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Geometrical Modelling of SWCNT by Tridimensional Extruding

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Abstract

Cylindrical nantube-like structures are obtained by three-dimensional extruding of specific cut off area from a plane (bidimensional structure). If in case of planar graphenic structure the elementary cell contain two carbon atoms, in our case we propose the existence of one such type of atom. The present paper confirm the existence of a plane structures, other then hexagonal ones, which lead to formation of cylindrical one-wall structures (SWNT-like).

Key words: *SWNT, cylindrical structures, graphene sheet, the extrude*

Introduction

In fig. 1a is presented a two-dimensional oblique net in which elementary cell is a parallelogram with the sizes $|\vec{a}_1|$ and respectively $|\vec{a}_2|$ having the little angle α.

Translated elementary cell on the axis directions $\mathrm{O}x$ and $\mathrm{O}\xi$ can build whole two- dimensional net.

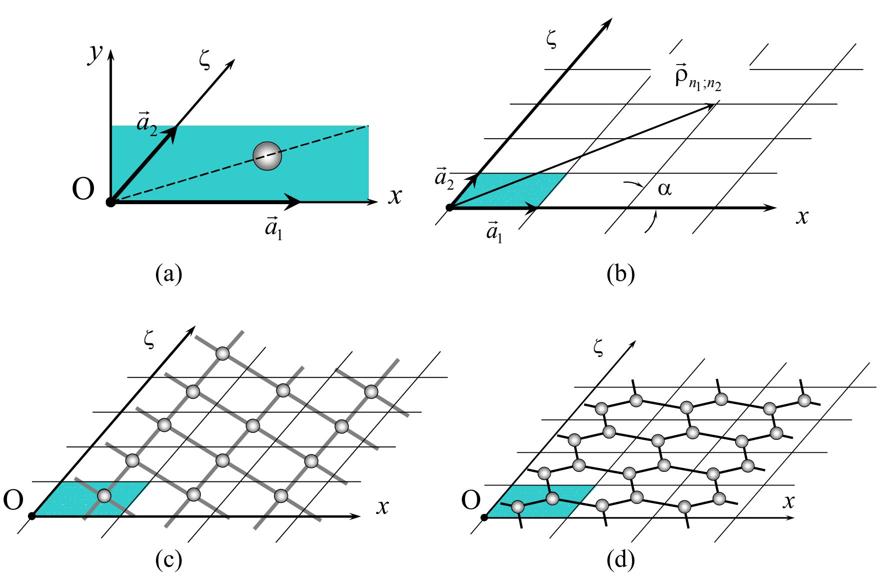


Fig. 1. Two-dimensional oblique net

This way of building involves the use of vector translational named forwards the chiral vector.

$$\vec{\rho}_{n_1;n_2} = n_1\vec{a}_1 + n_2\vec{a}_2, \quad (1)$$

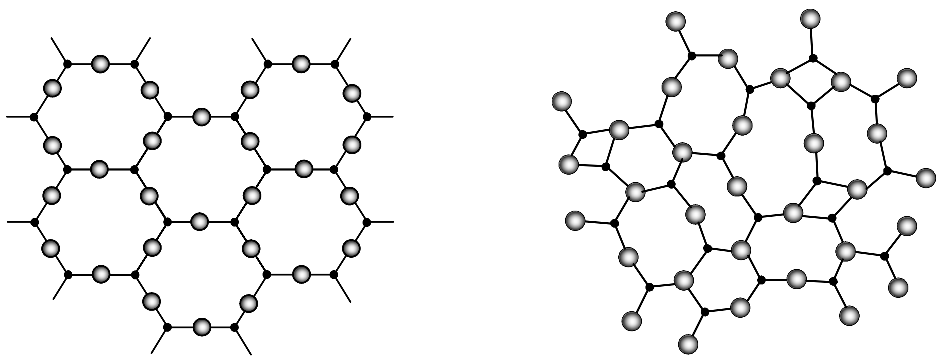
in which n_1 and n_2 are whole numbers.

Is presupposed that elementary cell contains only one atom in an immovable position reported to axis two-dimensional net (see fig. 1b). To obtain the image of atomic net, at all approached the reality, therefore each atom is necessary to form four bounds with the most approached four atoms neighbors (see fig. 1c).

If elementary cell contains two atoms in fixed positions to the axis net plane then, using only translations, is obtains a network of what atoms were hexagonal.

Accordingly, presupposing that each atom can form only three bounds with the most approached neighbors is obtained the image of a structures composed from irregular hexagons.

In fig. 2 is presented two-dimensional schematic analogue, after Zachariansen, which involve the difference among the regularly net of a crystal and one aleatory of a molten glass.



a) b)

Fig. 2. Two-dimensional schematic of net

Must be mentioned that the aleatory distribution of isotopes disturb the periodicity of crystalline net in terms of propagation of elastic waves.

In this case are will consider planed in which in effect isotopic are negligible completely.

For example, the existing isotope ^{14}C in little amounts can induct a deformation of graphenic net "pure" formed only from atoms ^{12}C.

The Formulation Problems

We have in view the build of a cylindrical structures selecting a rectangular zone from two-dimensional net and which is necessary to contain an integer number of elementary cell.

The borders of selected zones contain inevitably fractions of elementary cell, but after the operation of three-dimensional extruding, for forming a cylindrical surface is the necessity that the opposite borders to drive to the reciprocal completion of fragments of elementary cell. Also, the addition of a cylinder to other identical lengthwise axis of symmetry it must not presents the element of discontinuity in terms of the plane net.

Accordingly, if in the two-dimensional net is chosen a direction of the cutting-out, therefore he is necessary to built a second direction of cutting-out perpendicular to the first for breaking of a rectangular zone, which if is three-dimensional extruding roll permits the obtain of a cylinder with restrictions enforced above .

Is very easy to observe that the chiral vector $\vec{\rho}_{n_1;n_2}$ can enforce a direction of cutting-out.

Another direction of cutting-out of adequate by the vector $\vec{T}_{(A;B)}$ must be perpendicular to the chiral vector choose, that is:

$$\vec{T}_{(A;B)} \cdot \vec{\rho}_{n_1;n_2} = 0. \tag{2}$$

The notations A and B what appear to inferior index is allude to the component vectors $\vec{T}_{(A;B)}$ on two one direction translation Ox respectively $O\xi$:

$$\vec{T}_{(A;B)} = A\vec{a}_1 + B\vec{a}_2 . \tag{3}$$

The chiral vector represented in fact, the periodicity of two-dimensional net.

More than that, it can be considered being the length of bases of cylinder will be obtained after three-dimensional extruding.

$$\left|\vec{\rho}_{n_1;n_2}\right| = 2\pi r = \pi D , \tag{4}$$

in which r and D represents the ray of cylinder and respective the diameter of cylinder obtained after extruding.

Just as was affirmed, the fragments of elementary cell existing on two one direction of cutting-out is due to completed reciprocally after extruding, the components of vector $\vec{T}_{(A;B)}$ must have the qualities similar the vector $\vec{\rho}_{n_1;n_2}$ that is A and B being whole numbers.

Accordingly, the extruding can be done either by the direction adequate of $\vec{T}_{(A;B)}$ or by the direction of chiral vector $\vec{\rho}_{n_1;n_2}$.

If the extruding does so that, $\left|\vec{T}_{(A;B)}\right|$ be the length of bases of cylinder obtained after extruding then $\left|\vec{\rho}_{n_1;n_2}\right|$ will be the length of generatrix of cylinder.

This way of built the cylindrical nets from plane structures involve the transfer of property of symmetry from two-dimensional in three-dimensional necessary for characterization in terms of physical - chemical of nets SWCNT – like.

Discussion

Accomplishing the calculus enforced by the relation (2) is obtained immediately that:

$$\frac{A}{B} = -\frac{n_1\vec{a}_1\vec{a}_2 + n_2 a_2^2}{n_1 a_1^2 + n_2\vec{a}_1\vec{a}_2} . \tag{5}$$

In order to A and B being whole numbers then both numerator and the denominator is must be divided with $\left|\vec{a}_1\right|\left|\vec{a}_2\right|$, such that, the relation(5) becomes:

$$\frac{A}{B}=-\frac{n_1\cos\alpha+n_2|\vec{a}_2|/|\vec{a}_1|}{n_1|\vec{a}_1|/|\vec{a}_2|+n_2\cos\alpha}=\frac{(\text{whole number})}{(\text{whole number})}. \tag{6}$$

Noting $N_1=-(n_1\cos\alpha+n_2|\vec{a}_2|/|\vec{a}_1|)$ and $N_2=n_1|\vec{a}_1|/|\vec{a}_2|+n_2\cos\alpha$ as being, in the same time, some whole numbers, can as these have the greatest common divisor.

Noting L this greatest common divisor $N_1^*=N_1/L$ and $N_2^*=N_2/L$ is obtained immediately:

$$\frac{A}{B}=\frac{N_1^*}{N_2^*}. \tag{7}$$

Accordingly A can be identified with N_1^* and B can be identified with N_2^*.

Thus defined $\vec{T}_{(A,B)}$, this represents the minimum periodicity on the direction of axis cylinder obtained which permits the obtain of a nanotub with appreciable length (consider to be a multiple whole $|\vec{T}_{(A,B)}|$).

$$|\vec{T}_{(AB)}|=|\vec{\rho}_{n_1n_2}|\sin\alpha. \tag{8}$$

Or in the case when exists the divider L then:

$$|\vec{T}_{(AB)}|=\tfrac{1}{L}|\vec{\rho}_{n_1n_2}|\sin\alpha. \tag{9}$$

Lateral area cylinder obtained through extruding is:

$$A_{(cilindru)}=|\vec{T}_{(AB)}\times\vec{\rho}_{n_1n_2}|=|\vec{\rho}_{n_1n_2}|^2\sin\alpha \tag{10}$$

or

$$A_{(cilindru)}=\tfrac{1}{L}|\vec{\rho}_{n_1n_2}|^2\sin\alpha. \tag{11}$$

Must keep remarks “ $A_{cilindru}$ must be an whole number of areas of elementary cells $|\vec{a}_1|\cdot|\vec{a}_2|\sin\alpha$“. Noting with $N_{(celule)}$ the number of elementary areas existing on a cylindrical period then:

$$N_{(celule)}=\frac{A_{(cilindru)}}{|\vec{a}_1|\cdot|\vec{a}_2|\sin\alpha}=\frac{1}{L|\vec{a}_1|\cdot|\vec{a}_2|}|\vec{\rho}_{n_1\,n_2}|^2=$$

$$=\frac{1}{L|\vec{a}_1||\vec{a}_2|}(n_1^2|\vec{a}_1|^2+n_2^2|\vec{a}_2|^2+2n_1n_2|\vec{a}_1||\vec{a}_2|\cos\alpha). \tag{12}$$

If on each elementary cell exists n_0 atoms then the number of atoms contained on the lateral surface cylinder is:

$$N_{(atomi)}=\frac{n_0}{L|\vec{a}_1||\vec{a}_2|}|\vec{\rho}_{n_1n_2}|^2. \tag{13}$$

Particular Cases

The identification of A with N_1^* and B with N_2^* is possible only with the simultaneous of a achievement condition enforced about $\cos\alpha$ and ratio $|\vec{a}_2|/|\vec{a}_1|$.

Next we will take in question needle ascribable values of $\cos\alpha$ and ratio $|\vec{a}_2|/|\vec{a}_1|$ that let us does A and B be the component of vector $\vec{T}_{(A,B)}$.

As well, in all cases will be discussed it will consider $|\vec{a}_1|=|\vec{a}_2|=a$.

An interesting case is one of net plane (two-dimensional) quadratic for which $\alpha=\pi/2$ in which each cell contains an atomic entity capable to achieve 4 bounds with neighbor of the order I. Be know the vector $\left|\vec{\rho}_{n_1 n_2}\right|$ then for cutting-out portion from the plane net for extruding, is built the vector $\left|\vec{T}_{(A,B)}\right|=-n_2\vec{a}_1+n_1\vec{a}_2$. His components was established according with relations (6) and (7) (see the fig. 1 c). The result of extruding is represents in fig. 4. That could be considered that a real case when is the word of atomic remains able to form 4 bounds in plane and in different conditions of medium. In natural conditions those should be very unstable.

The most usual case is one of net plane in which $\alpha=\pi/3$ and each cell should be contains two atomic entities in what position divides the big diagonal of elementary cell in three equal portion.

If each atomic entity should be able to realize only 3 bounds with the neighbor of order I, then should be obtains, through extruding a cylindrical structure formed from regular hexagons.

This is the case most known and is used-up in modeling SWCNT (see the fig. 5).

Can be considerate interesting cases for $\cos\alpha=3/5$ $(\alpha\approx 53^\circ)$ and $\cos\alpha=4/5$ $(\alpha\approx 37^\circ)$.

Thus
$$A=-\left(n_1\frac{3}{5}+n_2\right)\ B=\left(n_2\frac{3}{5}+n_1\right), \tag{14}$$

respectively
$$A=-\left(n_1\frac{4}{5}+n_2\right);\ B=\left(n_2\frac{4}{5}+n_1\right). \tag{15}$$

Because A and B must be simultaneous whole numbers, n_1 and n_2 must be, also simultaneous divisible with 5. Practically, any value of $\cos\alpha$ equal with the ratio of two whole numbers (less numerator as the denominator) can drive to the cylindrical structures with the restrictions enforced.

If each cell contains an atomic entity is obtained a plane structure like the structure from fig. 1c.

If each cell should contains two atomic entities and each should be able to do just 3 bounds with the neighbor most approached should obtained a net of identical hexagons but irregular, see the fig. 1d.

The extruding result should be a cylindrical structure form from irregular hexagons. The same results it can be obtained from a cylindrical structure formed from regular hexagons (see first case considers) and then subdued of a stretches on the axial direction.

The Model Three-Dimensional Extruding

The extruding simulation from the plane structure of a SWCNT involve the element of space geometry and a proper program for calculate the positions of all atoms which intercede in formation of spatial structure. After the obtain of coordinates by a previous selected mark, using a visualization program of spatial structures we can create the three-dimensional images of the extruding steps. In fig. 3 is represented the hexagonal two-dimensional structure – in xOy plan were by line continuous - represented the nanotub borders surface which trace to obtained by extruding. With line dotty is represented the position at which lengthwise of the tubes begins the repeat position of put the atoms on nanotub.

The notations from the fig. 3 are following: R - the radius of nanotub, l - the length of nanotub and l_r - specific length of nanotub.

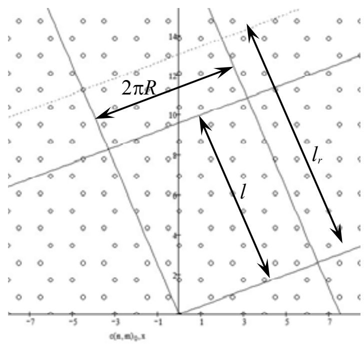
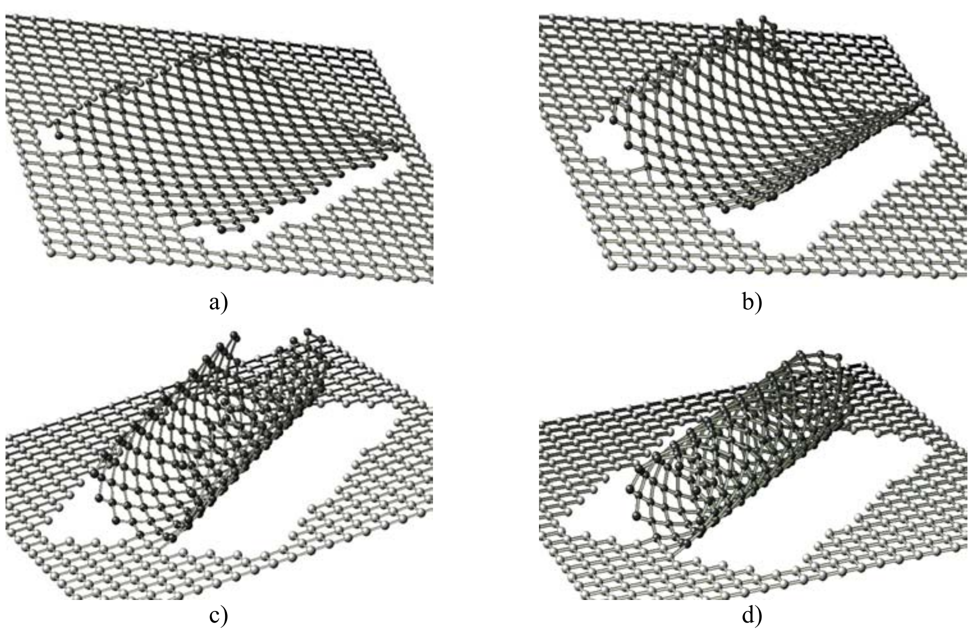


Fig. 3. Characteristic dimensions of the nanotub

It was studied two cases, the extruding of a nanotub from the plane quadratic structure and from the plane hexagonal structure. In fig. 4 we have represented some steps of the extruding in the case of quadratic net. In fig. 5 we have represented some steps of the extruding in the case of hexagonal net.



a) b)

c) d)

Fig. 4. The steps of the extruding in the case of quadratic net

In both cases it can realize the animation three-dimensional which show the methods where away it can realize a correspondence between a plane net (two-dimensional) and a nanotub(three-dimensional structure).

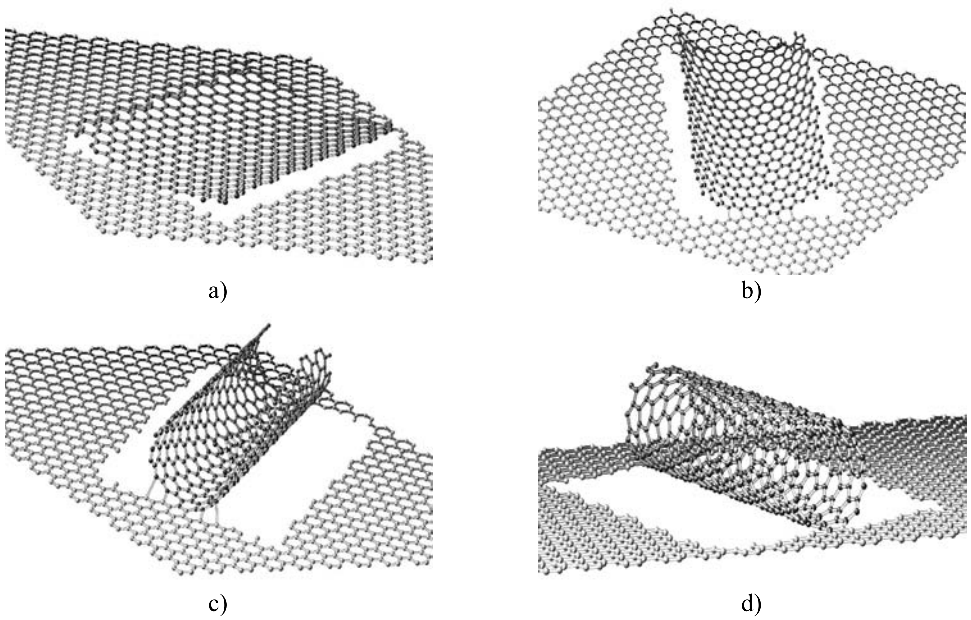


Fig. 5. The steps of the extruding in the case of hexagonal net

Conclusions

The method of extruding permits the transfer of geometric property of two-dimensional (plane) structures in the cylindrical (three dimensional) structures. Technical, this method can be used for obtaining of cylindrical structures to present certain straining on direction predefined of structure. Compose of ensemble from cylindrical concentric layers, with differed straining, "immersed" into filler, permits the obtain of cylindrical ensembles with a remarkable rigidity.

In present, the most intense studied and which presents the certain promises in the development of nanotechnology are single wall nanotubes (SWCNT). In domain of carbon nanotubes, the geometric modeling is alike of important directing to the fact that the electronic property are directly attached on their geometrical structure - the chiral vector. Depending on the choice of chiral vectors by extruding it can obtained, on principle, any cylindrical structure with any diameter. In the concrete case, the one of SWCNT, the diameter of the cylindrical structure it can not be much as little from cause of marked deformation of molecular orbits.

In principle, by extruding it can obtain any cylindrical structure starting from a plane structure, the work represents a generalization of theoretical applicable ascertainments in modeling of carbon nanostructures.

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Modelarea geometrică a structurilor tip SWCNT prin extrudare tridimensională

Rezumat

Obținerea unor stucturi cilindrice de tip nanotuburi de carbon se poate face prin roluirea (extrudare tridimensională) unei zone decupate dintr-o structură planară (bidimensională). Dacă în cazul unei structuri grafenice planare celula elementară conține doi atomi de carbon, în prezenta lucrare se presupune cazul existenței doar a unei entități atomice pe fiecare celulă elementară. Lucrarea confirmă existența unor stucturi planare, altele decât cele planar hexagonale, care conduc la formarea unor structuri cilindrice cu perete unic.