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Development of Embedded Atom Potential for Aluminum for Simulation of Materials at extreme conditions[1] CHANCE BROWN, East Tennessee State University, BRIAN DEMASKE, VASILY ZHAKHOVSKY, IVAN OLEYNIK, University of South Florida — An embedded atom potential (EAM) potential for aluminum was developed by fitting a wide range of zero-temperature stress tensor components calculated using density functional theory (DFT). The theoretical stress tensor components were calculated for isotropic compressions as well as uniaxial deformations along three principal crystal axes. A number of experimental properties were included within the fitting database to ensure the accuracy of the potential near equilibrium conditions. Out of many candidate potentials, the one that most closely reproduced the experimental melting point and shock Hugoniot data was selected as the final potential. This potential gives a good description of aluminum under extreme pressures and temperatures, making it well-suited for atomistic simulations of laser-matter interactions and shock compression.

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Chance Brown
East Tennessee State University

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