Computer Simulation of Melting and Orientational Transitions in Highly Compressed Solid Nitrogen

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Nosé-Hoover NVT molecular dynamics (MD) was applied to study stability of molecular phases of solid nitrogen at high pressures. Molecules forming the solid were considered as non-rigid strongly bound pairs of atoms. Intermolecular interaction was represented by the sum atom-atom and quadrupolar forces. We have determined the pressure dependence of melting temperature of highly compressed solid nitrogen and examined the influence of the quadrupole interaction on the stability of different solid phases. Results of two types of MD simulations: single-phase and two-phase in the box were compared. We observed turnover of the melting temperature at megabar pressure and discuss its possible explanations. Location of the vibration-rotation transitions between cubic phases in the solid nitrogen were located by monitoring the character of the orientational motion of molecules. The potential model reproduces the properties of dense solid nitrogen and the transition lines between orientationally ordered and disordered high pressure phases. It was found that quadrupolar forces have only a weak influence on the structure, energy and pressure, but significantly affect the stability of the crystalline structures and the location of the melting and orientational transitions on the phase diagram of nitrogen. The study of transitions between phases having different symmetry of crystalline lattice is a serious problem for MD simulation technique. We propose a method to solve this problem which combines MD simulation and theoretical equations of state. The efficiency of this method is demonstrated on prediction of the transition line between FCC and HCP phases at high pressures.