The Dependencies of Lattice Properties Versus of Size and Shape for the Nanocrystals of Diamond, Silicon and Germanium

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A model of nanocrystal in the form of a rectangular parallelepiped with a variable surface shape (RP-model) is used to study of the dependencies of the modulus of elasticity, Poisson's ratio, Young's modulus, shear modulus, coefficient of thermal expansion and heat capacity versus of size and shape of the free-standing nanocrystal of the simple matter. The concrete calculations are done for diamond, silicon and germanium. It is shown that at the isomorphous decrease of size for nanocrystals of diamond, Si or Ge the values: modulus of elasticity, Young's modulus, and shear modulus are decreasing, but functions: Poisson's ratio, coefficient of thermal expansion, and heat capacity are increasing along isotherm. Than nanocrystal shape deviates from the most energetically stable shape (for RP-model it is cube), the more noticeably the changes of mentioned functions at the decrease of the nanocrystal size along of isotherm. The calculations for the nanocrystal of silicon have shown that at the isomorphous reduction of size along isotherm of 100 K the coefficient of thermal expansion at defined size passes from the negative into the positive field.