Abstract Submitted
for the SHOCK07 Meeting of
The American Physical Society

Discussion Session: The Quality of Interaction Potentials in Molecular-Dynamics Calculations Under Extreme Conditions B.L. HOLIAN, Los Alamos National Laboratory — How good are the interaction potentials used in classical molecular-dynamics (MD) simulations at high pressures and temperatures? A variety of semi-emprical functional forms have been used in large-scale MD simulations of shockwave phenomena, for example. These potential functions make possible more efficient large-scale simulations of extreme conditions than will (at least for some time to come) be possible by ab-initio quantum-mechanical (QM) MD. The potential-function parameters have traditionally been fitted to experimental properties at low pressures and temperatures, with little information contributed from experiments under extreme conditions. As a result, one can legitimately worry about the quality of MD simulations in such regimes. Modern computational capabilities have enabled the use of many more high-quality QM calculations for high-pressure, zero-temperature properties, which could be of considerable use in extending the phase space for fitting empirical parameters. However, one can ask whether these QM calculations are sufficiently accurate to aid the fitting process, and even more fundamentally, whether the current set of semi-empirical potentials even have the right functional forms. In addition, the effects of high temperatures on the fundamental physics (or chemistry) of the potentials used is almost entirely unexplored territory. Small-scale QM MD could contribute a great deal to this topic, if one were convinced of the quality of those simulations. It is hoped that the members of the audience who have had experience in using any of these semi-empirical potentials, or in generating QM data for fitting their parameters, will share some comments. The time is ripe for new paradigms in the exchange of information between QM and classical MD.

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Date submitted: 27 Mar 2007 Electronic form version 1.4