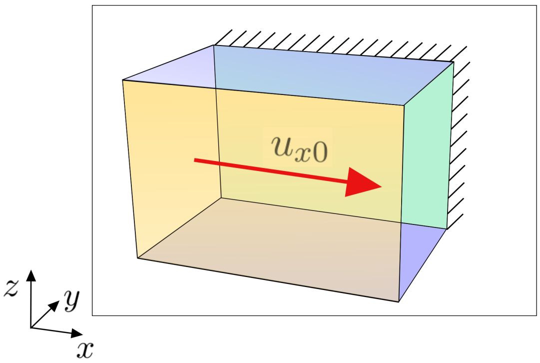
Master Thesis

Andreas Prahs

Misorientation dependent Resistance of Tilt Grain Boundaries against Plastic Flow



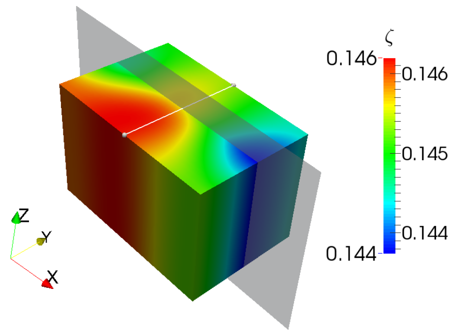


Fig.: Schematic illustration of the used boundary conditions for the simple shear test (left), exemplary result of the investigated bicrystal (right). The light gray plane illustrates the grain boundary.

Problem

In the context of microstructured materials it is essential to discuss non-local mechanical behavior of micro specimens. Strain gradient plasticity theories introduce an internal length scale and thus can be used to investigate size-dependent effects, e.g. the Hall-Petch effect. One major influence on the non-local behavior of crystals with a few grains is the presence of grain boundaries and their resistance against the transmission of dislocations through the grain boundary. This resistance, in general, may depend on a broad variety of micro-material properties like, e.g. , the crystallographic orientation of the adjacent grains. Within this work the misorientation dependency of grain boundaries against plastic flow is investigated.

Approach

Here, a simplified strain gradient plasticity model for small deformations, cf. Wulfinghoff et al. (2013), is extended by the dependency of the grain boundary resistance against plastic flow Ξ_0^C on the geometric mismatch between grains. For this purpose, the grain boundary dislocation density (GBD) according to Evers et al.

(2004) is used as a geometrical criterion to express the total mismatch between all glide systems of two adjacent grains. Hence, the grain boundary resistance is then formulated in dependency of the GBD. The applicability of the GBD for tilt and twist grain boundaries is investigated by analytical and numerical calculations of a bicrystal. For this purpose Finite-Element simulations of shear tests are performed. Further simulations show the difference between the GBD and the classical misfit angle, with respect to their usability as a measure of the misorientation between two grains.

Results

Numerical calculations for two selected twist grain boundaries confirm, that the classic misfit angle between two adjacent grains does not cover enough information to serve as a basis for a description of the misorientation dependency of the grain boundary resistance. A comparison of simulations, for tilt and twist grain boundaries, that consider Ξ_0^C, both, as a constant parameter and dependent on the GBD, is performed with focus on dislocation pile-ups at grain boundaries. It is observed that the used approach to model the dependency of Ξ_0^C on the misorientation of the grains leads to physically meaningful results, in case of tilt grain boundaries. By means of analytical calculations it can be shown, that the used approach only holds for tilt, however, not for twist grain boundaries.

Literature

(1) Wulfinghoff, S.; Bayerschen, E., Böhlke, T.: A gradient plasticity grain boundary yield theory *International Journal of plasticity*. **51**, 33–46, 2013

(2) Gurtin, M.E.; Fried, E.; Anand, L.: *The mechanics and thermodynamics of continua*. University Press, Cambridge, 2010

(3) Evers, L.P.; Brekelmans, W.; Geers, M.: Scale dependent crystal plasticity framework with dislocation density and grain boundary effects *International Journal of Solids and Structures*. **41**, 5209–5230, 2004

(4) Roters, F.; Eisenlohr, P.; Hantcherli, L.; Tjahjanto, D.D.; Bieler, T.R.; Raabe, D.: Overview of constitutive laws, kinematics, homogenization and multiscale methods in crystal plasticity finite-element modeling: Theory, experiments, applications *Acta Materialia*. **58**, 1152–1211, 2010

Advisers

Dipl.-Ing. Eric Bayerschen eric.bayerschen@kit.edu
Prof. Dr.-Ing. Thomas Böhlke thomas.boehlke@kit.edu