The Surface Pressure and the Fragmentation of a Nanocrystal

M.N. Magomedov[C,S]
Institute for Geothermal Research of Dagestan Scientific Centre RAS, Makhachkala, Dagestan, Russia
mahmag@iwt.ru

A nanocrystal in the form of a rectangular parallelepiped faceted by the {100} planes was considered. The nanocrystal is composed of N atoms, of which N_{po} atoms are arranged along the edge of the square base and $N_{ps} = f N_{po}$ atoms occupy the lateral edge of the parallelepiped. The total number of atoms in this system can be defined as $N = f N_{po}^3/\alpha$, where $f = N_{ps} / N_{po}$ is the shape parameter, $\alpha = \pi/(6k_y)$, and k_y is the packing coefficient. The crystal–vacuum interface is assumed to be a Gibbs geometric surface. Within the Einstein model of a vibrational spectrum, at the nearest neighbor approximation, the expression for the function of the surface pressure P_{sf} was obtained. The study of the dependencies $P_{sf}(x_\infty , k_3^*, T_e)$ at the various values of the «quantum parameter» x_∞ , the «size argument» k_3^*, and the relative temperature T_e, resulted in the following:

1. For any substance there is a particular «*temperature of inverse of the size dependence of the surface pressure*»: T_{ei}, where temperature dependences of the surface pressure for all size arguments k_3^* are intercrossed. At the dispersing of a crystal at $T_e < T_{ei}$ the surface pressure is increasing, and at the dispersing at $T_e > T_{ei}$ the surface pressure is decreasing with the diminution of the size argument.
2. For «classical» substances (where $x_\infty < 1$) for the nanocrystal with the given shape and the size there is a particular «*temperature of zero surface pressure*» T_{e0} where dependence of the surface pressure versus temperature is changing a sign: $P_w(k_3^*, T_{e0}) = 0$. At $T_e < T_{e0}$ the surface pressure is squeezing, and at $T_e > T_{e0}$ the surface pressure is stretching nanocrystal.
3. If the value of the surface pressure is sufficiently large, then it can result in the exothermal fragmentation of a nanocrystal. Moreover, the exothermal fragmentation can occur as under compressing, and under spraining surface pressure. Therefore the most optimum condition for the creature and exploitations of a nanocrystal will be such, under which the temperature of a nanocrystal $T_e = \mathrm{T} / \Theta(\infty)$ close to the «temperature of zero surface pressure» T_{e0}.