Thermodynamic Properties and Melting of Nanoparticles

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A self-consistent statistical method recently proposed for the calculation of thermodynamic properties of bulk anharmonic solids [1-3], is used for an investigation of the thermodynamic properties and the premelting phenomena of nanometer-sized particles composed of atoms interacting via central forces. It is shown that the size-dependent reconstruction of the vibrational spectrum in the nanocrystals introduces a particle–size dependence of the parameters of the binary distribution function of atomic displacement in crystals, and, consequently, of the average potential energy of the interaction with the nearest neighboring atoms. These corrections, together with the size-dependent decrease of the contributions to the energy of long-range interatomic interactions, are responsible for the size dependence of the thermodynamic properties of the nanoparticles and the particle-size dependence of the melting temperatures. The comparison of the theoretical results with available experimental data for nanostructures shows good mutual agreement.

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