

Abstract Submitted
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Atomistic simulation studies of plastic deformation and dislocation patterning as a function of temperature¹ N. SCOTT WEINGARTEN, Physics Dept., Catholic Univ., ROBIN SELINGER, Liquid Crystal Institute, Kent State Univ. — The mechanical properties of crystalline solids depend sensitively on the mechanisms controlling dislocation nucleation, motion, and patterning. To explore the role of thermal activation in these processes, we carry out atomistic Monte Carlo simulation studies of plastic deformation of 2-d single crystals at a range of temperatures. We find that at intermediate temperature, dislocations readily coalesce to form tilt boundaries, while at high temperature, the defects remain disordered in a gas-like phase, suggesting the possibility of an order-disorder phase transition. Conversely, near $T = 0$, dislocation mobility is too low to produce patterning on short time scales, again producing disordered structures. We study also the response of a polycrystalline solid under pure compression and look at the resulting distribution of stresses. We find that the defect-rich grain boundary regions bear higher stresses than those in the bulk, in agreement with Mughrabi's two-component composite theory. Results are compared with recent experiments by L. E. Levine et al.

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Robin Selinger
Liquid Crystal Institute, Kent State Univ.

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