Boron nitride nanosystems of regular geometry

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Abstract. The explicit expressions in term of B–N bond length are obtained for atomic site coordinates and intersite distances in regular boron nitride nanotubes and fullerenes. The radii of single-walled BN nanotubes and single-shelled BN fullerenes are estimated, and their most stable associations in form of double-walled nanotubes and double-shelled fullerenes are predicted. The differences between radii of regular boron nitride fullerenes with indexes of \((n+3)\) and \((n)\) are almost equal to the interlayer distance in layered boron nitride structures. Description made for the boron nitride nanosystems of regular geometries may serve as basis for further ground state and electron structure calculations.

1. Introduction
Boron nitride (BN) can be found in forms of one-dimensional diatomic molecule, two-dimensional nanotubular and fullerene surfaces and three-dimensional crystals, like the layered hexagonal h-BN and rhombohedral r-BN, cubic zinc-blende c-BN and wurtzite w-BN, etc. Boron and nitrogen atoms are tetrahedrally coordinated in both c-BN and w-BN crystals. However, unlike the zinc-blende case, in the wurtzite structure there are two different types of nearest-neighbor bonds (both bond lengths are almost equal, whereas the tetrahedral angles are distorted).

Any constituent atom of the h-BN crystal, which corresponds to the boron nitride ground state, may be considered as 3-coordinated because the strong covalent bonding occurs only within the layers, whereas weak van der Waals forces are mostly responsible for interlayer interactions. The h-BN crystal posses a “graphitic” structure with two-layer stacking sequence, while r-BN is characterized by a three-layer stacking. The layers in these layered structures consist of regular hexagons, i.e., 6-membered atomic rings, with vertexes alternatively occupied by B and N atoms. In h-BN crystal, B atoms are placed directly above N atoms and vice versa. Hence, it would be possible to think that the interlayer bonding has some ionicity. However, the electrostatic component is insignificant due to the large interlayer distance. Same is argued by the existence of layered r-BN crystal, in which each subsequent layer is turned, and also by the isolated plane defects and their bundles presented in real layered BN crystals, in which any given atom can be placed above the like atom. Besides, it is possible to obtain turbostratic t-BN and amorphous structures in form of mixtures of the various boron nitride crystalline phases, and multi-walled nanotubular and multi-shelled fullerene-like BN structures. Strong chemical bonding between atoms in given layer and weak interlayer interaction in layered boron nitrides specify an opportunity of the physical and chemical intercalations by various atoms and molecules.
Based upon the similarity of structures of the specified boron nitride phases with those of carbon, it was assumed [1] that alongside with C nanotubes and fullerenes, BN nanotubes and fullerenes should be stable. The latter are hexagonal or mixed BN layers wrapped into cylinders or spheres, respectively. A modified-neglecting-of-diatomic-overlap (MNDO) study of BN analogues of C fullerenes was presented in [2] and B\textsubscript{30}N\textsubscript{30} cage-molecule was predicted to be stable and, consequently, relatively simple to synthesize. In fact, by means of arc-discharge synthesis, BN nanosystems had been obtained both from carbon nanotubes [3] and in carbon-free plasma [4]. Like the bulk boron nitrides, the nanoscale ones are the materials with a diversity of technical and industrial applications. There are various synthesis methods and applications for the BN nanotubes and fullerenes. For those and also for electronic structure and physical properties of BN nanosystems see, for example, reviews [5-7] and references therein.

Design of devices based on nanostructured BN requires knowledge of the sizes of the nanotubes and fullerenes with given indexes. Here this task is solved for the most stable forms. Namely, in next sections, the geometries of regular BN nanotubes and fullerenes are presented. Note that in the figures below, B and N atoms are shown by the black and white circles, respectively; B–N bonds are shown by the solid lines, while auxiliary lines and arcs are dashed.

2. Geometry of regular boron nitride nanotubes

Primarily, the expressions of radii of the zigzag and armchair BN nanotubes in terms of B–N bond length have been obtained considering geometries of such structures (figures 1 and 2).

\[ r_{(n,0)} = \frac{\sqrt{3} d_{(n,0)}}{2} \]

\[ r_{(n,n)} = \frac{\sqrt{3}}{4 \sin \frac{\pi}{2n}} \]

**Figure 1.** Calculation of the zigzag nanotube radius.

The formulas for the radii of \((n,0)\) and \((n,n)\) BN nanotubes \(r_{(n,0)}\) and \(r_{(n,n)}\) are:

\[
\frac{r_{(n,0)}}{d_{(n,0)}} = \frac{\sqrt{3}}{4 \sin \frac{\pi}{2n}},
\]
Here \( d_{(n,0)} \) and \( d_{(n,n)} \) are the B–N bond lengths in zigzag and armchair nanotubes, respectively. Nanotube index \( n = 1, 2, 3, \ldots \) determines the number of atoms because its unit cell consists of \( 2n \) BN formula units.

\[
\frac{r_{(n,n)}}{d_{(n,n)}} = \frac{\sqrt{5 + 4 \cos \frac{\pi}{2n}}}{4 \sin \frac{\pi}{2n}}.
\]  

(2.2)

Figure 2. Calculation of the armchair nanotube radius.

On this basis, radii of the small single-walled BN nanotubes from \((1,0)\) to \((10,10)\) were estimated (table 1). Also, the most stable double-walled nanotubes from \((1,0)@(9,0)\) to \((5,5)@(10,10)\) were predicted (table 2) assuming bond lengths and inter-wall distances as \( d = 1.4457 \) Å and \( c/2 = 3.3306 \) Å, which are the experimental values of the B–N bond length in layers and interlayer distance in h-BN layered crystals, respectively. Actually, \( d_{(n,0)} \) and \( d_{(n,n)} \) depend on \( n \). Therefore, their equilibrium values can not be determined geometrically and can be found by maximizing binding energy of a given nanotube with respect to the B–N bond length. Evidently these dependences have to be weak, and in all cases, \( d_{(n,0)} \) and \( d_{(n,n)} \) can be substituted by the value \( d = 1.4457 \) Å. Analogously, inter-wall distances in all double-walled nanotubes can be approximated by \( c/2 = 3.3306 \) Å.

**Table 1.** Estimated radii \( r_{(n,0)} \) and \( r_{(n,n)} \) of small-sized boron nitride zigzag and armchair nanotubes.

| Nanotubes | Radii, Å |
|-----------|----------|
| \((1,0)\) | 0.63     |
| Double-walled nanotubes | Deviations of difference between radii |
|-------------------------|---------------------------------------|
| (1,0) @ (9,0)           | - 10.5 %                               |
| (1,0) @ (10,0)          | + 1.4 %                                |
| (1,1) @ (10,0)          | - 4.3 %                                |
| (1,1) @ (6,6)           | + 0.5 %                                |
| (2,0) @ (6,6)           | - 1.8 %                                |
| (2,0) @ (11,0)          | + 5.6 %                                |
| (3,0) @ (11,0)          | - 5.4 %                                |
| (3,0) @ (12,0)          | + 6.5 %                                |
| (2,2) @ (11,0)          | - 10.8 %                               |
| (2,2) @ (12,0)          | + 1.1 %                                |
| (4,0) @ (7,7)           | - 3.7 %                                |
| (4,0) @ (13,0)          | + 6.9 %                                |
| (5,0) @ (13,0)          | - 4.8 %                                |
| (5,0) @ (8,8)           | + 5.4 %                                |

**Table 2.** Predicted stable double-walled boron nitride nanotubes built up from regular single-walled ones.
Estimated radii of the single-walled BN nanotubes can be used for a prediction of their most probable combinations in multi-walled structures. Listed pairs as most suitable for formation of the stable double-walled BN nanotubes have been selected from the above calculated single-walled nanotubes. Remaining small divergences in sizes of the neighboring regular nanotubes can be compensated by defects and small chiral distortions. Such transformations of the zigzag or armchair nanotubes into chiral one will be accompanied, respectively, by increase or decrease in their radii. Hence, if the difference in radii between regular nanotubes are more (less) than $c/2$, the nanotube is favored in which the internal wall is zigzag (armchair) and the external wall has armchair (zigzag) structure.

Let us describe the geometries of the zigzag and armchair BN nanotubes using cylindrical coordinates $(\rho, \varphi, z)$.

![Figure 3. Lattice constant of the zigzag nanotube.](image)

\[
\begin{align*}
(3,3) @ (13,0) & \quad -7.2\% \\
(3,3) @ (8,8) & \quad +3.0\% \\
(6,0) @ (14,0) & \quad -4.8\% \\
(6,0) @ (15,0) & \quad +7.2\% \\
(4,4) @ (15,0) & \quad -3.8\% \\
(4,4) @ (9,9) & \quad +3.3\% \\
(7,0) @ (15,0) & \quad -4.7\% \\
(7,0) @ (9,9) & \quad +2.4\% \\
(8,0) @ (16,0) & \quad -4.7\% \\
(8,0) @ (17,0) & \quad +7.4\% \\
(5,5) @ (17,0) & \quad -0.5\% \\
(5,5) @ (10,10) & \quad +3.3\%
\end{align*}
\]
The constant of zigzag \((n,0)\) nanotube one-dimensional lattice equals to \(3d_{(n,0)}\) (figure 3). Its unit cell consists of 4 atomic rings in parallel planes perpendicular to the axis. There are 2 pairs of rings, each consisting of 2 planes with \(n\) boron or \(n\) nitrogen atoms. Evidently, cylindrical coordinate \(\rho\) for all atomic sites equals to the tube radius:

\[
\rho_B = \rho_N = r_{(n,0)},
\]

As for the coordinates \(\varphi\) and \(z\) in the first and second pairs of atomic rings, they equal to

\[
\varphi_B = \varphi_N = 2l\pi / n,
\]

\[
z_B = (3m + 1/2)d_{(n,0)},
\]

\[
z_N = (3m - 1/2)d_{(n,0)},
\]

and

\[
\varphi_B = \varphi_N = (2l + 1)\pi / n,
\]

\[
z_B = (3m - 1)d_{(n,0)},
\]

\[
z_N = (3m + 1)d_{(n,0)},
\]

respectively. Here \(l = 0,1,2,\ldots,n-1\) and \(m = 0,\pm 1,\pm 2,\ldots\) number atomic pairs in given pair of the atomic rings and these rings themselves, respectively.

The constant of the armchair \((n,n)\) nanotube one-dimensional lattice equals to \(2\sqrt{3}d_{(n,n)}\) (figure 4). Its unit cell consists of 2 atomic rings in parallel planes perpendicular to the tube axis. Each ring consists of \(n\) boron and \(n\) nitrogen atoms. Coordinate \(\rho\) for all atomic sites again equals the tube radius:

\[
\rho_B = \rho_N = r_{(n,n)},
\]

The other cylindrical coordinates in the first and second atomic rings, respectively, equal to

\[
\varphi_B = \varphi_1 + 2l\pi / n,
\]

\[
\varphi_N = -\varphi_1 + 2l\pi / n,
\]

\[
z_B = z_N = \sqrt{3}md_{(n,n)},
\]

and

\[
\varphi_B = -\varphi_1 - 2\varphi_2 + 2l\pi / n,
\]

\[
\varphi_N = \varphi_1 + 2\varphi_2 + 2l\pi / n,
\]

Figure 4. Lattice constant of the armchair nanotube.
Here

$$z_B = z_N = \sqrt{3}(m + 1/2)d_{(n,n)}.$$  \hfill (2.16)

Here

$$\sin \varphi_1 = \frac{2 \sin \pi / 2n}{\sqrt{5 + 4 \cos \pi / 2n}},$$  \hfill (2.17)

$$\sin \varphi_2 = \frac{\sin \pi / 2n}{\sqrt{5 + 4 \cos \pi / 2n}},$$  \hfill (2.18)

$l = 0, 1, 2, \ldots, n-1$ and $m = 0, \pm 1, \pm 2, \ldots$, number B or N atoms in atomic rings and these rings themselves, respectively. The geometry of angles $\varphi_1$ and $\varphi_2$ is shown in figures 5 and 6.

**Figure 5.** Geometry of angle $\varphi_1$. 
On this basis, the distances between given atomic site and sites in so-called central atomic pairs are expressed for zigzag tubes ($l = m = 0$ : $\varphi_B = \varphi_N = 0$, $z = d_{(n,0)} / 2$, and $z = -d_{(n,0)} / 2$):

$$\frac{(b_0^0 b_1 - (n,0))}{d_{(n,0)}^2} = \frac{3 \sin^2 \frac{l \pi}{n}}{4 \sin^2 \frac{\pi}{2n}} + 9m^2,$$  \hspace{1cm} (2.19)

$$\frac{(b_0^0 b_2 - (n,0))}{d_{(n,0)}^2} = \frac{3 \sin^2 \frac{(2l + 1) \pi}{2n}}{4 \sin^2 \frac{\pi}{2n}} + \frac{9(2m - 1)^2}{4},$$  \hspace{1cm} (2.20)

$$\frac{(b_0^0 n_1 - (n,0))}{d_{(n,0)}^2} = \frac{3 \sin^2 \frac{l \pi}{n}}{4 \sin^2 \frac{\pi}{2n}} + (3m - 1)^2,$$  \hspace{1cm} (2.21)

$$\frac{(b_0^0 n_2 - (n,0))}{d_{(n,0)}^2} = \frac{3 \sin^2 \frac{(2l + 1) \pi}{2n}}{4 \sin^2 \frac{\pi}{2n}} + \frac{(6m + 1)^2}{4},$$  \hspace{1cm} (2.22)

$$\frac{(b_0^0 b_1 - (n,0))}{d_{(n,0)}^2} = \frac{3 \sin^2 \frac{l \pi}{n}}{4 \sin^2 \frac{\pi}{2n}} + (3m + 1)^2,$$  \hspace{1cm} (2.23)

$$\frac{(b_0^0 n_1 - (n,0))}{d_{(n,0)}^2} = \frac{3 \sin^2 \frac{(2l + 1) \pi}{2n}}{4 \sin^2 \frac{\pi}{2n}} + \frac{(6m - 1)^2}{4},$$  \hspace{1cm} (2.24)

$$\frac{(b_0^0 n_2 - (n,0))}{d_{(n,0)}^2} = \frac{3 \sin^2 \frac{l \pi}{n}}{4 \sin^2 \frac{\pi}{2n}} + 9m^2,$$  \hspace{1cm} (2.25)

$$\frac{(b_0^0 n_2 - (n,0))}{d_{(n,0)}^2} = \frac{2 \sin^2 \frac{(2l + 1) \pi}{2n}}{4 \sin^2 \frac{\pi}{2n}} + \frac{9(2m + 1)^2}{4},$$  \hspace{1cm} (2.26)

and for armchair ($l = m = 0$ : $\varphi_B = \varphi_1$, $\varphi_N = -\varphi_1$, and $z_B = z_N = 0$) tubes:
3. Geometry of regular boron nitride fullerenes

Let us introduce the concept of a regular boron nitride fullerene. The structure of the BN fullerene may be considered regular if it meets certain conditions: (1) structure consists of equal numbers of B and N atoms; (2) only 3-coordinated chemical bonds are realized (i.e. as in layers of h-BN, r-BN, and t-BN crystals, as well as in regular BN nanotubes, but with distinguished valence angles); (3) atomic rings represent plane or broken (along diagonals between B and N sites) regular polygons with even number of vertexes alternatively occupied by B and N atoms. Given definition yields equal B−N bond lengths.

Let us denote this only structural parameter for \( (n) \)-fullerene \( (n=0, 1, 2, 3, \ldots) \) by \( d_{(n)} \).

In general, regular boron nitride \((n)\) fullerene consists of \( n+1 \) parallel atomic rings in northern hemisphere and \( n+1 \) parallel atomic rings in southern hemisphere. If the fullerene index \( n \) equals an integer power of 2 (i.e., \( 2^1=1, 2^2=2, 2^3=4, \ldots \)) then a pair of parallel atomic planes adjacent to the equatorial plane coincides in that plane. There are \( 2n \) atoms, \( n \) B atoms and \( n \) N atoms, in each plane. Then, the chemical formula of a regular BN fullerene should be \( B_2nN_2n \). Let us assume that index \( n \) serves as vertexes of the regular \( 2n \)-gon inscribed in circle with sides alternatively equal to certain parameters \( d_{B,n,m} \) or \( d_{N,n,m} \), which can be calculated as diagonals between certain B and N vertexes in regular \( 2k \)-gon \((k=1, 2, 3, \ldots)\) with vertexes alternatively occupied by B and N atoms and side of \( d_{(n)} \). In particular, when \( m=\pm(n+1) \), i.e., for polar circles, \( d_{B,n,m}=d_{N,n,m}=d_{(n)} \). In other words, polar circles present atomic rings in form of regular \( 2n \)-gons with side of \( d_{(n)} \). For planes with \( m=\pm1 \), which are adjacent or coincide with equatorial plane, only one from these two parameters equals to \( d_{(n)} \), while the remaining parameter designated as \( D_{(n)} \) should be determined separately.

Constructions carried out for small \((n)\) allows us to suggest that there is always a unique assembly of planes or broken (along diagonals between B and N sites) regular polygons with even number of vertexes, alternatively occupied by B and N atoms covering regular BN-fullerene surface without
overlaps or gaps. As the regular fullerene is inscribed in sphere, the spherical or, more precisely, geographical \((r, \varphi, \lambda)\) coordinates are useful to describe atomic site positions. Evidently, the geographical coordinate \(r\) for all atomic sites equals to fullerene radius \(r_{(a)}\),

\[
 r_B = r_N = r_{(a)}. \tag{3.1}
\]

The latitudes \(\varphi\) are determined as

\[
 \varphi_B = \varphi_N = \text{sgn } m \arccos \left( \frac{r_{n,m}}{r_{(a)}} \right), \tag{3.2}
\]

while longitudes \(\lambda\) are

\[
 \lambda_B = \arcsin \left( \frac{d_{B_{n,m}}}{r_{n,m}} \right) + \pi \left( \frac{4l - 3 - (-1)^n}{2n - 1} \right), \tag{3.3}
\]

\[
 \lambda_N = \arcsin \left( \frac{d_{N_{n,m}}}{r_{n,m}} \right) + \pi \left( \frac{4l - 3 - (-1)^n}{2n - 1} \right). \tag{3.4}
\]

Here index \(l = 1, \ldots, n\) numbers B and N atoms in planes.

---

**Figure 7.** Calculation of the radius of atomic ring in a parallel plane.
Figure 8. Calculation of the diagonal $d_{n,k,j}$ between certain B and N vertexes in regular $2k$-gon with vertexes alternatively occupied by B and N atoms and side of $d_{(n)}$.

Radius $r_{n,m}$ of the atomic ring in $m$-plane can be calculated from the following relation (figure 7),

$$r_{n,m}^2 = d_{B,n,m}^2 + 2d_{B,n,m}d_{N,n,m} \cos \frac{\pi \cdot n}{n} + d_{N,n,m}^2$$  \hspace{1cm} (3.5)

For planes with $m \neq \pm 1$, $d_{B,n,m}$ and $d_{N,n,m}$ are certain interatomic distances, which equal to a diagonals $d_{n,k,j}$ (figure 8) between certain B and N vertexes in regular $2k$-gon ($k = 1, 2, 3, \ldots$ and $j = 1, \ldots, k$) with vertexes alternatively occupied by B and N atoms and side $d_{(n)}$:

$$\frac{d_{n,k,j}}{d_{(n)}} = \frac{\sin \frac{\pi j}{2k}}{\sin \frac{\pi}{2k}}.$$  \hspace{1cm} (3.6)

If $m = \pm 1$, i.e., in planes adjacent or coincident with equatorial plane, one from the parameters $d_{B,n,m}$ and $d_{N,n,m}$ equals to $d_{(n)}$, while another equals to parameter $D_{(n)}$ expressed as

$$\frac{D_{(n)}}{d_{(n)}} = \frac{\sin \frac{\pi j_B}{2k_B}}{\sin \frac{\pi}{2k_B}} + \frac{\sin \frac{\pi j_N}{2k_N}}{\sin \frac{\pi}{2k_N}} - 1.$$  \hspace{1cm} (3.7)

where $j_B$ and $j_N$ are the $j$-values in planes with $m = \pm 2$. Stated relation is obtained taking into account that distance between closest atoms in planes with $m = \pm 2$ equals to square diagonal $\sqrt{2d_{(n)}}$ (corresponding drawing is analogous to that for fullerene radius case given below).

And finally, radius $r_{n,m}$ of regular ($n$) fullerene is determined as (figure 9)

$$\frac{2r_{(n)}^2}{d_{(n)}^2} = 1 + \frac{1}{8 \sin^2 \frac{\pi}{n}} \left( \frac{\sin \frac{\pi j_B}{2k_B}}{\sin \frac{\pi}{2k_B}} + \frac{\sin \frac{\pi j_N}{2k_N}}{\sin \frac{\pi}{2k_N}} \right)^2.$$  \hspace{1cm} (3.8)

In particular, in case of $n = 2^0, 2^1, 2^2, \ldots$, i.e., for fullerenes $B_4N_4$, $B_{12}N_{12}$, $B_{24}N_{24}$ etc, planes with $m = \pm 1$ coincide with the equatorial one, and one can obtain the simplified formula (figure 10):
\[ \frac{r_{(e)}^2}{d_{(e)}^2} = \frac{1}{\sin^2 \frac{\pi}{2n}} \left( \frac{3}{4} + \frac{\cos \frac{\pi}{2n}}{\sqrt{2}} \right) \]  

(3.9)

**Figure 9.** Calculation of the regular fullerene radius (general case).
Extrapolating this simplified formula over all regular BN fullerenes and again assuming $d_{(a)} = 1.4457 \, \text{Å}$, their radii have been calculated (table 3). Their most stable aggregates in form of double-shelled fullerenes predicted for inter-shell distances $c/2 \approx 3.3306 \, \text{Å}$ are shown in table 4.

Table 3. Estimated radii $r_{(n)}$ of regular boron nitride fullerenes.

| Regular fullerenes | Radii, Å |
|--------------------|---------|
| (1)                | 1.25    |
| (2)                | 2.29    |
| (3)                | 3.37    |
| (4)                | 4.48    |
| (5)                | 5.58    |
| (6)                | 6.69    |
| (7)                | 7.79    |
| (8)                | 8.90    |
| (9)                | 10.01   |
| (10)               | 11.12   |
| (11)               | 12.23   |
| (12)               | 13.34   |
| (13)               | 14.45   |
| (14)               | 15.56   |
| (15)               | 16.67   |
Table 4. Predicted stable double-shelled boron nitride fullerenes.

| Double-walled fullerenes | Deviations of difference between radii |
|--------------------------|----------------------------------------|
| (1) @ (4)                | −3.0 %                                 |
| (2) @ (5)                | −1.2 %                                 |
| (3) @ (6)                | −0.3 %                                 |
| (4) @ (7)                | −0.6 %                                 |
| (5) @ (8)                | −0.3 %                                 |
| (6) @ (9)                | −0.3 %                                 |
| (7) @ (10)               | 0.0 %                                  |
| (8) @ (11)               | ±0.0 %                                 |
| (9) @ (12)               | ±0.0 %                                 |
| (10) @ (13)              | ±0.0 %                                 |
| (11) @ (14)              | ±0.0 %                                 |
| (12) @ (15)              | +0.0 %                                 |
| (13) @ (16)              | +0.0 %                                 |
| (14) @ (17)              | ±0.0 %                                 |
| (15) @ (18)              | −0.0 %                                 |
| (16) @ (19)              | +0.3 %                                 |
| (17) @ (20)              | +0.3 %                                 |

From table 4 one can find that for regular fullerenes with indexes of \((n)\) and \((n+3)\), deviations of the difference between radii from the expected inter-shell distance value are almost zero. Explanation for that is at \(n \to \infty\) the radius of regular BN fullerene \(r_{(n)} \to \sqrt{3+2\sqrt{2}nd_{(n)}} / \pi\) and then \(r_{(n+3)} - r_{(n)} \to 3\sqrt{3+2\sqrt{2}}d_{(n)} / \pi\). Substituting \(d_{(n)} \to 1.4457\) Å we get \(r_{(n+3)} - r_{(n)} \to 3.3329\) Å which is the almost interlayer distance \(c/2 \approx 3.3306\) Å in layered BN crystals. This result does not seem accidental. Maybe the obtained formula for fullerene radius reveals general relation between intralayer and interlayer structural parameters \(a\) and \(c\) in all layered boron nitride structures, such as layered crystals, multi-walled nanotubes, and multi-shelled fullerenes, \(c/a \approx 2\sqrt{3(3+2\sqrt{2})}/\pi \approx 2.6621\) (in real h-BN layered crystals \(c/a \approx 2.6602\)).

On the basis of the stated relations, the explicit expressions (in term of B–N bond length \(d_{(n)}\)) of the interatomic distances in regular boron nitride fullerene have been obtained:

\[
(B \ n, m', l' - N \ n, m'', l'')^2 = 2r_n^2 - 2\text{sgn} \ m' m'' \sqrt{(r_n^2 - r_{n,m'})^2 + (r_n^2 - r_{n,m''})^2}
\]
4. Summary

From geometrical considerations, we have deduced the explicit expressions for the following parameters of zigzag and armchair BN nanotubes: radii, atomic sites coordinates and intersite distances in terms of $B-N$ bond length and index. We have also introduced concept of the regular BN fullerene and derived analogous expressions for them. In particular, the differences between radii of regular fullerenes with indexes of $n$ and $n'$ are close to the interlayer distance in layered BN crystals. It seems that formula of a regular fullerene radius reveals general relation between intralayer and interlayer structural parameters in all layered boron nitride structures. Using obtained expressions, we made numerical estimations for the small-sized boron nitride single-walled nanotubes and single-
shelled fullerenes and then, based on these estimations, predicted double-walled nanotubes and double-shelled fullerenes.

How can we solve the same task for multi-walled nanotubes or multi-shelled fullerenes? In such cases, it will be necessary to calculate radii of nanotubes or fullerenes with high indexes aiming at selection of the sequences of nanotubes or fullerenes, whose radii are close to an arithmetical progression with arithmetic ratio close to the interlayer distance in layered boron nitride structures. However, only geometrical consideration will be insufficient because in multi-walled or multi-shelled nanosystems there are intermediate layers as well. For this reason, the choice of the most stable structure should be made by comparing change in the binding energy caused by deviation from the equilibrium interlayer distance with that caused by the distortions of the regular structures.

Description made for the regular geometries of the boron nitride nanosystems may serve as basis for further ground state and electron structure calculations. In particular, quasi-classical approach may be used for this purpose (physical theory see in [8,9], and for related mathematical problems like the computing of matrix elements and solving of secular equation see [10-13]), which have already been applied to other structural modifications of boron nitride – diatomic molecule, isolated plane sheet, hexagonal h-BN, cubic c-BN, and wurtzite-like w-BN crystals [14-22]. Recently the relative stability of the ultra-small BN nanotubes has been studied by this approach, and a complex dependence of the molar energy on the radius was obtained [23]. Similar calculations for BN fullerenes should give answers to such questions as: whether the spheroid form or the flattened fullerenes containing defects are energetically more preferable; what are the maximal sizes of regular BN fullerenes, etc. In addition to the geometrical factors, such consideration needs to take into account features characterizing BN nanosystems in view of general equations derived [24] for fluctuations in energy of the small completely open (incompressible) systems. Those equations show that the fluctuations may be large, because there are no restraints on the size of the system; and, besides, fluctuations in total number or partial numbers of atoms in binary systems indirectly contribute to the fluctuations in their energy.

References

[1] Rubio A, Corkill J L and Cohen M L 1994 Phys. Rev. B 49 5081
[2] Xia X, Jelski D A, Bowsner J R and George Th F 1992 J. Am. Chem. Soc. 114 6493
[3] Weng-Seih Z, Cherrey K, Chopra N G, Blasé X, Miyamoto Y, Rubio A, Cohen M L, Louie S G, Zettl A and Gronsky R 1995 Phys. Rev. B 51 11229
[4] Chopra N G, Luyken R J, Cherrey K, Crespi V H, Cohen M L, Louie S G and Zettl A 1995 Science 269 966
[5] Chkhartishvili L S 2006 Thin Films in Optics and Nanoelectronics Neklyudov I M and Shulayev V M (Eds) Kharkiv (KhPTI) 2 367
[6] Chkhartishvili L S 2008 Nanomaterials Neklyudov I M and Shulayev V M (Eds) Kharkiv (KhPTI) 2 23
[7] Chkhartishvili L 2009 Boron Based Solids Chkhartishvili L (Ed) Trivandrum (Research Signpost) (in press)
[8] Chkhartishvili L 2004 Quasi-Classical Theory of Substance Ground State Tbilisi (GTU)
[9] Chkhartishvili L 2006 Quasi-Classical Method of Calculation of Substance Structural and Electronic Energy Spectrum Parameters Tbilisi (TSU)
[10] Chkhartishvili L S 2001 Math. Notes 69 421
[11] Chkhartishvili L S 2004 Trans. GTU 452 15
[12] Chkhartishvili L S 2005 Math. Notes 77 273
[13] Chkhartishvili L S 2009 Math. Notes (in press)
[14] Chkhartishvili L, Lezhava D, Tsagareishvili O and Gulua D 1999 Trans. AMIAG 1 295
[15] Chkhartishvili L, Lezhava D and Tsagareishvili O 2000 J. Solid State Chem. 154 148
[16] Chkhartishvili L and Lezhava D 2001 Trans. GTU 439 87
[17] Chkhartishvili L 2002 Proc. 1st Internat. Boron Symp. Erarslan K (Ed) Kütahya (DU) 139
[18] Chkhartishvili L S 2004 Phys. Solid State 46 2056
[19] Chkhartishvili L 2004 J. Solid State Chem. 177 395
[20] Chkhartishvili L 2006 Proc. TSU (Phys.) 40 130
[21] Chkhartishvili L 2006 Mater. Sci.: An Ind. J. 2 18
[22] Chkhartishvili L S 2006 Phys. Solid State 48 846
[23] Chkhartishvili L S 2009 Nanostruct. Mater. Sci. 1 33
[24] Hill T L and Chamberlin R V 2002 Nano Lett. 2 609