On mesoscale boundary conditions for gradient enhanced crystal plasticity in computational homogenization

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ABSTRACT

Gradient-enhanced crystal plasticity models introduce a length-scale dependency in the predicted inelastic response of polycrystals, whereby experimental findings such as the Hall-Petch effect can be accounted for. In this contribution, we consider variationally consistent selective homogenization (as described in [1]) to a polycrystalline material modeled by gradient-enhanced crystal plasticity. Thereby, the (homogenized) macroscale problem becomes that of a local continuum, while the internal variables "live" only on the underlying mesoscale. We consider both micro-free and micro-hard boundary conditions on the slip fields in the pertinent Statistical Volume Element (SVE). These choices both result in null micro-power expenditure through the boundary of the SVE, whereby a generalized macro-homogeneity condition can be met.

We perform a set of numerical investigations on three-dimensional polycrystalline SVE's of different size (i.e. number of crystal grains) and for different finite element discretization. Each grain has a fcc lattice structure. The orientation of the slip systems, as well as the shape and position of the crystal grains, are randomly generated to mimic an isotropic polycrystal. Several realizations are generated for each SVE-size, whereby statistical analysis of the homogenized response is allowed for. Of particular interest is the influence that SVE boundary conditions has on homogenized quantities, in particular, the macroscale stress. In a similar fashion as in [2], we consider all four different combinations of Dirichlet/Neumann boundary conditions on the displacement and slip fields, and investigate the convergence of the response with increasing size of the SVE and number of random realizations in order to validate bounding characteristics.

REFERENCES

[1] F. Larsson, K. Runesson and F. Su, Variationally consistent computational homogenization of transient heat flow, *Int. J. Num. Meth. Engng,* 2010; **81**:1659–1686

[2] K. Runesson, M. Ekh, F. Larsson, Computational homogenization of mesoscale gradient viscoplasticity, *Comput. Methods Appl. Mech. Engrg*. 2017; in press