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Anomalous plasticity in defect-mediated phase transformations[1]
PUNAM GHIMIRE, R. RAVELO, University of Texas - El Paso, T.C. GERMANN, Los Alamos National Laboratory — Large-scale molecular dynamics simulations of shocked wave propagation in metallic single crystals exhibit high elastic limits and are ideally suited for investigating the role defect nucleation and multiplication play on the kinetics of phase transformations. Here we report on the morphology and kinetics of shocked-induced phase transformations in Aluminum single crystals. The atomic interactions were modeled utilizing various embedded atom method (EAM) models of Aluminum, with most models exhibiting an artificial fcc→bcc phase transformation in the 25-30 GPa range. For cases where plastic deformation precedes the phase transformation, anomalous defect structures atypical of plastic deformation in bcc lattices nucleate early on but anneal out with time. In all cases, the defect-mediated phase transitions proceed at faster rates than defect-free ones.

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