# Nanocomposites and nanomaterials

## Modeling of the structure of boron nanocrystal. Equilibrium parameters and strength

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The crystal structure of boron is represented in the form of tetrahedron - $B_6$, where each atom forms bonds with neighboring 5-boron atoms. Such a connection is provided by the jumping of boron electrons from one bond to another. Complex $B_6$ involves stable triangular bonds, in contrast to the icosahedral structure. A complex can be ascribed to a cube with side $a$. The energy of the complex $\Phi_0$ is calculated using the a priori pseudopotential method. If $a_0$ is the distance between the boron atoms, then the centers of the complex are at a distance $a = (1+\sqrt{2})\cdot a_0$, where $a$ is the length of the edge of the cube. At minimum energy $\Phi_0$, the equilibrium parameter $a$ = 0,31887nm is determined. When stretching in the direction of Z (perpendicular to the plane (002) of the complex), the maximum strength value is $\sigma_0$ = 102 GPa, and the maximum deformation in this case is – 0.0987.

If the crystal has a limited size, then it is necessary to take into account the surface energy of the crystal when calculating the total energy of the electron-ion system. Because of the symmetric construction of the octahedron, we can state that for each facet of the cube the assigned complex accounts for 1/6 of the energy $\Phi_0$ of the $B_6$ complex, in which case it is possible to estimate the energy of the nanocrystal using a method similar to [1]. For a nanoplate with a thickness $d$ and an infinite basal plane, we have

$$\overline{\Phi} \approx \Phi_0 \left(1 - \frac{1}{3j}\right) \;;\quad j = d/a \;.$$

The average strength of a nanoplate with thickness $d$ will be

$$\bar{\sigma}_p = \sigma_{0.}\left(1 - K_p \cdot d^{-1}\right),$$

Where $\sigma_0$ is the theoretical strength of the bulk crystal in the $Z$ direction. Since the nanoscale is expressed in only one direction, the coefficient $Kp = a / 3$ depends only on the parameter ***a***.

1. Zakarian D. A. Nanoparticles with a diamond-like structure and the inverse Hall – Petch law // Raports of the National Academy of Sciences of Ukraine.-2014.-№ 10. -P.82-86.