Elastic-plastic structure of shock waves in single crystal copper

R. RAVELO, Univ of Texas, El Paso, B.L. HOLIAN, T.C. GERMANN, Los Alamos National Laboratory — Large-scale atomistic simulations of shock wave propagation in defect-free copper single crystals exhibit an orientation dependent elastic limit and elastic-plastic two-wave regimes for shock propagation along the (110) and (111) low-index directions but not along (100). By contrast, no orientational difference in the Us-Up profiles of single crystals compared with polycrystalline samples has been reported in shock experiments. The elastic-plastic response of copper shocked along (111) was examined via large-scale non-equilibrium molecular dynamics (NEMD) simulations employing samples of up to 3.5 microns in length and particle velocities between 0.5 and 2.5 km/s (20- 130 GPa). The longer time and length scales allow for a more accurate determination of the elastic limit, longitudinal and plastic wave speeds. Results show a steady elastic precursor for particle velocities below 1.6 km/s, which does not decay in time. The NEMD data for the plastic wave velocity in the split-wave regime extrapolates linearly in particle velocity to the shear-wave speed at zero pressure.

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