Abstract Submitted
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Atomistic simulation studies of dislocation patterning in plastic deformation N. SCOTT WEINGARTEN, Catholic University, ROBIN SELINGER, Catholic University — We present the first (to our knowledge) atomistic simulation study of dislocation pattern formation in a crystalline solid. The plastic response of a ductile single crystal under an applied bend depends on the nucleation, motion, and patterning of dislocations. The coalescence of dislocations to form microstructure is difficult to predict using mesoscale models because of the need to select arbitrary rules for defect nucleation, motion, and reactions. In the context of an atomistic simulation, no such approximations are needed. We simulate a Lennard-Jones crystal in two dimensions under an applied bend; the increasing strain gradient requires a growing density of geometrically necessary edge dislocations. When the dislocation density exceeds a threshold value, they coalesce to form tilt boundaries which subdivide the original single crystal into grains. We explore the relationship between rate and size effects in single crystal plasticity at the nanoscale where deformation is dislocation-source limited.

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