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Role of plastic deformation in shock-induced phase transitions[1]
PUNAM GHIMIRE, RAMON RAVELO, University of Texas at El Paso, Physics Department — 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. For phase transformations which proceed at pressures below the theoretical elastic-plastic transition pressure no plasticity accompanies the phase change. For cases where plastic deformation precedes the phase transformation, the defect-mediated phase transition proceeds nominally at faster rates than defect-free ones. We examined the effect of plastic deformation and shock propagation direction on shock-induced phase transformation employing large scale non-equilibrium molecular dynamics simulations. The atomic interactions were modeled utilizing embedded atom method (EAM) models, which exhibit a targeted $fcc \longrightarrow bcc$ phase transformation below and above the plastic deformation thresholds.

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