Strain-Rate Dependence of Material Strength: Large Scale Atomistic Simulations of Defective Cu and Ta Crystals

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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 modelled employing embedded-atom method (EAM) potentials. Quasi-isentropic uniaxial compression is achieved by incorporating a strain rate function in the positions and velocities equations of motion. In this new formalism the change in internal energy is exactly equal to the work done in compression. 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.