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Numerical Homogenization of Elastic and Plastic Properties of Polycrystalline Microcomponents

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ABSTRACT

The prediction of macro- and mesoscopic material properties of polycrystalline aggregates using numerical methods in combination with a micromechanical approach attains increasing attention since the effective material behavior can be modeled based on a sound physical basis and hence predicted much more accurately compared to phenomenological approaches. In this presentation we consider the elastic and plastic properties of polycrystalline metals and focus on microcomponents the grain size of which is of the same order of magnitude as the geometrical dimension of the component. As a result, the microstructure, i.e. the crystallographic and morphological texture [3,5] has a significant influence on the macroscopic mechanical behavior and the application of phenomenological material models fails. In order to develop highly stressable microcomponents, the correlation between microstructure and apparent and effective properties [2,7] is of great interest.

Based on the finite element method, we analyze the statistics of the elastic and the plastic properties of microcomponents and polycrystals made of cubic crystals. The predictions are compared to experimental data for Young's modulus, the yield stress, and other mechanical properties [1]. Furthermore, the numerical results are discussed and compared with predictions of classical homogenization theories such as simple and higher-order bounds as well as with perturbation estimates.

The material behavior in the grains is modeled with a crystal plasticity model taking into account elastic and viscoplastic effects [4,6]. The constitutive equations are integrated by the implicit Euler method and linearized consistently. In order to accurately capture the local stress and strain fields in the microcomponents, special emphasis is given to the meshing of the grain structure. A suitable approximation of random grains in the microcomponents is given by a three-dimensional Voronoi

tesselation. In this paper we propose a free meshing technique, which produces not only tri-periodic geometries but also triperiodic meshes. This allows for accurate computations using periodic boundary conditions. The meshing is performed with respect to several constraints which in result gives good quality tetrahedral meshes. In particular the distribution of stress and strain concentrations can only be determined using such free meshing techniques being a disqualifying argument for the so called multi-phase elements. They only deliver accurate mean values, however, no accurate information about the local stresses and strains can be obtained.

The results are as follows. The finite element simulations predict the mean elastic and plastic properties of the microcomponents. Also the scattering of Young's modulus and the yield stress is described accurately. It is found that the results for the specific material considered can be used for estimating the properties of other cubic materials if a proper scaling is applied.

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