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Petaflop simulations of shock-induced particulate ejection from copper TIMOTHY C. GERMANN, JAMES E. HAMMERBERG, GUY DIMONTE, Los Alamos National Laboratory — We present the results of several large-scale, Non-Equilibrium Molecular Dynamics (NEMD) simulations of shock-induced surface instability development. We consider single crystal Cu described by an embedded atom method (EAM) potential and driven by a shock wave along the [111] crystallographic direction, impinging upon a roughened Cu/vacuum or Cu/Ne interface. The initial temperature is 300K and the NEMD simulation cell is a quasi-2D $2.23\mu\text{m} \times 5.67\mu\text{m}$ slab geometry, 1.5 nm thick in the (periodic) third dimension. The first third of the sample length ($1.89\mu\text{m}$) is occupied by Cu (5.3×10^8 atoms), and the remainder either empty vacuum or Ne gas at a pressure of 0.67 MPa (1.95×10^8 atoms). The Cu/Ne (or Cu/vacuum) interface has an initial perturbation with average amplitude 30 nm and dominant wavelength of $0.74\mu\text{m}$. A shock wave is created by driving the free end of the Cu slab at a fixed particle velocity $u_p = 2.0$ to 3.5 km/s. Single-mode and multi-mode interfaces were considered using 212,992 CPUs of the LLNL BlueGene/L supercomputer for times approaching 1 ns. At the higher particle velocities, the Cu release state is in the fluid-solid mixed phase. We discuss the evolution of the density and velocity distributions of the ejected mass, the modes of particle breakup, and comparisons to source theories of ejecta formation and Richtmyer-Meshkov instabilities.

Timothy C. Germann
Los Alamos National Laboratory

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