Strain-Rate Dependence of Material Strength: Large-Scale Atomistic Simulations of Defective Cu and Ta Crystals[1] M. ABEYWARD-HANA, A. VASQUEZ, J. GAGLIONE, Univ of Texas, El Paso, T.C. GERMANN, Los Alamos National Laboratory, R. RAVELO[2], Univ of Texas, El Paso — Large-Scale molecular dynamics (MD) simulations are used to model shock wave (SW) and quasi-isentropic compression (QIC) in defective copper and tantalum crystals. The atomic interactions were modeled employing embedded-atom method (EAM) potentials. In the QIC simulations, the MD equations of motion are modified by incorporating a collective strain rate function in the positions and velocities equations, so that the change in internal energy equals the PV work on the system. We examined the deformation mechanisms and material strength for strain rates in the 10^9-10^{12} s^{-1} range For both Cu and Ta defective crystals, we find that the strain rate dependence of the flow stress in this strain rate regime, follows a power law with an exponent close to 0.40.

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