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MEAM potential for Al, Si, Mg, Cu, and Fe alloys BOHUMIR JELINEK, JEFF HOUZE, Mississippi State University, SEBASTIEN GROH, TU Bergakademie Freiberg, SEONG-GON KIM, MARK F. HORSTEMEYER, Mississippi State University, GREGORY WAGNER, Sandia National Laboratories, MICHAEL BASKES, University of California in San Diego — Modified Embedded Atom Method (MEAM) potential for Al, Si, Mg, Cu, and Fe alloys was developed as a combination of existing MEAM potentials for single elements. Pair parameters were constructed based on the structural and elastic properties of element pairs in the NaCl reference structure from ab-initio simulations, and then adjusted to reproduce heats of formation for binary compounds and defect formation energies. Some of the single element MEAM parameters were also improved to better match the generalized stacking fault curve. Validity and transferability of the new MEAM potential was tested by comparison with ab-initio simulations and experiments when available.

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