LINKING DISLOCATION DYNAMICS TO A CONTINUUM CRYSTAL PLASTICITY FORMULATION

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There are currently two paradigms within the multi-scale materials modeling framework. There is an embedding scheme in which fine scale models are embedded within coarse grained models, and both are solved simultaneously. There is also an information passing scheme in which coarse grained models are informed by the simulation results of fine scale models with both models run independently. Following the second paradigm, a dislocation density-based continuum model of crystal plasticity is developed to interpret dislocation dynamics simulation results. Evolution equations for the growth of crystallographic density and their average segment lengths are derived from observations in dislocation dynamics simulations, and the material constants are determined by fitting the slip activity and dislocation evolution on all of the slip-systems simultaneously from simple tension simulations on a single orientation.

The agreement of the fitted continuum model and dislocation dynamics simulations for another orientation demonstrates that continuum model captures the underlying physics in the dislocation dynamics simulations and that the fitting procedure is robust at the strain levels considered. Comparisons of the two models enabled efficient extraction of the critical phenomena and functional dependencies concerning the growth of dislocation density during the Stage 0 deformation of BCC metals characterized by the elongation of screw dislocations through the motion of edge dislocations and by the multiplication of dislocation sources with ensuing screw motion.

The strength of the current dislocation density-based continuum model lies in its ability to differentiate between the behavior of edge and screw densities providing a consistent framework to model all deformation stages of BCC single crystals; however, more work is needed to extend dislocation dynamics simulations to moderately larger strains and higher dislocation densities before the continuum model informed by information passing from the DD simulations will be able to accurately extrapolate the material behavior at large strains. This study focused mainly on the growth of dislocation density at strains on the order of 0.1 %. Studies must be conducted that also reflect dislocation recovery processes and dislocation forest interactions of screw dislocation densities whose influences were observed to be negligible in the Stage 0 deformation regime.

This work was performed under the auspices of the U.S. Department of Energy by the University of California, Lawrence Livermore National Laboratory under Contract No. W-7405-Eng-48.

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