Equation of State for the High-Pressure Polymeric Phase of Solid Nitrogen from Computer Simulation

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The polymeric cubic gauche phase of solid nitrogen, like other covalent structures, may exhibit both negative thermal expansion and essential deviations from the Dulong-Petit law. The thermodynamic behavior of solid nitrogen in the polymeric "cubic gauche" phase at high pressures and non-zero temperatures was studied earlier [1, 2] on the basis of a potential model representing the total energy of polymeric nitrogen crystals as a function of interatomic distances and angles between single chemical bonds attached to each atom. In this work, we present a new extensive set of Monte Carlo data covering the region of negative heat expansion and both negative and positive deviations from the Dulong-Petit law.

A new equation of state for solid polymerized nitrogen based on these simulation results is proposed. It combines the modified Mie-Gruneisen model and anharmonic corrections to the free energy of the solid. The parameters of the model are found on the basis of comparison with MC computer simulation data. An extension of the proposed model to other covalent solids at low temperatures and high pressures is discussed.

[1] L.N. Yakub, *J. Low. Temp. Phys.* **122**, 501 (2001).
[2] L.N. Yakub, *Low Temp. Phys.* **29**, 1032 (2003).