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Large-Scale Molecular Dynamics Simulations of Shock-Induced Plasticity in Tantalum Single Crystals[1] R. RAVELO[2], University of Texas, El Paso, TX , Q. AN, California Institute of Technology, Pasadena, CA, T.C. GERMANN, B.L. HOLIAN, Theoretical Division, Los Alamos National Laboratory —
We report on large-scale non-equilibrium molecular dynamics (NEMD) simulations of shock wave compression in Ta single crystals. The atomic interactions are modeled via a recently developed and optimized embedded-atom method (EAM) potential for Ta, which reproduces the equation of state up to 200 GPa. We examined the elastic-plastic transition and shock wave structure for wave propagation along the low index directions: (100), (110) and (111). Shock waves along (100) and (111) exhibit an elastic precursor followed by a plastic wave for particle velocities below 1.1 km/s for (100) and 1.4 km/s for (111). The nature of the plastic deformation along (110) is dominated by twinning for pressures above 41 GPa.

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