

Polyhedral Model of Carbon Nanotubes Analytically Describing their Geometry

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For carbon nanotubes, there is constructed a geometric model of polyhedral type, which allows the expressing their key structural parameters analytically, as functions of C–C bonds length and nanotube indices. In general, explicit formulas are obtained for 1D lattice constant and radius. Cylindrical coordinates of atomic sites and inter-site distances in carbon nanotubes are additionally found for achiral (zigzag and armchair) nanotubes. ‘Analytic’ geometric model will be useful for theoretical determination of ground-state and electronic structure parameters of carbon nanotubular materials, credible analysis of corresponding experimental data, as well as purposeful designing devices based on nanotubular carbon.

Keywords: Carbon nanotube, Polyhedral model, C–C bond, Nanotube index.

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1. INTRODUCTION

For theoretical determination of ground-state and electronic structure parameters of carbon nanotubular materials, credible analysis of corresponding experimental data, as well as purposeful designing devices based on nanotubular carbon, it is too important to be able to predict reliably the geometry of the nanotubes with given indices and C–C bonds length.

Usually, in studies dealing with carbon nanotubes these structures are assumed to be constructed by rolling up a plane sheet of graphene, which comprises a network of perfect hexagons with carbon atoms at vertices, in the sense that all bond lengths and all bond angles are identical. The rolled-up model [1 – 3] implies that the radius $r_{(n,m)}$ of (n,m) nanotube is given by the expression

$$\frac{r_{(n,m)}}{d_{(n,m)}} = \frac{\sqrt{3(n^2 + nm + m^2)}}{2\pi}, \quad (1)$$

where $d_{(n,m)}$ denotes the C–C bonds length, while $n = 1, 2, 3, \dots$ and $0 \leq m \leq n$ are nanotube indices. The rolled-up model with almost the same success can be applied to nanotubes of other materials with hexagonal structure, like the boron nitride (BN) nanotubes [4]. But, the conventional rolled-up model of nanotubes ignoring curvature effects does not apply to the very interesting case of small radii, for which these effects become significant.

Present work aims analytical determination of general (1D lattice constants and radii) and detailed (atomic sites coordinates and inter-site distances) geometric parameters of carbon nanotubes based on a geometric model of polyhedral type.

2. METHOD

Any real nanotubular surface is polyhedral, but not cylindrical. It was the reason why Cox, Hill and Lee had proposed [5, 6] (see also Review [7]) so-called ‘idealized’

geometric model, which accommodates the mentioned deficiency being based on the exact polyhedral-cylindrical structure. Their model’s basic assumptions give rise to a geometric structure for which all bonds in a nanotube play a truly equal role, unlike conventional one. In particular, according to the ‘idealized’ polyhedral model the Eq. (1) gives only the leading term in the expression of a nanotube radius which, however, should be added by the correction terms. In general, the smaller the tube radius, the larger these corrections become. The main disadvantage of the ‘idealized’ model is that within its frames, the geometric parameters of a given nanotube can be found only as numerical solutions of a complex system of transcendental equations.

For boron nitride nanotubes, Chkhartishvili had suggested [8-13] so-called ‘analytical’ geometric model – a different version of polyhedral model for achiral, i.e. zigzag and armchair, nanotubes with equal bond lengths and also rolled up from a hexagonal plane sheet, but at the same time allowing the explicit expressions of geometric parameters.

To describe a graphitic nanotube as a polyhedron one must begin with the tessellation of regular hexagons where the vertices of the tessellation represent the C-atoms and lines of the hexagons represent C–C chemical bonds. In their model, Cox, Hill and Lee overlay on this a second tessellation of equilateral triangles where the vertices of the triangles are the atoms and every second triangle also has an atom located at its center. The net effect of these two tessellations is a single tessellation of equilateral and isosceles triangles and by fixing the lengths of the sides, which represent bonds, it is possible to construct a truly faceted polyhedron, where all vertices are equidistant from an axis of symmetry and all the bond lengths and bond angles are equal for all atoms. Chkhartishvili’s model of BN-nanotubes geometry uses different method of tessellation: equilateral hexagons in zigzag and armchair sheets are divided into two isosceles trapeziums or one rectangle and two isosceles triangles, respectively. It means that all lines of tessellation are parallel to the tube axis and, therefore, all the atoms are placed on same cylindrical surface. Recently, an

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analogous approach we have successfully used [14] to construct a geometric model for all-boron nanotubes.

Present study is based on the ‘analytical’ geometric model. It is modified for carbon nanotubes and further developed to obtain geometric parameters of chiral nanotubes, analyze cases of ultra-small (degenerated) or ultra-large (asymptotical) radius nanotubes, determine atomic sites coordinates in carbon nanotubes, etc.

3. RESULTS AND DISCUSSION

As is known, a simple form for a single-walled carbon nanotube is a wrapped closed hexagonal atomic surface inscribed in a cylinder. Such nanotubes can be found in achiral, i.e. zigzag $(n,0)$ or armchair (n,n) , and also in chiral (n,m) forms. Here $n=1,2,3,\dots$ and $m=0,1,2,\dots,n$ are the tube indices.

Carbon nanotubes contain 4 different types of atomic sites. Denote them as C1, C2, C3 and C4, respectively. As for the number of atoms in 1D lattice of a nanotube, it equals to $4n$.

Below the detailed regular geometries of the zigzag and armchair carbon nanotubes are described using cylindrical coordinates (ρ, ϕ, z) .

3.1 Zigzag Nanotubes

3.1.1 General Geometric Parameters

1D lattice constant $a_{(n,0)}$ of a zigzag nanotube $(n,0)$ (Fig.1) and its radius $r_{(n,0)}$ are determined as follows:

$$\frac{a_{(n,0)}}{d_{(n,0)}} = 3 \quad (2)$$

and

$$\frac{r_{(n,0)}}{d_{(n,0)}} = \frac{\sqrt{3}}{4 \sin \frac{\pi}{2n}}, \quad (3)$$

where $d_{(n,0)}$ is the C–C bond length in such nanotubes.

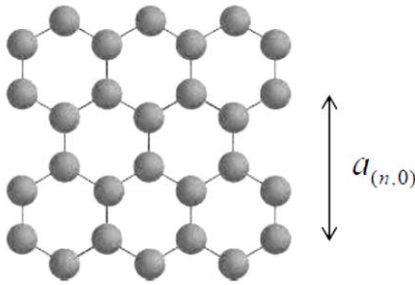


Fig. 1 – Lattice constant of a zigzag nanotube

At $n=1$, zigzag nanotube degenerates into the flat zigzag chain (Fig. 2). Coordination number of constituting atoms reduces from 3 to 2. Nevertheless Eq. (3) ‘works’ providing the true value of the radius of $(1,0)$ tube: $r_{(1,0)} / d_{(1,0)} = \sqrt{3} / 4$.



Fig. 2 – The $(1,0)$ nanotube – flat zigzag chain

Apparently, free-standing $(1,0)$ nanotube cannot exist, but it can exist as inner wall in multi-walled nanotubes or among larger nanotubes in nanotubular bundles.

According to ‘analytical’ model, at $n \gg 1$ the radius of a zigzag nanotube

$$\frac{r_{(n,0)}}{d_{(n,0)}} \approx \frac{\sqrt{3}n}{2\pi}, \quad (4)$$

i.e. being proportional to n asymptotically coincides with that predicted by conventional rolling-up model.

3.1.2 Atomic Sites Coordinates and Inter-site Distances

The 1D unit cell of a zigzag nanotube consists of 4 parallel atomic rings placed in different planes perpendicular to the tube axis. There are 2 pairs of identical rings; and each ring consists of n atoms. Positions of single representative-atoms of each of these rings are shown in Fig. 3. Let’s introduce the additional indices $l=0,1,2,\dots,n-1$ and $k=0,\pm 1,\pm 2,\dots$ numbering atomic pairs in given pair of the atomic rings and these rings themselves.

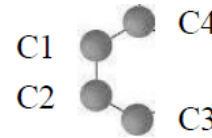


Fig. 3 – Non-equivalent atomic sites in a zigzag nanotube

Evidently, coordinate ρ for all the atomic sites equals to tube radius:

$${}_{(n,0)}^{lk}\rho_{C1} = {}_{(n,0)}^{lk}\rho_{C2} = {}_{(n,0)}^{lk}\rho_{C3} = {}_{(n,0)}^{lk}\rho_{C4} \equiv r_{(n,0)} = \frac{\sqrt{3}d_{(n,0)}}{4 \sin \frac{\pi}{2n}}. \quad (5)$$

As for the coordinates ϕ and z in the first and second pairs of atomic rings, they equal to

$${}_{(n,0)}^{lk}\phi_{C1} = {}_{(n,0)}^{lk}\phi_{C2} = \frac{2l\pi}{n}, \quad (6)$$

$${}_{(n,0)}^{lk}z_{C1} = 3\left(k + \frac{1}{6}\right)d_{(n,0)}, \quad (7)$$

$${}_{(n,0)}^{lk}z_{C2} = 3\left(k - \frac{1}{6}\right)d_{(n,0)}, \quad (8)$$

and

$${}_{(n,0)}^{lk}\phi_{C3} = {}_{(n,0)}^{lk}\phi_{C4} = 2\left(l + \frac{1}{2}\right)\frac{\pi}{n}, \quad (9)$$

$${}_{(n,0)}^{lk}z_{C3} = 3\left(k - \frac{1}{3}\right)d_{(n,0)}, \quad (10)$$

$${}_{(n,0)}^{lk}z_{C4} = 3\left(k + \frac{1}{3}\right)d_{(n,0)}, \quad (11)$$

respectively.

Let's fix l and k at $l=k=0$ to determine the zig-zag nanotube's "central" pair of atomic sites ${}_{(n,0)}^{00}C1$ and ${}_{(n,0)}^{00}C2$:

$${}_{(n,0)}^{00}\phi_{C1} = {}_{(n,0)}^{00}\phi_{C2} = 0, \quad (12)$$

$${}_{(n,0)}^{00}z_{C1} = \frac{d_{(n,0)}}{2}, \quad (13)$$

$${}_{(n,0)}^{00}z_{C2} = -\frac{d_{(n,0)}}{2}, \quad (14)$$

Now one can find the distances between current atomic sites ${}_{(n,0)}^{lk}C1$, ${}_{(n,0)}^{lk}C2$, ${}_{(n,0)}^{lk}C3$ and ${}_{(n,0)}^{lk}C4$, and fixed ones called by us as "central":

$$\frac{({}_{(n,0)}^{lk}C1 - {}_{(n,0)}^{00}C1)^2}{d_{(n,0)}^2} = \frac{3\sin^2\frac{l\pi}{n}}{4\sin^2\frac{\pi}{2n}} + 9k^2, \quad (15)$$

$$\frac{({}_{(n,0)}^{lk}C2 - {}_{(n,0)}^{00}C1)^2}{d_{(n,0)}^2} = \frac{3\sin^2\frac{l\pi}{n}}{4\sin^2\frac{\pi}{2n}} + 9\left(k - \frac{1}{3}\right)^2, \quad (16)$$

$$\frac{({}_{(n,0)}^{lk}C3 - {}_{(n,0)}^{00}C1)^2}{d_{(n,0)}^2} = \frac{3\sin^2\left(l + \frac{1}{2}\right)\frac{\pi}{n}}{4\sin^2\frac{\pi}{2n}} + 9\left(k - \frac{1}{2}\right)^2, \quad (17)$$

$$\frac{({}_{(n,0)}^{lk}C4 - {}_{(n,0)}^{00}C1)^2}{d_{(n,0)}^2} = \frac{3\sin^2\left(l + \frac{1}{2}\right)\frac{\pi}{n}}{4\sin^2\frac{\pi}{2n}} + 9\left(k + \frac{1}{6}\right)^2, \quad (18)$$

$$\frac{({}_{(n,0)}^{lk}C1 - {}_{(n,0)}^{00}C2)^2}{d_{(n,0)}^2} = \frac{3\sin^2\frac{l\pi}{n}}{4\sin^2\frac{\pi}{2n}} + 9\left(k + \frac{1}{3}\right)^2, \quad (19)$$

$$\frac{({}_{(n,0)}^{lk}C2 - {}_{(n,0)}^{00}C2)^2}{d_{(n,0)}^2} = \frac{3\sin^2\frac{l\pi}{n}}{4\sin^2\frac{\pi}{2n}} + 9k^2, \quad (20)$$

$$\frac{({}_{(n,0)}^{lk}C3 - {}_{(n,0)}^{00}C2)^2}{d_{(n,0)}^2} = \frac{3\sin^2\left(l + \frac{1}{2}\right)\frac{\pi}{n}}{4\sin^2\frac{\pi}{2n}} + 9\left(k - \frac{1}{6}\right)^2, \quad (21)$$

$$\frac{({}_{(n,0)}^{lk}C4 - {}_{(n,0)}^{00}C2)^2}{d_{(n,0)}^2} = \frac{3\sin^2\left(l + \frac{1}{2}\right)\frac{\pi}{n}}{4\sin^2\frac{\pi}{2n}} + 9\left(k + \frac{1}{2}\right)^2. \quad (22)$$

3.2 Armchair Nanotubes

3.2.1 General Geometric Parameters

1D lattice constant $a_{(n,n)}$ of an armchair nanotube (n,n) (Fig. 4) and its radius $r_{(n,n)}$ are determined as follows:

$$\frac{a_{(n,n)}}{d_{(n,n)}} = \sqrt{3} \quad (23)$$

and

$$\frac{r_{(n,n)}}{d_{(n,n)}} = \frac{\sqrt{5 + 4\cos\frac{\pi}{2n}}}{4\sin\frac{\pi}{2n}}, \quad (24)$$

where $d_{(n,n)}$ is the C-C bond length in such nanotubes.

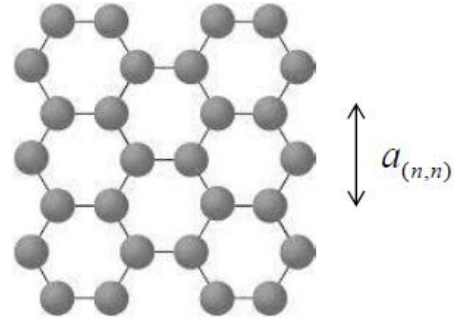


Fig. 4 – Lattice constant of an armchair nanotube

Even the smallest ($n=1$) armchair nanotube does not degenerate: coordination number of atoms constituting (1,1) tube remains 3, as normally. This tube is faceted by 2 pairs of planes (Fig. 5). Its radius is determined by the Eq. (24): $r_{(1,1)} / d_{(1,1)} = \sqrt{5} / 4$.

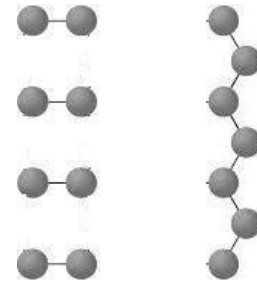


Fig. 5 – Facets of the (1,1) nanotube

Because of strong curvature effects, forming of a free-standing (1,1) nanotube seems to be too doubtful. However, it can exist as inner wall in multi-walled nanotubes or among larger nanotubes in nanotubular bundles.

According to the "analytical" model, at $n \gg 1$ the radius of an armchair nanotube

$$\frac{r_{(n,n)}}{d_{(n,n)}} \approx \frac{3n}{2\pi}, \quad (25)$$

i.e. asymptotically is proportional to n and coincides with that predicted by conventional model.

3.2.2 Atomic Sites Coordinates and Inter-site Distances

The 1D unit cell of an armchair nanotube consists of 2 parallel atomic rings in planes perpendicular to the tube axis. From its part, each ring consists of n pairs of carbon atoms. Positions of pairs of representative atoms of each of these rings are shown in Fig. 6. Now indices $l=0,1,2,\dots,n-1$ and $k=0,\pm 1,\pm 2,\dots$ number atomic pairs in atomic rings and these rings.

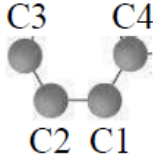


Fig. 6 – Non-equivalent atomic sites in an armchair nanotube

The coordinate ρ for all the atomic sites should equal to the tube radius:

$$\begin{aligned} \rho_{(n,n)C1}^{lk} &= \rho_{(n,n)C2}^{lk} = \rho_{(n,n)C3}^{lk} = \\ &= \rho_{(n,n)C4}^{lk} \equiv r_{(n,n)} = \frac{\sqrt{5 + 4 \cos \frac{\pi}{2n}} d_{(n,n)}}{4 \sin \frac{\pi}{2n}}, \end{aligned} \quad (26)$$

while the rest cylindrical coordinates in the first and second atomic rings equal to

$$\phi_{(n,n)C1}^{lk} = \phi_1 + \frac{2l\pi}{n}, \quad (27)$$

$$\phi_{(n,n)C2}^{lk} = -\phi_1 + \frac{2l\pi}{n}, \quad (28)$$

$$z_{(n,n)C1}^{lk} = z_{(n,n)C2}^{lk} = \sqrt{3}kd_{(n,n)}, \quad (29)$$

and

$$\phi_{(n,n)C3}^{lk} = -\phi_1 - 2\phi_2 + \frac{2l\pi}{n}, \quad (30)$$

$$\phi_{(n,n)C4}^{lk} = \phi_1 + 2\phi_2 + \frac{2l\pi}{n}, \quad (31)$$

$$z_{(n,n)C3}^{lk} = z_{(n,n)C4}^{lk} = \sqrt{3} \left(k + \frac{1}{2} \right) d_{(n,n)}, \quad (32)$$

respectively. Here

$$\sin \phi_1 = \frac{2 \sin \frac{\pi}{2n}}{\sqrt{5 + 4 \cos \frac{\pi}{2n}}} \quad (33)$$

and

$$\sin \phi_2 = \frac{\sin \frac{\pi}{2n}}{\sqrt{5 + 4 \cos \frac{\pi}{2n}}}. \quad (34)$$

Let's fix l and k at $l=k=0$ to determine the armchair nanotube's "central" pair of atomic sites ${}_{(n,n)}^{00}C1$ and ${}_{(n,n)}^{00}C2$:

$$\phi_{(n,n)C1}^{00} = \phi_1, \quad (35)$$

$$\phi_{(n,n)C2}^{00} = -\phi_1, \quad (36)$$

$$z_{(n,n)C1}^{00} = z_{(n,n)C2}^{00} = 0. \quad (37)$$

The distances between current atomic sites ${}_{(n,n)}^{lk}C1$, ${}_{(n,n)}^{lk}C2$, ${}_{(n,n)}^{lk}C3$ and ${}_{(n,n)}^{lk}C4$, and fixed "central" sites are determined as:

$$\frac{({}_{(n,n)}^{lm}C1 - {}_{(n,n)}^{00}C1)^2}{d_{(n,n)}^2} = \frac{\left(5 + 4 \cos \frac{\pi}{2n}\right) \sin^2 \frac{l\pi}{n}}{4 \sin^2 \frac{\pi}{2n}} + 3k^2, \quad (38)$$

$$\frac{({}_{(n,n)}^{lm}C2 - {}_{(n,n)}^{00}C1)^2}{d_{(n,n)}^2} = \frac{\left(2 \sin \left(l - \frac{1}{2}\right) \frac{\pi}{n} + \sin \frac{l\pi}{n}\right)^2}{4 \sin^2 \frac{\pi}{2n}} + 3k^2, \quad (39)$$

$$\begin{aligned} \frac{({}_{(n,n)}^{lm}C3 - {}_{(n,n)}^{00}C1)^2}{d_{(n,n)}^2} &= \\ &= \frac{\left(5 + 4 \cos \frac{\pi}{2n}\right) \sin^2 \left(l - \frac{1}{2}\right) \frac{\pi}{n}}{4 \sin^2 \frac{\pi}{2n}} + 3 \left(k + \frac{1}{2}\right)^2, \end{aligned} \quad (40)$$

$$\begin{aligned} \frac{({}_{(n,n)}^{lm}C4 - {}_{(n,n)}^{00}C1)^2}{d_{(n,n)}^2} &= \\ &= \frac{\left(\sin \left(l + \frac{1}{2}\right) \frac{\pi}{n} + 2 \sin \frac{l\pi}{n}\right)^2}{4 \sin^2 \frac{\pi}{2n}} + 3 \left(k + \frac{1}{2}\right)^2, \end{aligned} \quad (41)$$

$$\frac{({}_{(n,n)}^{lm}C1 - {}_{(n,n)}^{00}C2)^2}{d_{(n,n)}^2} = \frac{\left(2 \sin \left(l + \frac{1}{2}\right) \frac{\pi}{n} + \sin \frac{l\pi}{n}\right)^2}{4 \sin^2 \frac{\pi}{2n}} + 3k^2, \quad (42)$$

$$\frac{({}_{(n,n)}^{lm}C2 - {}_{(n,n)}^{00}C2)^2}{d_{(n,n)}^2} = \frac{\left(5 + 4 \cos \frac{\pi}{2n}\right) \sin^2 \frac{l\pi}{n}}{4 \sin^2 \frac{\pi}{2n}} + 3k^2, \quad (43)$$

$$\begin{aligned} \frac{({}_{(n,n)}^{lm}C3 - {}_{(n,n)}^{00}C2)^2}{d_{(n,n)}^2} &= \\ &= \frac{\left(\sin \left(l - \frac{1}{2}\right) \frac{\pi}{n} + 2 \sin \frac{l\pi}{n}\right)^2}{4 \sin^2 \frac{\pi}{2n}} + 3 \left(k + \frac{1}{2}\right)^2, \end{aligned} \quad (44)$$

$$\begin{aligned} \frac{({}_{(n,n)}^{lm}C4 - {}_{(n,n)}^{00}C2)^2}{d_{(n,n)}^2} &= \\ &= \frac{\left(5 + 4 \cos \frac{\pi}{2n}\right) \sin^2 \left(l + \frac{1}{2}\right) \frac{\pi}{n}}{4 \sin^2 \frac{\pi}{2n}} + 3 \left(k + \frac{1}{2}\right)^2. \end{aligned} \quad (45)$$

3.3 Chiral Nanotubes

From above obtained expressions of achiral nanotubes' 1D lattice constants and radii, it is easy to construct extrapolation formulas for a chiral nanotube (n, m) lattice constant $a_{(n,m)}$ and radius $r_{(n,m)}$:

$$\frac{a_{(n,m)}}{d_{(n,m)}} \approx \sqrt{3 \left(3 - \frac{2m}{n} \right)} \quad (46)$$

and

$$\frac{r_{(n,m)}}{d_{(n,m)}} \approx \frac{\sqrt{3 + \frac{2m}{n} \left(1 + 2 \cos \frac{\pi}{2n} \right)}}{4 \sin \frac{\pi}{2n}}, \quad (47)$$

where $d_{(n,m)}$ is the C–C bond length in this nanotube.

Thus, according to the ‘analytical’ model at $n \gg 1$ the radius of a chiral nanotube

$$\frac{r_{(n,m)}}{d_{(n,m)}} \approx \frac{\sqrt{3n(n+2m)}}{2\pi}, \quad (48)$$

i.e. asymptotically approximates that predicted by conventional rolling-up model.

3.4 Example of Geometric Model Based Structural Analysis

It has been reported [15] an on-chip Rayleigh imaging technique using wide-field laser illumination to measure optical scattering from individual single-walled carbon nanotubes with high spatial and spectral resolution. This method in conjunction with calibrated atomic force microscopy accurately measures the diameters $2r_{(n,m)}$ for a large number of tubes in parallel. The technique was applied for fast mapping of key structural parameters, including the chiral indices (n, m) for individual single-walled carbon nanotubes. The values of diameters and indices experimentally determined are listed in Table 1.

Table 1 – Experimental and theoretical diameters of single-walled carbon nanotubes

No	Chiral indices	Experimental diameter, nm	Theoretical diameter, nm	Relative deviation
1	(13, 1) [(11, 3)]	1.07	1.10 [1.07]	2.7 % [0.0 %]
2	(15, 0)	1.19	1.18	0.8 %
3	(12, 11)	1.58	1.58	0.0 %
4	(20, 4) [(19, 4)]	1.77	1.85 [1.77]	4.3 % [0.0 %]
5	(22, 2) [(20, 4)]	1.83	1.87 [1.85]	2.1 % [1.1 %]
6	(15, 14)	1.99	1.99	0.0 %
7	(20, 9) [(18, 10)]	2.04	2.16 [2.05]	5.6 % [0.4 %]
8	(23, 5) [(21, 6)]	2.05	2.16 [2.06]	5.1 % [0.5 %]
9	(16, 15)	2.13	2.13	0.0 %
10	(25, 10) [(24, 9)]	2.48	2.62 [2.49]	5.3 % [0.4 %]

In the present work, we have calculated same nanotubular diameters based on the ‘analytical’ polyhedral model for given indices and C–C bonds length of 0.142 nm, the bond length value in graphene. These theoretical results also are shown in Table 1. One can see that for all these species relative deviations from theory do not exceed 5.6 %. Agreement with experiment can be radically improved – made all deviations less than 1.1 % – if slightly, not more than in ± 2 , change chiral indices of some nanotubes. Refined values of chiral indices, radii and corresponding deviations are shown in brackets. Note that, within the frames of experimental errors, the refined theoretical diameters of a half of examined species are indistinguishable (with relative deviation 0.0 %) from that of measured ones.

The possibility of refinement in nanotube’s chiral indices based on its geometric model reveals the experimentally obtained fact that frequent chirality-changing structural defects accompanied with only slight diameter-changes are characteristic for single-walled carbon nanotubes. Consequently, it is not improbable that measured values of diameter, on the one hand, and chiral indices, on the other hand, are attributed to different parts of the same nanotube.

Such a possibility seems to be very important because electronic and other physical properties of single-

walled nanotubes depend on their structure, which may be characterized by the diameter and the chirality encoded by two integers – nanotube indices. Usually, for the synthesis of carbon nanotubes one may achieve some control over their diameters but little control over their chiralities. As such tubes may be either metallic or semiconducting this poor structural control implies a rather poor control over their electronic properties. This is a basic problem of carbon nanotechnology. It was stated and clearly explained elsewhere [16].

4. CONCLUSION

In conclusion, we have introduced the ‘analytic’ geometric model of polyhedral type for single-wall carbon nanotubes. The model provides with expressions of nanotubes 1D lattice constant and radius, and cylindrical coordinates of constituent C-atoms and corresponding inter-atomic distances as explicit functions of C–C bond length and chiral indices. Radii of carbon nanotubes calculated on the basis of this model are in excellent agreement with measured ones. Besides, the model is able to refine the chiral indices of these nanotubes.

‘Analytic’ geometric model will be useful in calculations of electronic structure and key physical properties of carbon nanotubular materials, as well as designing novel nanodevices based on nanotubular carbon.

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