Size effects in fullerites nanoparticles

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Using the correlative method of unsymmetrized self-consistent field for anharmonic crystals we study structural, dynamical and thermodynamic properties of high-temperature modifications of fullerites. Here we present the results for size effects in C_{70} fine crystalline particles. The intermolecular potential derived by Vertheijen *et al.* is utilized. Anharmonic terms up to the fourth order are taken into account. We have considered three highly symmetrical forms of particles with singular faces: cubical, spherical and octahedral, and calculated size dependences of their mean lattice parameters a and thermal expansion coefficients. Influences of the surface tension and of the lattice relaxation near surfaces have been taken into account. For all three forms of nanoparticles, both values increase with decreasing size, that is a consequence of anharmonicity. This effect is appreciable enhanced when the temperature increases. We also note a dominant contribution of the lattice relaxation to the size dependence of the lattice parameter.