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Challenges in the discrete-continuum transition in a crystal plasticity framework

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The need for predicting the behavior of crystalline materials on small-scales has led to the development of physically based descriptions of the motion of dislocations. Several dislocation-based continuum theories have been introduced, but only recently rigorous techniques have been developed for performing meaningful averages over systems of moving, curved dislocations, yielding evolution equations for a dislocation density tensor, see [1]. Those evolution equations provide a physically based framework in describing the motion of curved dislocations in three-dimensional systems. However, unresolved challenges in the transition regime between discrete modeling and continuum approaches come in with the homogenization of stress fields and stress interactions in a dislocation network.

Regarding a self-consistent coarsening of dislocation modelling in order to construct an efficient numerical implementation, several issues have to be solved including calculation of the stress field of a system of dislocations, correlation functions, and boundary conditions. Accurate solutions have been found for one and two dimensional systems [2,3]. However, the understanding and investigation of predictive modelling techniques for determining the dislocation stress interaction over several slip systems on the overall 3D response of a material is a central aspect for the design of new materials and the optimization of currently used materials.

In this presentation, we discuss the role of different dislocation based stress formulations for flow stress and strain hardening in a 3D continuum representation of dislocation microstructures. We consider different approaches of dislocation multiplication mechanisms pointing out the challenges induced by dislocation transport between different slip systems for a continuum formulation. The results are compared to discrete dislocation distributions and discussed with respect to different representative microstructures.

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