THE RESEARCH OF GEOMETRICAL CHARACTERISTICS OF CARBON NANOTUBES BY THE COEFFICIENT OF CHIRALITY

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***Summary*. The article considers the properties of chirality coefficients (HF) and their practical application. The research indicates on a proven by analytical method dependence of basic geometric characteristics of nanotubes from chirality values. The article confirms loyalty of formulas that allow to find the interatomic distances of nanotubes by using of the above-mentioned coefficients.**

***Keywords:* nanotube chirality ratios, geometric properties of nanotubes and methods of applied geometry.**

Formulation of the problem. Systematics disparate data on the geometry of the nanotubes, which are found mainly in the scientific literature only an auxiliary element, currently seems highly relevant. Also, there is a need for introductory studies to further the use of systematic information in the modeling of nanostructures.

Analysis of recent research. The practical significance of HF described in detail in the works [1,2]. Proceedings [3,4] have mostly applied character. The sources [5,6] highlights the fundamental knowledge about the structure of nanotubes, which have become a fundamental principle of our research work. If we consider the source [7-9], it is worth noting thoroughly examined the practical application of carbon structures, but there had been no important parallels regarding dependence of the electrical and electrochemical characteristics of nanotubes on their geometric structure.

The wording of Article purposes. In this work the aim is to find out a set of geometric characteristics of carbon nanotubes that directly depend on HF.

Main part. Consider the process of folding the graphite tube in the plane [1].

Let two orthogonal vectors $\boldsymbol{C}$ and $\boldsymbol{L}$ (Fig. 1), expressed in basis ($\mathbf{a_1}$, $\mathbf{a_2}$), set in graphite plane rectangle that moves when minimized to the cylindrical surface. Then the vectors $\mathbf{a_1}$ and $\mathbf{a_2}$ pass into the winding turns $S_1(\Delta\varphi_1; \Delta z_1)$ and $S_2(\Delta\varphi_2 ; \Delta z_2)$, which are generatrices of symmetry tube radius $R=\frac{|C|}{2\pi}$.

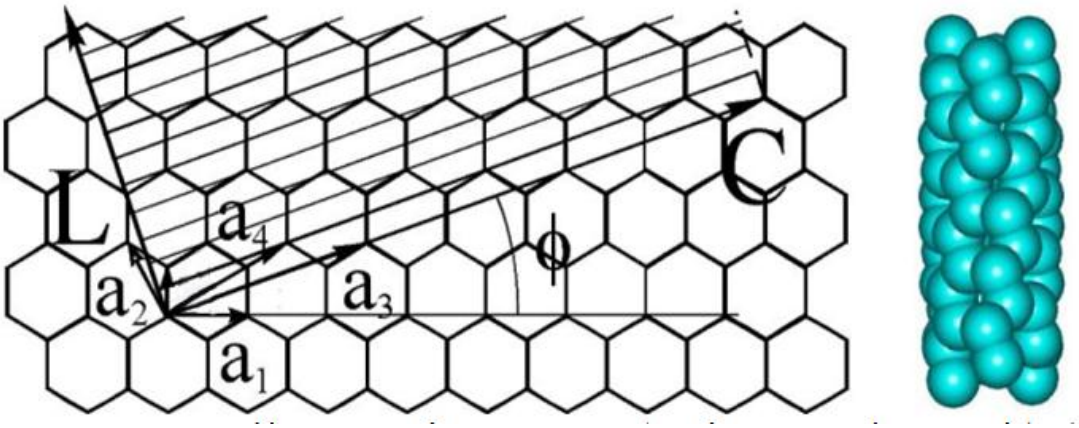

Fig. 1. A graphite layer and carbon tube with chirality indices (9,3) basis vectors ($\mathbf{a_1}$, $\mathbf{a_2}$), ($\mathbf{a_3}$, $\mathbf{a_4}$), chirality angle $\boldsymbol{\varphi}$.

Chirality nanotubes denote character set (i_1, i_2), or, respectively, (n, m). They point coordinates hexagon that as a result of folding plane should coincide with the hexagons located at the origin [5]. Easy to follow a direct link coefficients chirality of the tube diameter:

$$D = \sqrt{m^2 + n^2 - n \cdot m} \cdot \frac{3d_0}{\pi}, \qquad (1)$$

where $d_0 = 0{,}142$ *нм* - the distance between the carbon atoms in the hexagonal grid of graphite. We know about the direct dependence of the strength of single-walled nanotubes, the diameter of which is defined by the formula (1). Since the diameter of the nanotubes is close to the size of the cross-molecule polymers, single-layer nanotubes as the most recent members strong. [7] Thus, it may be noted that the coefficients of chirality widely used to solve applications that will be confirmed further. Research group symmetry tube is convenient to consider using operator turns screw $S_3(\Delta\varphi_3; 0)$ and $S_4(\Delta\varphi_4 ; \Delta z_4)$ [1]. The number of carbon atoms on the rings, set up representing a given basis, depending on the order of the symmetry axis S_3 and $\Delta\varphi_3$. The latter is determined by the rotary axis determines nanotubes:

$$\Delta\varphi_3 = \frac{2\pi}{n}, \qquad (2)$$

where n – an integer that specifies the order of the axis of symmetry and equal GCD ($\mathbf{i_1}$, $\mathbf{i_2}$). Parameter Δz_4 equivalent value shift atoms relative to each other in the upcoming rings. On the one hand, the product $\Delta z_4 \Delta\varphi_3 R$ equal to the area of the unit cell, the other - it is determined through basis ($\mathbf{a_1}$, $\mathbf{a_2}$). It is not difficult to express:

$$\Delta z_3 = \frac{3}{2} \frac{n \cdot a_0}{\sqrt{i_1^2 - i_1 i_2 + i_2^2}}, \qquad (3)$$

where $\mathbf{a_0}$ = 1.42 and distance between the nearest carbon atoms of a graphite plane, n = GCD ($\mathbf{i_1}$, $\mathbf{i_2}$). Mirror plane exist tubes in the case where the angle of chirality (Fig. 2) carbon tubes (the angle between the vectors $\boldsymbol{C}$ and a_1), depending on the index ($\mathbf{i_1}$, $\mathbf{i_2}$), a multiple of $\pi/6$ [1]. These values correspond to the corners of tubes configuration zigzag (n, 0) and armchair (2n, n).

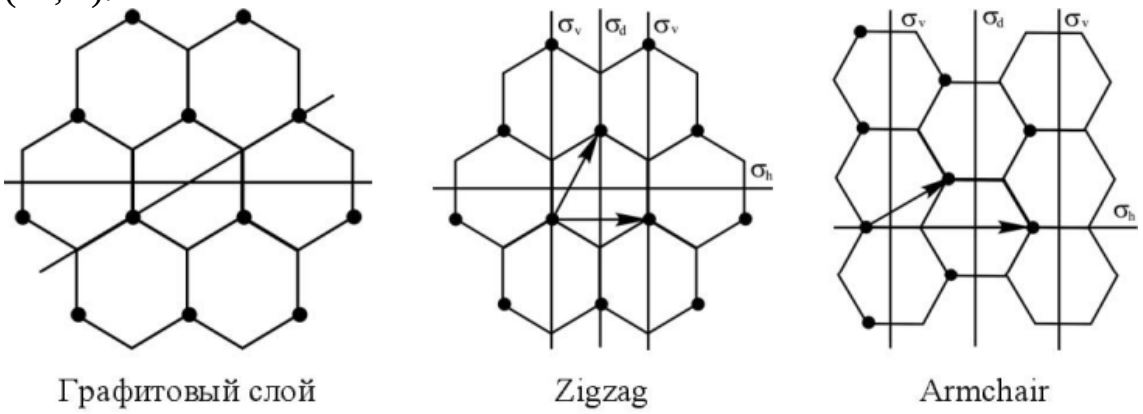

Fig. 2. The plane mirror images
for graphite layer with elements of symmetry σ_v and σ_d
(inherited tube when minimized).

May withdraw the formula [2] through *a* (bond length B-B (N-N)) and *n* (chirality index) to determine the coordinates of nuclear sites and interatomic distances in ideal boron nitride nanotubes. These relations are suitable for any structural analog, particularly for carbon nanotubes.

Consider finding interatomic distances in the sample zigzag (Fig. 3). Dark and bright points appear relevant atoms B and N.

According to [2] The unit cell N-nanotubes (n, 0) consists of 4 atomic circles orthogonal axis of the tube with n atoms each. Circles of atoms are alternately oppositely and form pairs at a distance and $a/2\sqrt{3}$ (distance between adjacent pairs of atoms of the same name - and $a/\sqrt{3}$).

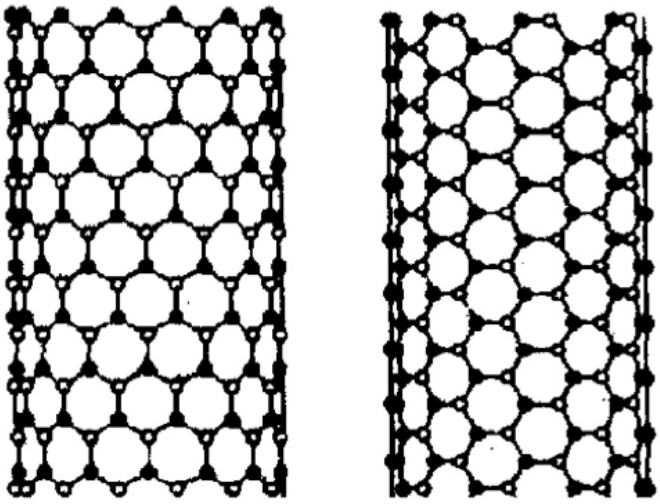

Fig. 3. Zigzag - 1 and armchair - 2 tubes of boron nitride.

In order to determine the coordinates of which are necessary to solve the problem of finding the crystallographic interatomic distances, spend xOz plane through the fracture surface of the sheet forest, and the plane xOy - in the middle of a B-N-ties, which lies on this line. Polar angle and height units ${}^{lm}_{(n,0)}\mathrm{B1}$ и ${}^{lm}_{(n,0)}\mathrm{N1}$ in the vicinity of nuclear power, equivalent to the vicinity of the central pair, will be equal to:

$$\varphi = 2/\pi/n, \quad z = (6m+1)a/2\sqrt{3} \quad u \quad \varphi = 2/\pi/n, \quad z = (6m-1)a/2\sqrt{3}, \tag{4}$$

where $l = 0,1,2\ldots,n\text{-}1$ i $m = 0,\pm1,\pm2,\ldots$ – Indexes pairs of atoms of boron and nitrogen. For the central pair (${}^{00}_{(n,0)}\mathrm{B1}$ и ${}^{00}_{(n,0)}\mathrm{N1}$) are zero. It is not difficult to calculate the polar radius and height units ${}^{lm}_{(n,0)}\mathrm{B2}$ и ${}^{lm}_{(n,0)}\mathrm{N2}$. Indeed, spending and using the calculations found in [3] to the radius zigzag - nanotubes $R_{(n,0)} = \dfrac{a}{4\sin\ \pi/2n}$, can find interatomic distance from the central couple:

$$\frac{({}^{lm}_{(n,0)}\mathrm{B1}-{}^{00}_{(n,0)}\mathrm{B1})^2}{a^2}=\frac{\sin^2 l\pi/n}{4\sin^2\pi/2n}+3m^2,\qquad \frac{({}^{lm}_{(n,0)}\mathrm{B1}-{}^{00}_{(n,0)}\mathrm{N1})^2}{a^2}=\frac{\sin^2 l\pi/n}{4\sin^2\pi/2n}+\frac{(3m+1)^2}{3},$$

$$\frac{({}^{lm}_{(n,0)}\mathrm{B2}-{}^{00}_{(n,0)}\mathrm{B1})^2}{a^2}=\frac{\sin^2(2l+1)\pi/2n}{4\sin^2\pi/2n}+\frac{3(2m-1)^2}{4},\quad \frac{({}^{lm}_{(n,0)}\mathrm{B2}-{}^{00}_{(n,0)}\mathrm{N1})^2}{a^2}=\frac{\sin^2(2l+1)\pi/2n}{4\sin^2\pi/2n}+\frac{(6m-1)^2}{12},$$

$$\frac{({}^{lm}_{(n,0)}\mathrm{N1}-{}^{00}_{(n,0)}\mathrm{B1})^2}{a^2}=\frac{\sin^2 l\pi/n}{4\sin^2\pi/2n}+\frac{(3m-1)^2}{3},\quad \frac{({}^{lm}_{(n,0)}\mathrm{N1}-{}^{00}_{(n,0)}\mathrm{N1})^2}{a^2}=\frac{\sin^2 l\pi/n}{4\sin^2\pi/2n}+3m^2,$$

$$\frac{({}^{lm}_{(n,0)}\mathrm{N2}-{}^{00}_{(n,0)}\mathrm{B1})^2}{a^2}=\frac{\sin^2(2l+1)\pi/2n}{4\sin^2\pi/2n}+\frac{(6m+1)^2}{12},\quad \frac{({}^{lm}_{(n,0)}\mathrm{N2}-{}^{00}_{(n,0)}\mathrm{N1})^2}{a^2}=\frac{\sin^2(2l+1)\pi/2n}{4\sin^2\pi/2n}+\frac{3(2m+1)^2}{4} \qquad (5)$$

Conclusions. Thus, in the study highlights the symmetry group of carbon nanotubes with operators helical turns S_3 and S_4. Conceptuality analyzed for the existence of chirality angle mirror planes tubes. The process of determining coordinates nuclear units and interatomic distances nanotubes. Established that as chirality of nanotubes determine their electrical properties, which are used, for example, in the creation of semiconductor heterostructures is urgent further study of nanostructures modeling methods applied geometry and computer graphics based on the studies.

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