Abstract Submitted
for the SES06 Meeting of
The American Physical Society

Development and Testing of MEAM Potential for Al-Mg Alloys
BOHUMIR JELINEK, SUNGHO KIM, JEFFERY HOUZE, SEONG-GON KIM, MARK HORSTEMEYER, Mississippi State University, MICHAEL BASKES, Los Alamos National Laboratory — A MEAM potential for Al-Mg alloys was developed based on the elastic and structural properties determined from ab-initio calculations. Transferability of the new potential was tested by comparing various bulk, surface, and point defect properties with ab-initio simulations. Volume-energy dependence of Al and Mg in fcc, hcp, bcc and simple cubic crystal structures from MEAM and ab-initio simulations was determined. Heat of formation for Al-Mg crystals with several different stoichiometries and structures was calculated using both methods. Surface formation, stacking faults, and adsorption energies were also compared. For point defects calculations, a close agreement of vacancy formation energies, interstitial and substitutional point defect energies was found.

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Date submitted: 21 Aug 2006 Electronic form version 1.4