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The Generalization of the Polyhedral Model for Carbon Nanotubes

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Abstract

In the present work a few expresions have been established in order to determine nanotubes subnanometer diameter type "armchair" and "zig-zag" proposing a different geometrical configuration than the one used to elaborate the polyhedral model in the speciality literature. The geometrical configuration proposed implies the mathematical demonstrations from the distorted graphene sheet,the cutting of the graphene sequence from the distorted network being made the same way as the conventional model.

Key words: *SWNT, cylindrical structures, polyhedral model*

Introduction

The recent studies in the carbon nanostructure domain mark a special interest in the nanotubes subnanometer category (the nanotubes diameter contained in the domain 3-7 Å) [1], [2], [3]. The existence of a nanotube with 3Å diameter has been confirmed [1],[3] situated in the multi-wall nanotubes (MWNT) interior obtained with the arc discharge method in alternating current into the atmosphere with a low content of hydrogen. The results of the probability density function minimization demonstrates that the nanotube with the approximate 3Å diameter has a configuration type „armchair" with the chiral indices (2;2) [4]. The interatomic bonds formed by each hybrid atom sp^2 with the first grade neighbours have different lenghts: $l_{C_2C_3} = l_{C_2C} \equiv l_1 = 1{,}50\,\text{Å}$, $l_{C_1C_2} \equiv l_2 = 1{,}38\,\text{Å}$, while the angles between the bonds have the values: $\gamma_{C_2C_3C_4} \equiv \gamma_1 = 119{,}7^\circ$, and $\gamma_{C_1C_2C_3} \equiv \gamma_2 = 110{,}8^\circ$.

In accordance with the configuration suggested by other autors [4] we obtain the layout of the carbon atoms in the top of a triangular pyramid with only one symmetrical plan in the mirror (fig. 1, *b*). By accepting the representative polyhedral model for the subnanometer nanotubes [5], this imposes the configuration of a regulated triangular pyramid with three symmetrical planes in the mirror (fig. 1, *a*), where the interatomic bond lengths are equal and the angles between them are equal.

In this work a few expresions have been established to determine the nanotubes diameter type „armchair" and „zig-zag" considering as a geometrical configuration a tiangular pyramid with only one symmetrical plan in the mirror.

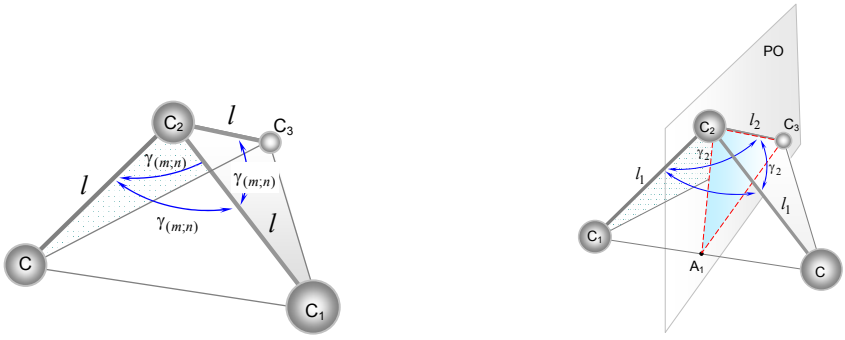


Fig. 1. (a) The noncomplanar configuration formed by an sp^2 hybrid carbon atom with his first grade neighbours (b) noncomplanar distorted configuration formed by an sp^2 hybrid atom with his first grade neighbours

The Establishment of the Nanotubes Diameter Type Armchair

Knowing that the establishment of the chirality of one nanotube is made by cutting off a graphene sequence followed by its rolling, the geometrical configuration proposed initiations the mathematical demonstrations from the distorted graphene sheet (fig. 2). The cutting of the graphene sequence from the distorted network is made similar to the conventional model [6].

Fig. 2 presents a distorted grephene network which by rolling will lead to the obtaining of a nanotube type „armchair" C(4,4) (fig. 3 (a)). The 3D image of the triangular pyramide obtained after the rolling of the graphene sheet is presented in figure 3 (b). The grey arrows point the conversion from 2D to 3D after rolling. For the understanding of the pyramid model application for the subnanometer nanotubes case, in figure 3(c) is presented the triangular pyramid layout in a configuration type „armchair".

In figure 3 (c) we can notice that $\overline{C_2C_1} = l_2$, $\overline{C_2C_3} = \overline{C_2C} = l_1$, $\overline{C_3C_1} = \overline{CC_1} = d_2$, $\angle C_3C_2C = \gamma_1$, $\angle C_1C_2C_3 = \angle C_1C_2C = \gamma_2$. In the triangles ΔC_3C_2C and ΔC_3C_1C, $\overline{C_2A_1}$ and $\overline{C_1A_1}$ are heights and results that $\overline{C_3A_1} = \overline{A_1C} = \frac{d_1}{2}$, $\angle C_3C_2A_1 = \angle A_1C_2C = \frac{\gamma_1}{2}$, $\angle C_3C_1A_1 = \angle A_1C_1C = \frac{\alpha}{2}$.

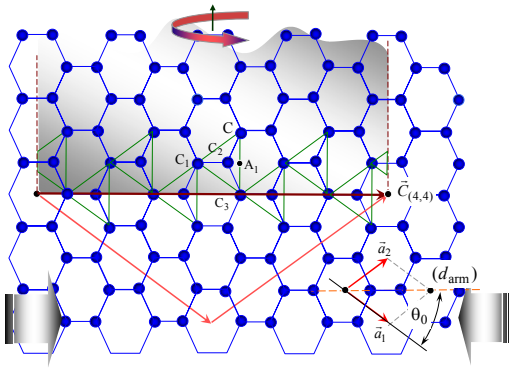
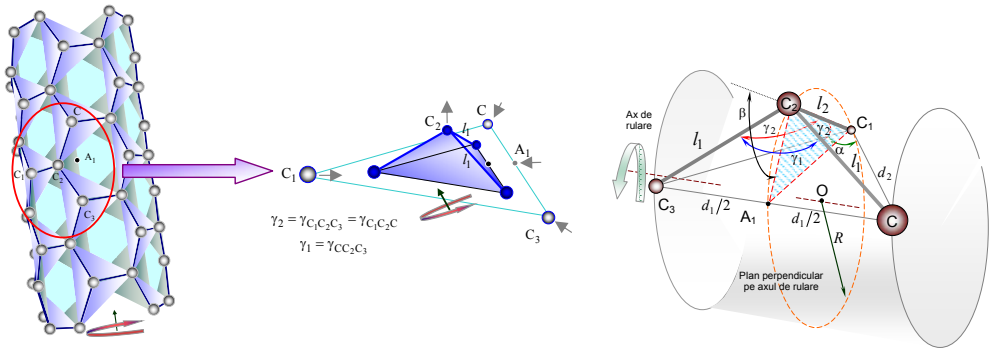


Fig.2. The distorted graphene network



(a) (b) (c)

Fig.3. The representation of the „armchair" type nanotube with the chiral indices (4,4) according to the polyhedral model.
(a) SWNT nanotube C(4,4) type
(b) 3D image of the triangular pyramide,
(c) The pyramides layout in a „armchair" type configuration

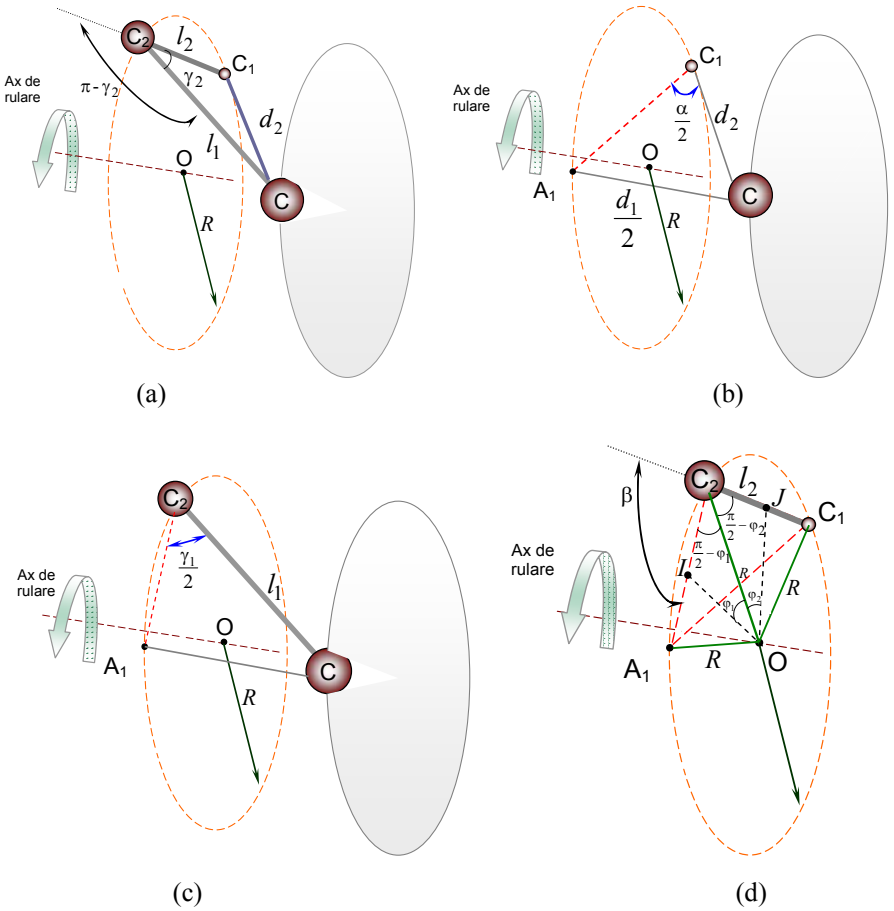


Fig. 4. Fragments from figure 3 (c)

To calculate the "armchair" type nanotube diameter, figure 4 presents representative fragments for the mathematical demonstration from figure 3 (c).
Using Pitagora's generalized theorem for the triangle from figure 4 (a) results:

$$\left.\begin{array}{l}\overrightarrow{C_1C} = \overrightarrow{C_1C_2} + \overrightarrow{C_2C} \\ \angle\left(\overrightarrow{C_1C_2}, \overrightarrow{C_2C}\right) = \pi - \gamma_2\end{array}\right\} \Rightarrow d_2^2 = l_2^2 + l_1^2 + 2l_1 l_2 \cdot \cos(\pi - \gamma_2) = l_2^2 + l_1^2 - 2l_1 l_2 \cdot \cos\gamma_2 \,. (1)$$

In figure 4 (b) we can observe that from the right-angled triangle ΔA_1C_1C with $\angle C_1A_1C = \frac{\pi}{2}$,

$$\sin\frac{\alpha}{2} = \frac{\overline{A_1C}}{d_2} \Rightarrow \overline{A_1C} = d_2 \sin\frac{\alpha}{2}, \tag{2}$$

$$\cos\frac{\alpha}{2} = \frac{\overline{A_1C_1}}{d_2} \Rightarrow \overline{A_1C_1} = d_2 \cos\frac{\alpha}{2} = d_2\sqrt{1-\sin^2\frac{\alpha}{2}}\,. \tag{3}$$

In figure 4 (c) from the right-angled triangle ΔA_1C_2C with $\angle C_2A_1C = \frac{\pi}{2}$ results that:

$$\sin\frac{\gamma_1}{2} = \frac{\overline{A_1C}}{l_1} \Rightarrow \overline{A_1C} = l_1 \sin\frac{\gamma_1}{2}, \tag{4}$$

$$\cos\frac{\gamma_1}{2} = \frac{\overline{A_1C_2}}{l_1} \Rightarrow \overline{A_1C_2} = l_1 \cos\frac{\gamma_1}{2}\,. \tag{5}$$

From figure 4 (d) we can observe that the right-angled triangle $\Delta A_1C_2C_1$ is inscribed in a circle and by drawing a radius from each point from the circle results two triangles ΔC_2OA_1 and ΔC_2OC_1.

From the triangles ΔC_2OA_1 and ΔC_2OC_1 with the heights $\overline{OI}$ and $\overline{OJ}$ results:

$$\overline{A_1I} = \overline{IC_2} \Rightarrow \overline{IC_2} = \frac{\overline{A_1C_2}}{2}, \tag{6}$$

$$\overline{C_2J} = \overline{JC_1} \Rightarrow \overline{C_2J} = \frac{\overline{C_2C_1}}{2}\,. \tag{7}$$

Bearing in mind the expressions (6) and (7) and noting with $\angle C_2OI = \varphi_1$ and $\angle C_2OJ = \varphi_2$, from the right-angled triangle ΔC_2IO and ΔC_2JO results that:

$$\sin\varphi_1 = \frac{\overline{IC_2}}{C_2O} = \frac{\overline{IC_2}}{R} = \frac{\overline{A_1C_2}}{2R} = \frac{\overline{A_1C_2}}{D}, \tag{8}$$

$$\left.\begin{array}{l}\sin\varphi_2 = \dfrac{\overline{JC_2}}{C_2O} = \dfrac{\overline{JC_2}}{R} = \dfrac{\overline{C_2C_1}}{2R} = \dfrac{\overline{C_2C_1}}{D} \\ \overline{C_2C_1} = l_2\end{array}\right\} \Rightarrow \sin\varphi_2 = \frac{l_2}{D}, \tag{9}$$

where *D* represents the circles diameter.

From the expressions (5) and (8) it results that:

$$\sin \varphi_1 = \frac{l_1}{D} \cos \frac{\gamma_1}{2}. \tag{10}$$

Knowing that $\overline{C_2C_1} = l_2$ and bearing in mind the expressions (2) and (3) results that:

$$\overline{A_1C_1} = \sqrt{d_2^2 - \overline{A_1C}^2}. \tag{11}$$

From the expressions (4) and (11) results that:

$$\overline{A_1C_1} = \sqrt{d_2^2 - l_1^2 \sin^2 \frac{\gamma_1}{2}}. \tag{12}$$

Using Pitagora's generalized theorem for the triangle $\Delta A_1C_2C_1$ and considering the expressions (5) and (12) results that:

$$\left.\begin{array}{l} \overrightarrow{A_1C_1} = \overrightarrow{C_1C_2} + \overrightarrow{A_1C_2} \\ \angle\left(\overrightarrow{C_1C_2}, \overrightarrow{C_2A_1}\right) = \beta \end{array}\right\} \Rightarrow d_2^2 = l_2^2 + l_1^2 + 2\, l_2\, l_1 \cdot \cos \frac{\gamma_1}{2} \cdot \cos\beta. \tag{13}$$

From the expressions (1) and (13) results that:

$$\cos\beta = -\frac{\cos\gamma_2}{\cos\frac{\gamma_1}{2}}. \tag{14}$$

In figure 4 (d) we can observe that:

$$2\beta_{(\text{fotoliu})} = 2(\varphi_1 + \varphi_2) = \frac{2\pi}{2m}, \tag{15}$$

where, 2*m* is the number of sides of equal lenght of $\overline{A_1C_1}$ from the regular polygon which is inscribed in the nanotubes circumference and at the same time, *m* represents the chiral nanotubes indices (*m*, *m*).

Considering the expressions (9), (10) and (14) we obtain the nanotubes „armchair" type diameter:

$$D_{(\text{"armchair"})} = \sqrt{\frac{l_1^2 \cdot \cos^2 \frac{\gamma_1}{2} + l_2^2 - 2 l_1 l_2 \cdot \cos\gamma_2}{1 - \frac{\cos^2\gamma_2}{\cos^2\frac{\gamma_1}{2}}}}. \tag{16}$$

Establishing the Nanotube Type „Zig-zag" Diameter

Given the diameter of a „zig-zag" type nanotube generated by rolling a graphene sequence where the chiral vector is $\vec{C}_{(m,0)}$ type is establised in the same way. The afferent drawing for this case is custom for $m = 5$. In a distorted graphene network there are multiple circumstances to define a elementary cells vectors $\vec{a}_1$ and $\vec{a}_2$. It is demonstrated that whichever the pair $\vec{a}_1$

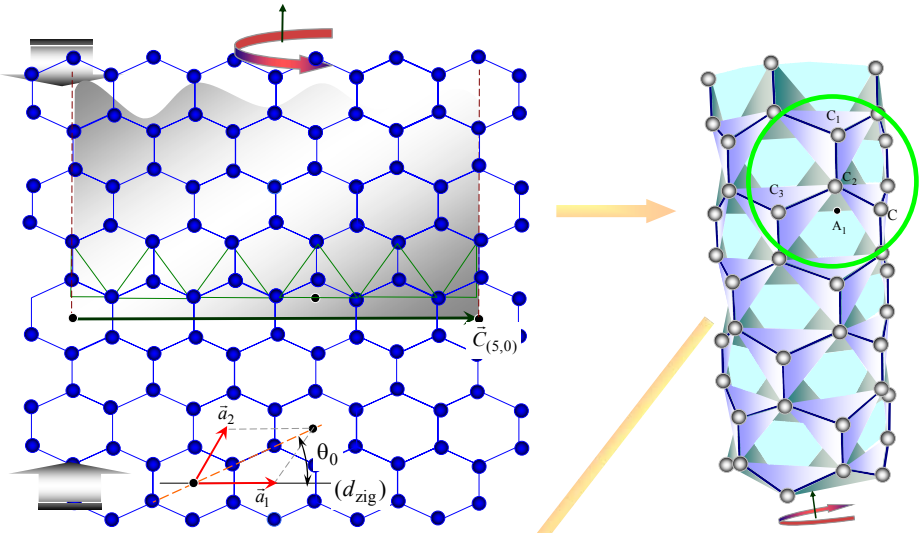
and $\vec{a}_2$ may be the elementary cells area is the same, this contains two carbon atoms in positions dependent on the choice made.

However the zig-zag configuration as it was defined in the applicable conventional model on the ideal graphene sheet points the fact that one of the interatomic bonds needs to be situated along the cylinders generatix obtained by rolling.

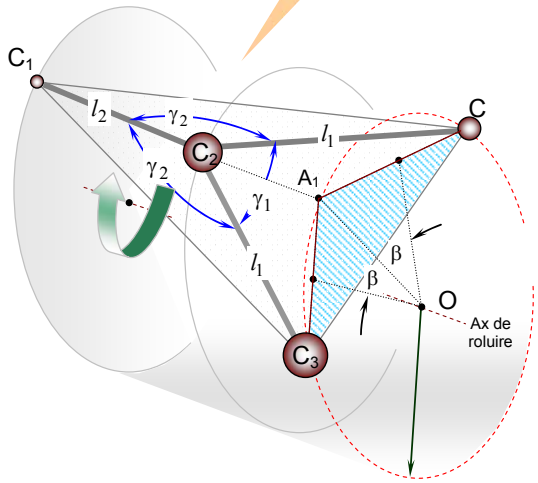
For this reason the „zig-zag" configuration will be obtained by a adequate choice of the $\vec{a}_1$ and $\vec{a}_2$ elementary vectors (figure 5, *a*).

If we cut out a sequence from the distorted graphene sheet defined by the $\vec{C}_{(5;0)}$ chiral vector and this is rolled according to the polyhedral model, all five aquilateral triangles "listed" along the chiral vector will be transformed in triangular pyramides (figure 5, *b*).

In figure 5 (c) the pyramides orientation is presented so that every top side is situated on the rolling cylinder.



(a) graphene distorted network (b) C(5,0) type SWNT nanotube



(c) The pyramides layout in a "zig-zag" configuration

Fig.5. The „zig-zag" type representation of the nanotube with the (5,0) chiral indices, according to the polyhedral model

The pyramid layout on the cylinders rolling surface shows that the $\overline{C_3C}$ chord view angle is $4\beta_{(\text{zig-zag})}$ and it needs to be *m* times 2π rad more to obtain a regulary polymonial in the nanotubes transverse section namely:

$$\beta_{(\text{zig-zag})} = \pi / 2m \,, \tag{17}$$

where *m* is the chiral indice of the vectors $\vec{C}_{(m,0)}$ for the general case.

Using the same demonstration as the one used for the „armchair" type nanotube, by analysing figure 5 (c) we obtain:

$$\cos\beta_{(m;0)} = \sin(\gamma_1 / 2) / \sin\gamma_2 \tag{18}$$

and the diameter of the „zig-zag" type nanotube marked with $D_{(m;0)}$ is:

$$D_{(m;0)} = l_1 \sin\gamma_2 / \sqrt{1-[\sin(\gamma_1 / 2) / \sin\gamma_2]^2} \,. \tag{19}$$

By replacing $l_{C_2C_3} = l_{C_2C} \equiv l_1 = 1{,}50\,\text{Å}$, $l_{C_1C_2} \equiv l_2 = 1{,}38\,\text{Å}$, and $\gamma_{C_2C_3C} \equiv \gamma_1 = 119{,}7^\circ$, $\gamma_{C_1C_2C_3} = \gamma_{C_1C_2C} \equiv \gamma_2 = 110{,}8^\circ$, the nanotubes calculated diameter with the expression (16) is $D_{(2;2)} = 2{,}8075\text{Å}$. This result is identical with the one obtained by a energy bond minimization method and confirmed by the HRTM measurings ($2{,}81\text{Å}$) [1], [7]. For the chirality establishment for this nanotube the expression (16) will be kept in mind. So, the accounts lead to the result $\beta_{(\text{fotoliu})} = 45^\circ$. Therefore, in the presented configuration in the reference [4], $m = 180/[2\beta_{(\text{fotoliu})}] = 2$ value adequate for an „armchair" type nanotube with the chiral indices (2,2). If the same results are used in a „zig-zag" type arranging then it's established that $\beta_{(m;0)} = 22{,}33^\circ$, so that, $m = 4$ will result a „zig-zag" type nanotube diameter, $D_{(4;0)} = 3{,}6904\,\text{Å}$.

By replacing in expression (16) $l_1 = l_2 = l = 1{,}44\,\text{Å}$, considering $\gamma_1 = \gamma_2 = \gamma$ and marking $D_{(\text{"}armchair\text{"})}$ with $D_{(m,m)}$ will obtain:

$$D_{(m,m)} = 0{,}5\sqrt{3}\, l_{CC^{(2)}} \sin\gamma_{(m,m)} / \sqrt{\cos^2[\gamma_{(m,m)} / 2] - \cos^2\gamma_{(m,m)}} \tag{20}$$

and

$$\cos\beta_{(m,m)} = -\cos\gamma_{(m,m)} / \cos[\gamma_{(m,m)} / 2] \,, \tag{21}$$

$$2\beta_{(m,m)} = 2(\varphi_1 + \varphi_2) = \pi / m \,. \tag{22}$$

As we can observe,the expressions (20), (21) and (22) are established for the nanotubes obtained by rolling ideal graphene sheet.

By considering the different chiralitys of the armchair type nanotube we obtain the values from table 1. The values from the lines 1, 2 and 3 according to the (2,2), (3,3) and (4,4) chirality established according to the expressions (19), (20) and (21) are identical with the ones obtained with the polyhedral model proposed in the reference [5]. This showes that the expressions proposed in this work can be used for the diameter calculation for all „armchair" type nanotubes.

The (2,2) nanotubes diameter doesn't match with the value established in the reference [4], forasmuch the described nanotube in this reference comes from the rolling of a distorted graphene sheet.

Table 1. Data ragardind the regulary triangular faced pyramide of the "armchair" type nanotube with three symmetrical layouts in the mirror

Chiral index	$\beta_{(m;m)} = 90/m$	$\gamma_{(m;m)}$ (°)	$D^{(p)}_{(m;m)}$ (Å)	$R^{(p)}_{(m;m)}$ (Å)
(2;2)	**45.00**	**112.9787**	**2.9410**	**1.4705**
(3;3)	30.00	**116.9321 (̊)**	**4.2517**	**2.1258(̊)**
(4;4)	22.50	**118.2852 (̊)**	**5.5950**	**2.7975(̊)**
(5;5)	18.00	**118.9058**	**6.9511**	3.4755
(6;6)	15.00	**119.2414**	**8.3135**	4.1568
(7;7)	12.86	**119.4432**	**9.6796**	4.8398
(8;8)	11.25	**119.5740**	**11.0480**	5.5240
(9;9)	10.00	**119.6635**	**12.4178**	6.2089
(10;10)	9.00	**119.7276**	**13.7887**	6.8944
(11;11)	8.18	**119.7749**	**15.1604**	7.5802
(12;12)	7.50	**119.8109**	**16.5326**	8.2663
(13;13)	6.92	**119.8389**	**17.9053**	8.9526
(14;14)	6.43	**119.8611**	**19.2783**	9.6392
(15;15)	6.00	**119.8790**	**20.6516**	10.3258
(16;16)	5.63	**119.8937**	**22.0251**	11.0126
(17;17)	5.29	**119.9058**	**23.3989**	11.6994
(18;18)	5.00	**119.9160**	**24.7727**	12.3864
(19;19)	4.74	**119.9246**	**26.1467**	13.0734
(20;20)	4.50	**119.9320**	**27.5208**	13.7604

$D^{(p)}_{(m;m)}$, $R^{(p)}_{(m;m)}$ - established diameters and radius according to the polyhedral model considering $l_{CC^{(2)}} = 1{,}44\,\text{Å}$.

For the armchair type nanotubes for which $m > 14$ (for example) the $\gamma_{(m,m)}$ angles values are very close to $120°$ involving more "relaxed" interatomic bonds regarding the subnanometer nanotubes.

Thus the l_{CC} interatomic bond length can be identified with the one experimental established for the graphene sheet case from a $l_{CC} = 1{,}426\,\text{Å}$ microcrystal and not the value used by [5].

For this kind of nanotubes the established diameter values according to the polyhedral model are very close to the one established according to the conventional model.

By replacing $l_1 = l_1 = l = 1{,}44\,\text{Å}$, in expression (19) considering $\gamma_1 = \gamma_2 = \gamma$ the diameter $D_{(m,0)}$ is:

$$D_{(m,0)} = l_{CC^{(2)}} \sin\gamma_{(m,0)} / \sqrt{1 - \sin^2[\gamma_{(m,0)}/2] / \sin^2\gamma_{(m,0)}}\,. \tag{23}$$

Expressions (17) and (18) will become:

$$\beta_{(m,0)} = \pi/2m\,, \tag{24}$$

$$\cos\beta_{(m,0)} = \sin[\gamma_{(m,0)}/2] / \sin\gamma_{(m,0)}\,. \tag{25}$$

Using $l = 1{,}44\,\text{Å}$ as a interatomic bond length will result the zig-zag nanotubes primary characteristic, presented in table 2.

Table 2. Data ragardind the regulary triangular faced pyramide of the "zig-zag" type nanotube with three symmetrical layouts in the mirror

Chiral Indices	$D^{(p)}_{(m;0)}$ (Å)	$R^{(p)}_{(m;0)}$ (Å)	$\gamma_{(m;0)}$ (°)	$\beta_{(m,0)}$ (°)
(2;0)	**2.0365**	**1.0182**	**90.0000**	**45.0000**
(3;0)	**2.9057**	**1.4529**	**109.4712**	**30.0000**
(4;0)	**3.4249**	**1.7125(*)**	**114.4698(*)**	**22.5000**
(5;0)	**4.1680**	**2.0840(*)**	**116.5651(*)**	**18.0000**
(6;0)	**4.9283**	**2.4641(*)**	**117.6521(*)**	**15.0000**
(7;0)	**5.6983**	**2.8492(*)**	**118.2912(*)**	**12.8571**
(8;0)	**6.4744**	**3.2372(*)**	**118.6996(*)**	**11.2500**
(9;0)	**7.2545**	3.6273	**118.9767**	10.0000
(10;0)	**8.0374**	4.0187	**119.1736**	9.0000
(11;0)	**8.8224**	4.4112	**119.3185**	8.1818
(12;0)	**9.6088**	4.8044	**119.4283**	7.5000
(13;0)	**10.3964**	5.1982	**119.5135**	6.9231
(14;0)	**11.1849**	5.5924	**119.5809**	6.4286
(15;0)	**11.9741**	5.9871	**119.6352**	6.0000
(16;0)	**12.7639**	6.3820	**119.6796**	5.6250
(17;0)	**13.5542**	6.7771	**119.7164**	5.2941
(18;0)	**14.3449**	7.1725	**119.7471**	5.0000
(19;0)	**15.1360**	7.5680	**119.7731**	4.7368

Bearing in mind that the angle formed by the sp^2 hybrid carbon atom is 120^o and for the sp^3 hybridized carbon atom is $109,47^o$, results that a „zig-zag" type nanotube with the indices (2,0) can't be obtained experimentaly.

For a graphene sheet defined by the $\vec{C}_{(3;0)}$ chiral vector particular case, after its rolling, the angles between the interatomic bonds have the same $\gamma_{(3;0)} = 109,47^\circ$ value according to the expression (24), specific angle for the sp^3 hybridized carbon atom from a diamantiferous structure.

By replacing $l_{CC^{(3)}} = 1,541\text{Å}$ in the expression (19), the rolling cylinders diameter is $D_{(3;0)} = 2,9054\,\text{Å}$. Three out of four bonds of the sp^3 hybrid atoms are used to forme the (3,0) nanotube remaining one uncompensated.

Such a nanotube presents on its' surface uncompensated bonds, which involves dominant contour effects regarding with the ones presented at a diamond crystal.

Conclusions

This work referes to the SWNT small diameter geometrical modelling bearing in mind the importance of the length of the bond formed by the sp^2 hybrid carbon atoms.

Such as it was elaborated, the polyhedral model appears as a completion for the conventional geometrical model, both of them having the same start point: the rolling of the graphene lay-out sequence defined by the $\vec{C}_{(m;n)}$ chiral vector with $m \geq n = 0,1,2...$ [5].

The results obtained based on the polyhedral model become notable for the nanotubes with extremely small diameters $3-7\,\text{Å}$.

The difference between the results provided by the two models becomes ingsignificant for the

nanotubes with very big diameters when the angle between the bonds formed by a atom with the first grade neighbour, marked with γ, are very close to $\gamma_{(\text{planar})} = 120^{\circ}$.

In this work some expressions have been established to determine the „zig-zag" and „armchair" type subnanometer nanotubes diameters proposing a different geometrical configuration than the one used to elaborate the polyhedral model related in reference [5].

The proposed geometrical configuration presupposes the introduction of the mathematical demonstrations from a graphene sheet distorted, the cut out of the graphene sequence from the distorted network is made in the same way as the one for the conventional geometrical model [6].

The proposed mathematical expressions are different than the ones proposed in the speciality literature, but they lead to the same result for diameters and angles for the „zig-zag' type nanotubes with m=4, 5, 6, 7, 8 [5].

The results identity suggests the fact that this expressions are correct and more easy to use regarding the expressions established in the reference [5], which in fact, represents the solutions of a transcendental equation, solutions which include a term named arrearage of the expansion in series.

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Generalizarea modelului poliedral pentru nanotuburi de carbon

Rezumat

În prezenta lucrare au fost stabilite expresii pentru determinarea diametrelor nanotuburilor subnanometrice de tip „fotoliu" şi „zig-zag" propunând o configuraţie geometrică diferită de cea utilizată în elaborarea modelului poliedral relatat în literatura de specialitate. Configuraţia geometrică propusă presupune iniţierea demonstraţiilor matematice de la o fâşie grafenică planară distorsionată, decuparea secvenţei grafenice din reţeaua distorsionată făcându-se la fel ca în modelul convenţional.