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Micromechanical investigations and modelling of a Copper–Antimony-Alloy under creep conditions

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ABSTRACT

In many practical applications, creep damage is the limiting factor of a component's lifetime. A micromechanical model of creep induced grain boundary damage is proposed, which allows for the simulation of creep damage in a polycrystal within the framework of finite element analysis. The model considers grain boundary cavitation and sliding according to a micromechanically motivated cohesive zone model while creep deformation of the grains is described following the slip system theory. The model can be applied to idealised polycrystalline structures, such as a Voronoi tessellation or, like demonstrated here, to real grain structures of miniature creep specimens. Creep tests with pure Cu single crystals and with a coarse-grained polycrystalline Cu-1 wt.% Sb alloy at 823 K have been performed and used to calibrate the polycrystal model. The grain structure of the polycrystalline Cu–Sb specimens has been revealed by the EBSD method. Extensive grain boundary sliding and cavitation has been observed in the crept specimens. Grain boundary sliding has been found to promote wedge-type damage at grain boundary triple junctions and to contribute significantly to the total creep strain. Furthermore, the assumed stress sensitivity of the models grain boundary cavity nucleation rate strongly influences the development of wedge-type damage.

1. Introduction

The description of the mechanical behaviour of polycrystalline materials that are stressed under creep conditions is an objective in the field of both research and application. Most models rely on a phenomenological description of the macroscopic strain rate in dependency of the applied stress for the prediction of creep rates within a component, like the commonly used Norton law. Some empirical models, such as, e.g., the Wilshire equations provide an effective way for modelling the stress and temperature dependences of the minimum creep rate and of the creep life for a wide range of applied creep conditions (Holmström and Auerkari, 2009; Whittaker and Wilshire, 2010; Wilshire and Battenbough, 2007). However, these and similar models usually consider only uniaxial stress states, which complicates the assessment of real components on the basis of experimental creep curves. Also the extrapolation capabilities are limited since the equations usually have no micromechanical background and therefore can only describe the observed macroscopic behaviour.

The use of continuum damage mechanics is a different way to describe the degradation of creeping materials. Thereby, the constitutive description of the material behaviour is enriched by damage variables, which evolve in dependency of the deformation history. Whereas it was intended in the pioneering works (Kachanov, 1958;

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Rabotnov, 1969), to assign a physical meaning to the damage variables, e.g., the damaged area fraction, the physical meaning of damage variables is often smeared out within practical applications, since the fitting of models usually bases upon the macroscopic creep strain rather than on real damage measurements.

Especially for the description of the long term creep behaviour of polycrystalline materials, a micromechanically motivated creep model is expected to improve the predictions. At low applied stresses, the development of creep damage is related to the nucleation and growth of cavities on grain boundaries (GBs).

One sophisticated approach for modelling creep damage development in polycrystals was proposed by Van der Giessen and co-workers (Onck and van der Giessen, 1997a,b; van der Giessen et al., 1997; van der Giessen and Tvergaard, 1991, 1994a,b,c), who used a cavitation model based on equisized and equispaced cavities (axisymmetric cavity arrangement) to model cavitating GBs within simple polycrystalline structures. An axisymmetric cavity arrangement was first considered by Hull and Rimmer (1959) to estimate the growth rates of cavities by GB diffusion and the initial model has been extended in further investigations, e.g., for the combined influence of GB diffusion and dislocation creep of the adjoining grains on GB cavity growth (Needleman and Rice, 1980). The model of Van der Giessen and co-workers did not consider effects resulting from not equispaced cavities, such as the reduction of cavity growth rates for a clustered cavity arrangement (Chyou and Delph, 1988; Fariborz et al., 1985; Vöse et al., 2012; Yu and Chung, 1990). In turn, it already incorporated cavity growth, cavity nucleation and constraints from the surrounding material by considering a plane strain unit cell of a simple polycrystal. The latter is important, since the constraints exerted by the surrounding material are known to substantially slow down GB cavitation (Dyson, 1976; Eggeler, 1991; Needleman and Rice, 1980; Rice, 1981).

The modelling of an explicit microstructure consisting of several grains allows the calculation of stress redistributions within the polycrystal in consequence of creep deformations. Beside the deformation in the interior of each grain and the deformations caused by GB cavitation, GB sliding can play an important role as well (Onck and van der Giessen, 1997b; Tvergaard, 1985). A Newtonian viscous relation is often applied to GB sliding (Ashby, 1972; Raj and Ashby, 1971), but additional effects can be taken into account, e.g., a threshold stress under which no sliding occurs (Du et al., 2008), or the influence of misorientation between adjacent grains, which was investigated through molecular dynamics simulations (Qi and Krajewski, 2007). Finally, the consideration of a hardening mechanism for GB sliding, which was observed in an experimental study (Raj, 1991), could also improve the physical description of a GB.

In the present work, results of creep tests that have been performed with pure Cu single crystals as well as a coarse-grained polycrystalline Cu-1 wt.% Sb alloy are presented. The single crystal creep tests provide the necessary data to calibrate a crystal viscoplasticity model for Cu under the conditions considered here. The creep tests with the polycrystalline Cu–Sb alloy have been used to characterise the development of creep damage at the scale of the grain structure, with special regard to GB cavitation.

A micromechanical model of a polycrystal has been developed in order to describe the creep damage behaviour of the Cu–Sb alloy. It allows for the simulation of general three-dimensional polycrystalline structures within the framework of finite element analysis (FE analysis), wherein the effects of GB cavitation and sliding are accounted for by a cohesive zone model. Cohesive zone models and elements were originally introduced into FE analysis for the investigation of crack propagation. Cohesive zone models are often called traction-separation laws because the traction vector, which describes the stress state of the interface, is given as a functional relation of the displacement jump (separation). A phenomenological potential function is often used to formulate thermodynamically consistent models (e.g. Turon et al., 2006), in which the traction vector follows from a potential with respect to the displacement jump.

In contrast, the present cohesive model has been derived from detailed simulations of GB cavitation successively developed in Fedelich and Owen (2009), Vöse et al. (2012) and Vöse and Fedelich (2012). The simulations accounted for cavity birth, growth by GB diffusion, coalescence and sintering. It was found that the simulation results could be synthesised by an analytical model of GB thickening under normal stress, which forms the basis of the present work. The resulting GB damage model has been fitted to the experimental data of the Cu–Sb specimens. This data includes estimations of GB sliding as well as direct measurements of GB cavities. The calibrated polycrystal model can be used to simulate creep tests, e.g., in order to investigate the interactions of different creep mechanisms at the microscale under more general loading conditions.

2. Experimental methods

2.1. Materials

A cylindrical Cu–Sb ingot containing 1.01 wt.% Sb (which is henceforth referred to as Cu-1 wt.% Sb for simplicity) was produced using vacuum induction melting. For detailed information on the ingot metallurgy that was used to produce the Cu–Sb ingot the reader is referred to Otto et al. (2011), where the microstructural evolution during casting, annealing and subsequent thermomechanical processing is carefully documented. The cylindrical section of the cast ingot had an outer diameter of 39.4 mm and a length of approximately 90 mm. The as-cast ingot was then encapsulated into a quartz tube under a pure Ar pressure of 500 mbar and annealed for 192 h at 1223 K in order to (a) remove the dendritic features of the as-cast state, (b) dissolve all Sb in the Cu matrix, and (c) coarsen the grain structure. This treatment resulted in a mean grain diameter bigger than 1 mm. A subsequent 48 h anneal was conducted at 823 K in order to establish near-equilibrium segregation of Sb to the GBs. Significant amounts of excess Sb have been shown to be present at