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**MEAM Potentials for Al and Mg Alloys and Interfaces** BOHUMIR JELINEK, SEONG-GON KIM, MARK F. HORSTEMEYER, Mississippi State University, M.I. BASKES, Los Alamos National Laboratory — The ab-initio calculations based on density functional theory (DFT) are performed for the Al and Mg crystals and their alloy in reference structures, such as NaCl structure. The lattice constant (volume), bulk modulus and shear moduli for each element and the alloy are determined from the total energy calculations. These material parameters are then used to determine the Modified Embedded Atom Method (MEAM) potentials for these elements and their alloys. The transferability of these parameters are tested by obtaining relevant physical quantities on structures different than the reference structures and compare them with the results from ab-initio calculations. MEAM potentials determined for these materials are also used to study the properties of alloys and interfaces.

Seong-Gon Kim
Mississippi State University

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