon}_{ij} = \int_S \left\{ \dot{\rho} b f_{ij} - \rho b \dot{\vec{R}} \bullet \vec{\nabla} f_{ij} \right\} dS$, where $(\dot{\ }) = \partial(\ )/\partial t$, $f = f\left(\vec{r}-\vec{R}\right)$, and $\vec{r}$ is the vector $(x, y, 0)$ while $\vec{R}$ is the vector $(X, Y, 0)$. The integration is performed over the coordinates $(x, y, 0)$. If ρ, $\dot{\rho}$, and $\dot{\vec{R}}$ are constant throughout the area S then $\dot{\varepsilon}_{ij} = \dot{\rho} b \int_S f_{ij} dS - \rho b \dot{\vec{R}} \bullet \oint_C f_{ij} \vec{n} dC$ where the contour C surrounds the area S, and use has been made of the divergence theorem.

We can find an approximate value for the second integral by considering the case of a circular contour of radius a surrounding the area S, and all of the dislocations moving with velocity v. Then the maximum engineering strain rate for edge dislocations with $\dot{\rho} = 0$ is given by $\dot{\gamma}_{\max} = \rho_e b v$, which exactly matches the Orowan equation. We now need an estimate for the term proportional to $\dot{\rho}$. Consider again the case of a circular area of radius a. An integration yields $\dot{\gamma}_{\max} = 2\dot{\rho}_e b a + \rho_e b v$. Our proposal is to make the term $2a$ in the $\dot{\rho}$ term proportional to the average distance between pinned dislocations. That is, if the pinned dislocation density is ρ_p then the distance is proportional to $1/\sqrt{\rho_p}$.

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