Effect of crystal orientation on porosity evolution in a creeping single crystal

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A B S T R A C T

The effect of crystal orientation on porosity evolution in a face centered cubic (fcc) single crystal subject to tensile creep loading is analyzed. The matrix material is characterized by a rate power law viscous crystal plasticity constitutive relation. Three dimensional finite deformation finite element analyses of initially cubic unit cells containing a single initially spherical void are carried out for three crystal orientations of the main loading direction together with two other cases analyzed to study the effect of secondary orientations. The calculations are carried out for three values of the stress triaxiality and for each stress triaxiality value three values of the Lode parameter are considered. Two of the crystal orientations are significantly anisotropic orientations. Symmetry boundary conditions are imposed consistent with the crystal symmetry; the sides of the unit cell are not constrained to remain straight. For an anisotropic orientation, the Lode parameter can have a significant effect on the evolution of creep strain and porosity even at relatively high values of the stress triaxiality. An overall enhanced creep rate can occur with no void growth or even accompanying void collapse. Also, whether or not a stress concentration greater than the elastic stress concentration develops depends on crystal orientation.

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1. Introduction

The motivation for our modeling of porosity evolution in creeping single crystal stems from the experimental observations of tensile creep fracture of a single crystal superalloy in Srivastava et al. (2012) that indicated that porosity evolution could play an important role in the creep fracture of such materials. Porosity evolution in viscous solids has been analyzed to model creep fracture and/ or compaction, see for example Budiansky et al. (1982), Banks-Sills and Budiansky (1982), Nemat-Nasser and Hori (1987), Lee and Mear (1994), Needleman et al. (1995), Mohan and Brust (2000), Srivastava and Needleman (2012, 2013).

There is a large literature on porosity evolution in inelastic solids that has been aimed at modeling room temperature ductile fracture in metals, see Tvergaard (1990) and Benzerga and Leblond (2010) for reviews. The majority of such studies have been carried out for plastically isotropic solids, but some analyses of porosity evolution have been carried out accounting for plastic anisotropy; for example, using a Hill-type yield criterion for the matrix material (Benzerga et al., 2004; Kysar et al., 2005; Monchiet et al., 2008) or using continuum slip crystal plasticity (Orsini and Zikry, 2001; Schacht et al., 2003; Wan et al., 2005; Potirniche et al., 2006; Liu et al., 2007; Yang and Dong, 2009; Ha and Kim, 2010; Yerra et al., 2010; Yu et al., 2010; Lebensohn and Cazacu, 2012; Han et al., 2013).

The primary orientation of single crystal superalloys used in turbine airfoils in jet engines (which have an fcc-like crystal structure) is close to a $\langle 001 \rangle$ crystal

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orientation. The tensile creep response of a voided fcc single crystal with this orientation relative to the principal stress axes is nearly isotropic due to the slip system symmetry (Srivastava and Needleman, 2012). However, owing to their complicated structure turbine airfoils often encounter more complex stress states in service so that the principal stress axes are oriented along a variety of crystal orientations. Recently, Sabnis et al. (2012) suggested that even the secondary orientations can have important consequences for crack nucleation. In addition, a finite element analysis of a tensile creep specimen cross section with an oxide layer in Srivastava et al. (2012) indicated that the presence of an oxide layer could significantly change the near-surface values of the stress triaxiality (the ratio of the first to second stress invariants) and of the Lode parameter (a measure of the third stress invariant) from those corresponding to uniaxial tension (a stress triaxiality value of 1/3 and a Lode parameter value of -1). Furthermore, analyses in Srivastava and Needleman (2012, 2013) for $\langle 001 \rangle$ oriented voided fcc single crystals showed that, depending on the value of the stress triaxiality, the value of the Lode parameter, the void spacing and the initial void volume fraction, either void growth or void collapse can occur under tensile creep loading conditions. Hence, analyses of the response of porous single crystals with various crystal orientations subject to a range of tensile creep loading conditions are of interest.

Strain controlled analyses of void evolution in single crystals have been carried out in Schacht et al. (2003), Potirniche et al. (2006), Liu et al. (2007), Yang and Dong (2009) to investigate the effect of crystal orientation. In these calculations, the values of the stress triaxiality and the Lode parameter vary during the deformation history. Calculations exploring the effect of crystal orientation at various stress triaxiality values using three-dimensional cell models are reported in Wan et al. (2005), Yu et al. (2010), Ha and Kim (2010), Yerra et al. (2010), Han et al. (2013). In Wan et al. (2005), Yu et al. (2010), Ha and Kim (2010), the faces of the cubic unit cell are constrained to remain planar during the deformation which can over constrain the deformation mode for some orientations. To avoid such over constraining (Yerra et al., 2010) applied fully periodic boundary conditions on the faces of the unit cell. In Yerra et al. (2010) the effect of crystal orientation on void growth was analyzed for a range of stress triaxiality values for a body centered cubic single crystal matrix. Their results suggest that for low stress triaxiality, the void shape evolution, void growth, and strain at the onset of coalescence are strongly dependent on the crystal orientation, while under high stress triaxiality, only the void growth rate is significantly affected by the crystal orientation. However, in Yerra et al. (2010) the effect of varying the Lode parameter was not explored.

Here, the effect of crystal orientation on porosity evolution under creep loading is studied using an initially cubic unit void cell model that represents a regular array of initially spherical voids, with a 1% volume fraction, in a face centered cubic (fcc) crystal. Uniaxial creep rupture of single crystal superalloys has been analyzed along $[100]$, $[110]$ and $[111]$ crystallographic orientations (for example, Qi and Bertram (1999)). Hence calculations are

carried out for fcc crystals oriented with the $[100]$, $[110]$ and $[111]$ directions parallel to the main loading direction. Two secondary orientations are also analyzed for the $[110]$ and $[111]$ crystals. For each crystal orientation, three values of the stress triaxiality, $\chi = 3$, $2/3$ and $1/3$ and three values of the Lode parameter, $L = -1$, 0 and 1 are considered. The boundary conditions on the faces of the unit cell are applied in accordance with the symmetry along the crystal orientation normal to it. Our calculations show that the crystal orientation can have a strong effect both on the evolution of creep strain and on the evolution of porosity as well as on the evolution of void shape. Most notably we find that the effect of the Lode parameter, for a given stress triaxiality value, depends on the crystal orientation and that for certain crystal orientations the Lode parameter has a significant effect on the evolution of creep strain and porosity even at high stress triaxiality values. This is in contrast to results for porosity evolution in $\langle 001 \rangle$ oriented fcc single crystals and in isotropic solids with a Mises flow potential where the Lode parameter only significantly affects porosity evolution at low stress triaxiality values.

2. Problem formulation

Three dimensional finite element calculations are carried out to model the response of a regular array of voids under constant true stress creep loading conditions using a unit cell model. The unit cell is initially cubic with an initially spherical void at the center. A single crystal superalloy contains crystallographically coherent fcc-based ordered $L1_2$ precipitate in a fcc matrix. Here, as in Srivastava and Needleman (2012, 2013), the homogenized matrix material of the unit cell is modeled as an fcc single crystal with the potentially active slip systems taken to be the twelve primary octahedral slip systems $\{111\}\langle 110 \rangle$. Isothermal conditions are assumed and attention is confined to the circumstances where diffusion effects are negligible. For polycrystalline metals, grain boundary diffusion often plays a significant role. However, for single crystals this mechanism is ruled out and, at sufficiently low temperatures (Srivastava et al., 2012) bulk diffusion also is not significant in single crystal superalloys so that dislocation creep is the main deformation mechanism. Finite deformation finite element analyses are carried out using a rate dependent crystal plasticity constitutive relation for power law creep. For each crystal orientation considered, calculations are carried out for several fixed values of stress triaxiality and Lode parameter.

2.1. Constitutive relation

The crystal constitutive formulation follows that in Asaro and Needleman (1985) and the implementation is based on the UMAT due to Huang (1991).

The deformation gradient, $\mathbf{F}$, is written as

$$\mathbf{F} = \mathbf{F}^* \cdot \mathbf{F}^P \tag{1}$$

where $\mathbf{F}^*$ is due to stretching and rotation of the crystal lattice and $\mathbf{F}^P$ is due to crystallographic slip. Differentiating Eq. (1) with respect to time and combining terms gives