Variational-statistical calculation of the gaseous medium density field in the vicinity of a spherical crystalline nanoparticle

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Using a two-level statistical method for describing the properties of inhomogeneous systems, calculations were performed to determine the micro- and macrostructure, as well as the thermodynamic characteristics of a molecular heterogeneous system consisting of a crystalline nanoparticle, which is in equilibrium with a gaseous macroscopic medium. The interaction between molecules are described using the Lennard-Jones potential. The calculations were performed taking into account the radial spatial relaxation of the parameters of the FCC lattice of a defect-free nanoparticle with site occupation numbers equal to unity ($n = 1$). This means that in a crystalline spherical nanoparticle containing 15 coordination spheres, the presence of thermal vacancies was not taken into account. Near the boundary near the nanoparticle, the radial density profile of the gas medium was approximated using the two-parameter function $n(r_p)$ containing the hyperbolic tangent, i.e. $n(r_p) = a-(a-n_0)th(\kappa\Delta r_p)$. Where p–coordination sphere index number; a and κ–variation parameters; n_0–value of the occupation numbers far from the nanoparticle, which determines the density of the bulk gas homogeneous medium. At the nanoparticle boundary $p = 15$, and its radius is $r_{15} = 4.38\sigma$, σ–linear parameter of the Lennard-Jones potential. For example, for argon $\sigma = 0.3405$ nm, so the radius of the nanoparticle is $r_{15} = 1.49$ nm. The functional $\Omega\{n_p\} = F\{n_p\} - \mu\Sigma n_p$ was varied for different values of the parameters a and κ at a temperature of $\theta = 0.6$, which corresponds to a phase transition between a nanoparticle and a gaseous medium.