# Master Thesis

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# Finite Element Discretization of the Energy of Inclined Grain Boundaries within a Gradient Plasticity Model

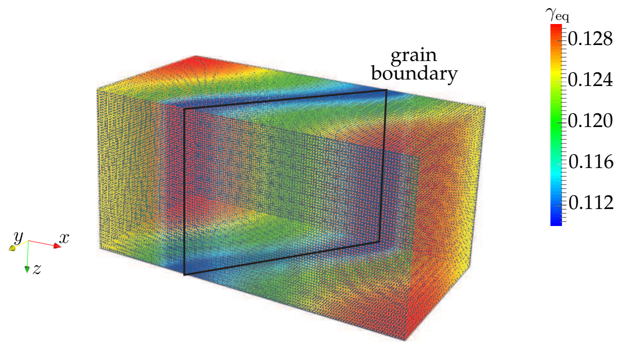


Fig.: Exemplary distribution of the equivalent plastic shear for a non-coplanar grain boundary.

## Problem

A significant contribution to the overall mechanical behaviour of microstructural materials is provided by the interaction of dislocation movement and grain boundaries. As a consequence, polycrystals are observed to respond with a higher strength for smaller grain sizes, a phenomenon which can not be modeled with classical single crystal plasticity theories. Gradient plasticity theories have been developed to describe this size dependency, assuming that grain boundaries commonly either act as impenetrable obstacles or allow unrestricted dislocation movement, cf. Gurtin (2002). By means of an energetic grain boundary energy approach, the grain boundary conditions can be generalized (see, e.g., Wulfinghoff et al., 2013) to allow for a behaviour in between the two idealized limits. The additional energy contribution rises with increasing plastic flow, and consequently stores energy associated to the plastic or defect state of the grain boundary. In order to extend the in-house finite element implementation to incorporate inclined grain boundaries, a discretization strategy is developed.

## Approach

For the discretization of inclined grain boundaries, three discretization approaches are compared and a suitable grain boundary node mapping algorithm including various node weight approaches is developed. The influence of the discretization approaches on the mechanical response is investigated in tensile test simulations of bicrystals for several grain boundary orientations. In addition, the results obtained with the different approaches are compared to results with an exact discretization of the grain boundary.

## Results

An investigation of the influence of various grain boundary orientations shows a linear dependency of the nominal stress at the end of the last time increment on the grain boundary surface area. The parameters to describe this linear behaviour are identical for the investigated discretization approaches, as well as for an exact grain boundary discretization. The increase of the amount of plastically active grain boundary nodes takes place at different rates, which can be explained by the width of each grain boundary implementation and the resulting differences in nodal weights. Regarding the stress-strain curves, it is found that two discretization approaches yield similar results as the exact reference discretization. All three considered approaches offer the benefit to not remesh the geometry if the inclination of the grain boundary is changed, as it would be necessary in the case of an exact discretization.

## 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.: A gradient theory of single-crystal viscoplasticity that accounts for geometrically necessary dislocations *Journal of the Mechanics and Physics of Solids* **50** (1), 5–32, 2002

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