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Numerical Implementation of Continuum Dislocation Dynamics and Comparison with Discrete Dislocation Simulations

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Plastic deformation of metals is the result of the motion and interaction of dislocations, line defects of the crystalline structure. Dislocation density based modeling of crystal plasticity remains one of the central challenges in multi scale materials modeling. Continuum dislocation dynamics(CDD) is originally based on a higher dimensional dislocation density tensor comprised. We employ a simplified version of CDD obtained by closing a tensor expansion of the higher dimensional theory at low order which yields a CDD of curved dislocations based on only three internal state variables per slip system. These equations define a dislocation flux based crystal plasticity law which does not require distinguishing geometrically necessary and statistically stored dislocations. The evolution equations are solved by a three-dimensional discontinuous Galerkin method guaranteeing the conservation of the total number of dislocations. Different boundary conditions including closed and open boundary conditions are modeled in this work. Closed boundary conditions result in dislocation pile ups at the boundaries of the domain; free boundary conditions allow for out-flow of dislocations through the pillar surfaces. We compare the plastic slip and the resulting dislocation microstructure in simulations of torsion and compression of micro-pillars with results of 3D discrete dislocation dynamics simulations and find that salient features of the dislocation microstructure can be predicted by the continuum dislocation dynamics theory.

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