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Micromechanical modeling of creep damage in a Copper-Antimony Alloy

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Abstract

A micromechanical model of creep induced grain boundary damage is proposed, which allows for the simulation of creep damage in a polycrystal with the finite element method. Grain boundary cavitation and sliding are considered via a micromechanically motivated cohesive zone model, while the grains creep following the slip system theory. The model has been calibrated with creep test data from pure Cu single crystals and a coarse-grained polycrystalline Cu-Sb alloy. The test data includes porosity measurements and estimates of grain boundary sliding. Finally, the model has been applied to Voronoi models of polycrystalline structures. In particular the influence of grain boundary sliding on the overall creep rate is demonstrated.

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Keywords: Creep damage; grain boundary sliding; cohesive zone; micromechanical model; polycrystal.

1. Introduction

In many practical applications, creep damage is the limiting factor of a component's lifetime. In an ongoing research, a model has been developed to bridge the scales of the individual creep cavities and of the polycrystal. The link between these scales is a cohesive zone model that accounts for the effective mechanical behavior of the Grain Boundaries (GB) subjected to normal and tangential stresses. It accounts for GB thickening as well as GB sliding.

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The development of the model has been previously presented (Fedelich and Owen, 2009; Vöse et al., 2012; Vöse et al., 2014). The present paper summarizes the model equations and its calibration and introduces first applications to Representative Volume Elements (RVE) of polycrystals.

2. A cohesive zone model for grain boundary creep damage

2.1. Model summary

For an exposition of the theory of GB cavitation under creep loading in metals, the reader may refer to the seminal textbook of Riedel (1987). In the following, the local state of damage on a GB is represented by two variables:

- The surface cavity density $\rho = N_S / S_0$, where N_S is the number of cavities in an element S_0 of the GB surface
- The dimensionless damage variable $\beta = V_S / S_0 \sqrt{\rho}$, where V_S is the cumulated volume of the cavities contained in S_0

Note that the quantity defined by $u_n^{\,p} = V_S / S_0$ corresponds to the average thickening of the GB. Accordingly, β can also be written as $\beta = u_n^{\,p} \sqrt{\rho}$ and thus regarded as the GB thickening scaled by the average cavity spacing. Evolutions equations for these variables

$$\begin{aligned} \dot{\rho} &= \dot{\rho}\left(\rho, \beta; a_{\text{init}}, \tilde{D}_{gb}, \gamma_s, a_p, b_p, \psi\right), \\ \dot{\beta} &= \dot{\beta}\left(\rho, \beta; a_{\text{init}}, \tilde{D}_{gb}, \gamma_s, a_p, b_p, \psi\right), \end{aligned} \tag{1}$$

have been derived by Vöse et al. (2012), and modified and presented in their final form in Vöse et al. (2014). They rely on the detailed simulations of cavitation in an element of GB following the procedure developed by Fedelich and Owen (2009) and Vöse et al. (2012). Cavity growth by GB diffusion and cavity coalescence are considered herein. Cavity nucleation is random and stress driven according to the power law

$$\dot{\rho}^{nucleation} = a_p \left(\frac{\sigma_n}{\sigma_p} \right)^{b_p} \tag{2}$$

for the nucleation rate, where σ_n is the normal stress acting on the GB, σ_p is a reference stress and a_p and b_p are two adjustable model parameters. The remaining parameters in equ. (1) are a_{init} the initial radius of new cavities, ψ the dihedral angle, γ_s the specific energy per unit area and $\tilde{D}_{gb}$ the GB diffusion coefficient. To bridge the cavity scale and the polycrystal scale, the contributions of the individual cavities to GB thickening and stiffness decrease are smeared over the GB, as proposed by Onck and Van der Giessen (1997). The net effect of cavitation at the polycrystal level is represented by the displacement jump

$$\mathbf{u} = \mathbf{u}^{\text{grain 1}} - \mathbf{u}^{\text{grain 2}} = u_n \, \mathbf{n} + u_t \, \mathbf{t}, \tag{3}$$

where $\mathbf{u}^{\text{grain 1}}$ and $\mathbf{u}^{\text{grain 2}}$ are the displacements of material points attached to the adjoining grains along the GB (see Fig. 1) and $\mathbf{n}$ resp. $\mathbf{t}$ is the normal resp. a tangential vector to the GB.