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A new nickel EAM potential for atomistic simulations of ablation, spallation, and shock wave phenomena BRIAN DEMASKE, VASILY ZHAKHOVSKY, University of South Florida, CARTER WHITE, Naval Research Laboratory, IVAN OLEYNIK, University of South Florida — A new embedded atom method (EAM) interatomic potential for nickel was developed with the goal to improve upon the predictive power of atomistic simulations of materials at extreme conditions. In contrast to standard approaches for the development of potentials, our methodology focused on accurate sampling of stress tensor components calculated in a wide range of isotropic and uniaxial compression and tensile strains. Also included in the fitting database were experimental properties at standard conditions, such as elastic constants, cohesion energy, vacancy formation, and stacking fault energies. In order to validate the new potential, the liquid-vapor coexistence line, melting line, and shock Hugoniot were calculated. In each case, the new EAM potential was found to be in good agreement with experiment. Preliminary results from simulations of ablation, spallation, and shock wave propagation will be discussed.

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