Abstract

In order to include the processes on the scale of the grain structure into the description of the creep behaviour of polycrystalline materials, the damage development of a single grain boundary has been initially investigated in the present work. For this purpose, a special simulation method has been used, whose resolution procedure based on holomorphic functions. The mechanisms taken into account for the simulations include nucleation, growth by grain boundary diffusion, coalescence and shrinkage until complete sintering of grain boundary cavities. These studies have then been used to develop a simplified cavitation model, which describes the grain boundary damage by two state variables and the time-dependent development by a mechanism-oriented rate formulation. To include the influence of grain boundaries within continuum mechanical considerations of polycrystals, an interface model has been developed, that incorporates both damage according to the simplified cavitation model and grain boundary sliding in dependence of a phenomenological grain boundary viscosity. Furthermore a micromechanical model of a polycrystal has been developed that allows to include a material’s grain structure into the simulation of the creep behaviour by means of finite element simulations. Thereby, the deformations of individual grains are expressed by a viscoplastic single crystal model and the grain boundaries are described by the proposed interface model. The grain structure is represented by a finite element model, in which the grain boundaries are modelled by cohesive elements. From the evaluation of experimental creep data, the micromechanical model of a polycrystal has been calibrated for a copper-antimony alloy at a temperature of 823 K. Thereby, the adjustment of the single crystal model has been carried out on the basis of creep rates of pure copper single crystal specimens. The experimental determination of grain boundary sliding and grain boundary porosity for coarse-grained copper-antimony specimens, on the other hand, have been used for the adjustment of the interface model. The calibrated model has finally been used in combination with artificially generated grain structures to investigate influences resulting from numerical and modelling issues. It was found that the mesh size has only a relatively small influence on the macroscopic creep behaviour. But because of the nearly incompressible deformation behaviour of the single crystal model, the use of special purpose continuum element types was necessary to avoid the occurrence of volumetric locking. Also the creep behaviour of polycrystalline materials, which includes the damage development leading to failure, has been analysed for different material and loading parameters. Especially for the copper-antimony alloy under consideration, it becomes evident that the creep behaviour was affected by grain boundary sliding. In particular, stress redistributions at the grain boundaries were comparable to the behaviour of free grain boundary sliding. Furthermore, simulations for multiaxial loading conditions indicated that the damage development is significantly influenced by the maximum principal stress and the von Mises stress.