

Size Influence on Melting and Thermodynamic Properties of Free Nanocrystals

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A self-consistent statistical method is used to describe thermodynamic properties of free spherical nanocrystals. It is shown that size influence on thermodynamic properties of nanocrystals is caused by a size-dependent modification of the vibration spectrum affecting the parameters of a statistical distribution function of atomic displacements and, thus, governing size dependence of average values of energetic contributions to the Gibbs free energy of the system. For Cu and Au nanocrystals, we present calculated size dependences of the Debye temperature, heat capacity, interatomic distance, melting temperature, etc. We show a possibility of reverse heat transfer in a system of nanoparticles – a “heat pump.”