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Role of plastic deformation in shock-induced phase transitions[1]
PUNAM GHIMIRE, Univ of Texas, El Paso, T.C. GERMANN, Los Alamos National Laboratory, R. RAVELO[2], Univ of Texas, El Paso — Non-equilibrium molecular dynamics (NEMD) simulations of shock-wave propagation in fcc single crystals exhibit high elastic limits and large anisotropies in the yield strength. They can be used to explore the role of plastic deformation in the morphology and kinetics of solid-solid phase transformations. We report on large-scale atomistic simulations of defect-mediated phase transformations under shock and quasi-isentropic compression (QIC). An analytical embedded atom method (EAM) description is used to model a fcc-bcc phase transition (PT) boundary fitted to occur below or above the elastic-plastic threshold in order to model systems undergoing a PT with and without plasticity. For cases where plastic deformation precedes the phase transformation, the defect-mediated PT proceeds at faster rates than the defect-free ones. The bcc fraction growth rate can be correlated with a sharp decrease in the dislocation densities originally present in the parent phase.

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