

Abstract Submitted
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Molecular Dynamics Studies of Dynamical High-Pressure Phase Transitions in Rare-Gas Solids EUGENE PECHENIK, School of Physics and Astronomy, The Raymond and Beverly Sackler Faculty of Exact Sciences, Tel Aviv University, Tel Aviv 69978, Israel, GUY MAKOV, Department of Physics, NRCN, P.O. Box 9001, Beer Sheva, Israel — The phase diagram of pair potential models of rare-gases was studied with respect to the effect of the choice of potential on the nature of the phase diagram. In particular the existence of a high-pressure bcc phase is shown to be potential sensitive. We show using molecular dynamics that the fcc-bcc phase transition cannot be reproduced with the Lennard-Jones (12-6) pair potential, though it is reproduced with the Buckingham pair potential. We propose a simple analytical technique, based on the Einstein theory of a harmonic solid, for predicting an fcc-bcc phase transition in a given system. Using the atomic volume and the pair potential as input, we were able to predict the transition temperature. These findings agree with an earlier work by A. B. Belonoshko et al., Phys. Rev. Lett. 87, 165505 (2001). Additionally, shock wave simulations of several model systems were conducted. The structure of shock wave in this model was examined as a function of shock strength and the existence of a dynamic phase transition was explored.

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