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A multi-scale, atomistic-based strength model for tantalum and molybdenum DANIEL ORLIKOWSKI, Lawrence Livermore National Laboratory, LIN YANG, JOHN A. MORIARTY — For the description of bcc tantalum and molybdenum strength at the continuum level, we have combined several extensive sets of quantum-based, atomistic calculations into a new parameterization of the Steinberg-Lund (SL) and mechanical threshold stress (MTS) strength models. This model is then used to simulate recent gas-gun shock experiments. The atomistic calculations that determine the parameters of these model were derived from two disparate methods but both based on quantum-based model generalized pseudopotential theory (MGPT) for the ion-ion interactions. In one method, Green's function boundary conditions are used to relax dynamically the boundary forces in molecular dynamics simulations of the kink-pair activation enthalpy and Peierls stress for $(a/2) < 111 >$ screw dislocations. The other method combines MGPT Monte Carlo simulations with full potential linear muffin-tin orbital (FP-LMTO) method of density functional theory to determine the temperature and pressure dependence of the shear modulus. We discuss the new parameterization of the models and hydrodynamic simulation results.

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