STRAIN GRADIENT CRYSTAL PLASTICITY INCORPORATING GRAIN BOUNDARY EFFECTS

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Summary This paper focuses on the micromechanical description of the mechanical response of an FCC multi-crystal microstructure on the basis of geometrical details (grains, orientations, internal/external boundaries) and the physics of the underlying plastic deformation (dislocation driven crystal plasticity). A strain gradient dependent crystal plasticity approach is presented to model the constitutive behavior of polycrystal FCC metals under large plastic deformations. The model is applied to predict the non-homogeneous deformation of a polycrystalline sample including grain boundary effects. The resulting response naturally leads to grain size effects and strengthening of the Hall-Petch type.

INTRODUCTION

Conventional single and polycrystal plasticity models do not explicitly incorporate the influence of inter– and intragranular inhomogeneities in the constitutive description, whereas it is the basic origin of scale dependent behaviour and associated size effects. In general, such inhomogeneities at the microscale can be caused by externally applied macroscopic gradients of plastic deformation, by the presence of grain boundaries locally obstructing the plastic deformation, or by a combination of both. The occurring non-uniform plastic deformations give rise to the development of geometrically-necessary dislocation (GND) densities (preserving crystallographic lattice compatibility) and statistically-stored dislocation (SSD) densities (carrying the crystallographic slip), which physically differ in their role only.

In this paper, a strain gradient enhanced crystal plasticity framework is outlined, based on an extended slip law incorporating a slip resistance and a back-stress, that emerge from the evolution of the SSD, GND, and “grain boundary dislocation” (GBD) densities. Particularly the latter contribution is original, since it has not been addressed in related frameworks like e.g. [1, 2, 4]. The framework is next applied to an example that emphasizes the role of the grain size and grain boundaries in developing hardening effects in plasticity.

STRAIN GRADIENT CRYSTAL PLASTICITY

A non-local crystal plasticity framework has been developed, which incorporates the distinct interactions of various types of dislocation densities. This has been accomplished by including a phenomenological flow rule at the slip system level, which depends on an effective resolved shear stress (τ^{α}_{eff}) and a slip resistance term (s^{α}) [3]. The first one is composed of the ordinary Schmid stress, yet in this case “corrected” by a newly developed back-stress measure, which represents the long-range interactions that are characteristic of GND density fields, because of their specific dislocation sign and relatively large range of influence. It naturally incorporates a kinematic hardening contribution and includes dependencies between various slip systems based on their spatial orientation. The second term –the slip resistance– depends on the short-range interactions between all dislocations on all slip systems present in the material. Whereas the SSD densities are controlled by a “generation-annihilation” evolution equation adopted from literature, the GND densities follow directly

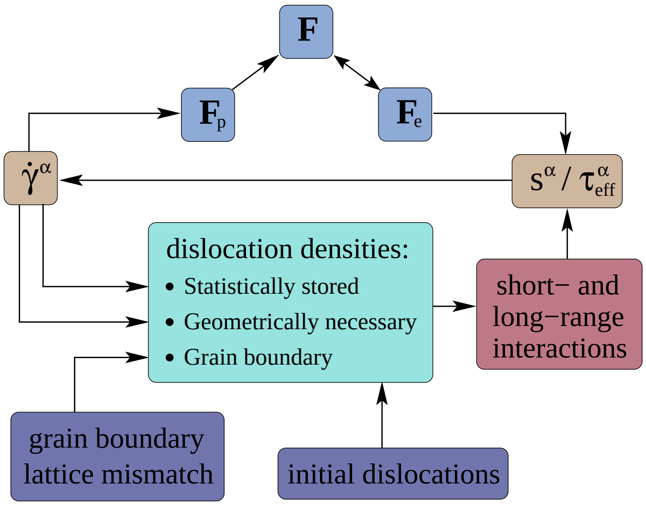


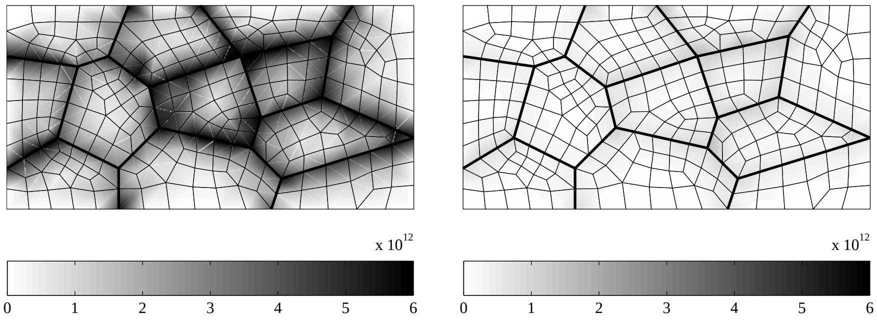
Figure 1. Sketch of the dislocation density based crystal plasticity framework

from the spatial gradients of crystallographic slip (γ^α). Finally, grain boundary dislocation densities (GBD's) have been determined as well, based on the crystallographic lattice mismatch at the grain boundaries. These GBD densities constitute an initial GND density field at the grain boundaries. The dislocation density based crystal plasticity model is outlined schematically in figure 1. Next to the slip resistance as caused by the (short-range) interactions of all SSD's and GND's, any heterogeneity in the GND density field also causes a long-range influence on crystallographic slip, namely through the resulting back-stress contribution. This second influence of the GND densities is caused by the fact that, at a length scale of several orders of magnitude larger than the individual dislocation size, the net effect of the GND densities does not vanish (in contrast to the SSD densities).

The implementation of the entire SSD/GND/GBD density based crystal plasticity framework has been established by means of a weak formulation, consistent linearization and discretization of the governing equations, i.e. the ordinary stress equilibrium condition completed with the GND evolution expression, resulting in a global system of equations to be solved iteratively. Extra nodal degrees of freedom are introduced – i.e. the GND densities– that allow for the specification of various additional boundary conditions which closely approach reality, i.e. dislocation free outer surfaces, strongly obstructed plastic deformation between grains, and an initial GND density field near the grain boundaries.

DEFORMATION OF A POLYCRYSTALLINE SAMPLE, INCLUDING GRAIN BOUNDARY EFFECTS

The mechanical response of a polycrystal sample under plane stress conditions has been simulated for various sample sizes, preserving the grain morphology and the crystallographic orientations. An assembly of grains is therefore considered, in which each grain is discretized in finite elements in order to be able to describe the intragranular inhomogeneities. Obstructing plastic slip at grain boundaries within a plane stress simulation on a polycrystalline sample leads to a grain size dependent flow curve, consistent with a Hall-Petch behaviour. Furthermore, at the grain boundaries, a grain boundary dislocation (GBD) density has been inserted as well, which causes the initial yield stress to be grain size dependent as well. As an example, a plane stress analysis of a polycrystal aluminum sample is presented, for which the geometrical and material parameters are given in [3]. The distribution of the GND's for two different sizes are depicted in figure 2. The SSD density field appears to be nearly size independent, where the largest SSD densities are found in the crystal core, related to the unhindered crystallographic slip in that region. The GND field appears to be strongly size dependent (figure 2), as the plastic inhomogeneities between the grain boundaries and the cores have to be accommodated by the GND field within a varying distance for the different sample sizes. This leads to the observed strengthening.



(a) $L = 1.0$ mm. **(b)** $L = 10$ mm.

Figure 2. Distribution of the characteristic GND density for two sample lengths at an equivalent strain of 1%.

CONCLUSIONS

A strain gradient enhanced crystal plasticity model that incorporates the intrinsic role of dislocations in their various roles (SSD, GND, GBD) provides meaningful micromechanical predictions of inter- and intragranular deformations and associated size or strengthening effects.

References

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