

Thermodynamic Properties of Solid Polymeric Nitrogen

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We discuss the problem of constructing the equation of state (EOS) for polymeric phase of solid nitrogen at extremely high pressures and temperatures. Helmholtz free energy is represented as a sum of the quasi-harmonic contribution described by the modified Mie-Grüneisen model and anharmonic corrections. EOS describes the behavior of the internal energy, thermal expansion, isothermal compressibility, heat capacity, speed of sound, as well as such specific features of polymeric nitrogen as negative thermal expansion and significant deviations of the heat capacity from the Dulong-Petit law, found in our Monte Carlo computer simulation of the nitrogen cubic gauche polymeric phase [1]. Thermodynamic properties predicted on the basis of this EOS are in good agreement with the experimental data measured at extreme pressures [2]. The possibilities of application of the proposed EOS to other substances, with polymerization of the molecules at high densities are discussed.