Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Theoretical Approach for Developing Accurate Potentials for Molecular Dynamics Simulations: Thermoelastic Response of Aluminum
J.M. WINEY, Wash. State Univ., A. KUBOTA, Lawrence Livermore Nat. Lab., Y.M. GUPTA, Wash. State Univ. — To achieve the correct thermoelastic response of solids in classical simulations, a new approach is presented for developing accurate interatomic potentials. In this approach, the potentials are fitted to values for the atomic volume and the second- and third-order elastic constants at T = 0K by extrapolating the room temperature values, using classical thermo-mechanical relations. This procedure avoids the low- temperature quantum regime, enabling recovery of the correct response in classical simulations to higher temperature. As an example of this approach, an EAM potential was developed for aluminum. Results using this potential provide consistently better agreement with thermoelastic data at higher temperature compared to previous EAM potentials. Our approach is applicable to the development of other types of potentials as well and is amenable to incorporating the results of first principles calculations performed using the classically extrapolated volume for T = 0K. Work supported by DOE.

Michael Winey
Washington State University

Date submitted: 27 Nov 2007 Electronic form version 1.4