Optimization of Calculation of Parameters of Tubes from a One-Dimensional Hexagonal Lattice

Felix A. Desyatirikov
Dept. of Gymnasium named after Academician N. Basov
Voronezh State University
Voronezh, Russia
felixdes@ieee.org

***Abstract*— A mechanism is proposed for optimizing the calculation of the geometric dimensions of pipe structures from a hexagonal web, for example, carbon nanotubes. The algorithm uses the three axes of symmetry of the matrix of values of the tube diameters found for different directions of folding. The application of the algorithm is shown on the example of the calculation of detonation in a nanotube in a gaseous medium, which can be used for pointwise doping the surface with an inactive substance.**

Keywords*— *symmetric matrix; optimization of the calculation; structure of a carbon nanotube; detonation in a gaseous medium

I. INTRODUCTION

Carbon nanotubes are the object of research for various applications. The carbon nanotube is a permeable structure made of hexagonal cloth, which can be considered as a model of various objects – from the construction structure, to the shell of the missile [1]. The proposal of such a model is one of the objects of research. The thrust in such a construction must be created by chemical reaction products that leave the tube, the initial components of which freely penetrate through the surface of the nanotube. Such a construction can be used to introduce an impurity into the surface layer of a dense material [2, 3]. Calculation of the properties of the tube requires knowledge of its geometric parameters, so it is important to increase the efficiency of such calculations [4, 5]. The paper presents a method for accelerated calculation of the diameters and lengths of single-walled nanotubes.

The purposes of the work are, at first, to determine the regularities in calculating nanotube parameters and to find a way to accelerate the calculation of the geometric parameters of nanotubes; and the second – development of a model of the process of point introduction of a solid substance (doping) into the near-surface layer of the material as a result of detonation of a gas mixture in a carbon nanotube.

II. OPTIMIZATION OF CALCULATION OF GEOMETRIC PARAMETERS

A carbon nanotube is obtained by folding a fragment of a graphene plane (consisting of regular hexagons) in the direction of the folding vector. This vector ***R*** is called the chirality vector (Fig. 1).

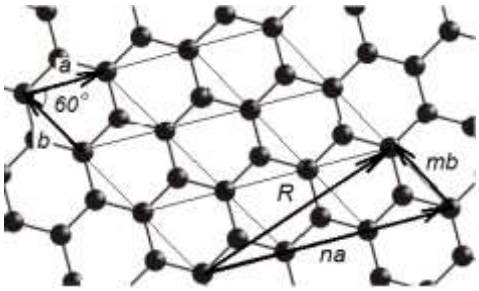

Fig. 1. The folding vector of a graphene plane

When the fragment of the graphene plane is minimized, the end of ***R*** must coincide with its origin, and the corresponding hexagons coincide and the tube is seamless. The folding vector R is defined as follows: ***R = na + mb***, where ***n*** and ***m*** are integers (chirality indices), and ***a*** and ***b*** are the defining vectors of the graphene plane.

In this case, the chirality indices ***n*** and ***m*** are the main characteristic of single-walled nanotubes, which determines all the main geometric parameters. We will show this by the example of determining the diameter of a nanotube, for which we distinguish from Fig. 1 triangle, constructed on the chirality and folding vectors, i.e. Fig. 2.

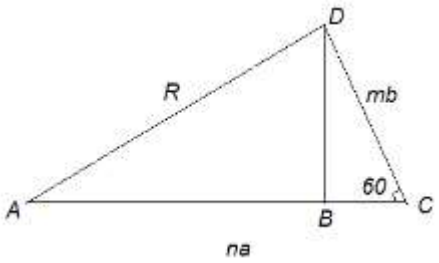

Fig. 2. The folding vector of a graphene plane

In Fig. 2 we draw the height ***BD***. From the right triangle ***BDC***: angle ***BDC=90°-60°=30°***. Then ***BC***, as lying against the angle of ***30°***:

$$BC = \frac{1}{2} mb \cdot$$

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We find the ***DB*** by the Pythagorean theorem:

$$DB^2 = (mb)^2 - BC^2 = \frac{3}{4}(mb)^2.$$

From the right triangle ***ADB***, taking into account that ***a=b***:

$$R = \sqrt{AB^2 + DB^2} = \sqrt{(na - BC)^2 + DB^2} = \sqrt{(na - \frac{1}{2}mb)^2 + \frac{3}{4}(mb)^2} =$$

$$= \sqrt{(na)^2 - abnm + (mb)^2} = a\sqrt{n^2 - nm + m^2} \quad ,$$

For a rolled tube, ***R*** is the circumference of the tube, so the tube diameter:

$$D = \frac{R}{\pi} = \frac{a}{\pi}\sqrt{n^2 - nm + m^2} \quad , \qquad (1)$$

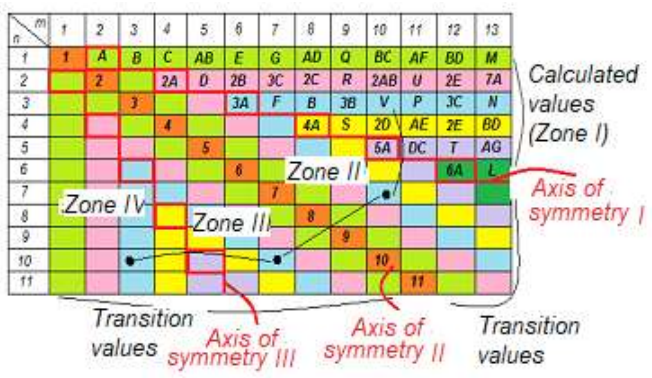
where ***a*** – is the cell parameter of the graphite plane: $a=2{,}46A^o$. We denote the root expression in formula (1) by ***đ.***

The value of the radicand is also used to determine the length of a nanotube. In determining the length of a nanotube, the term "translation vector ***T*** " is used to mean a minimum-length vector connecting two identical nodes along the axis of the nanotube. Accordingly, the length of the nanotube is some integer number of the lengths of the translational vector. The length of the translational vector is determined by the following formula [6]:

$$T = \frac{\sqrt{3}\, a\sqrt{n^2 - nm + m^2}}{GCD(2n - m,\, 2m - n)} \quad ,$$

here ***GCD*** is the greatest common divisor of two numbers.

In Fig. 3 shows the calculated values of the radicand ***đ*** for various chirality indices ***m*** and ***n*** (in one color, the equivalent values of ***đ*** are shown):



A	B	C	D	E	F	G	S	R	Q	V	P	U	T	L	N	M
3	7	13	19	31	37	43	61	67	73	79	97	103	109	127	139	157

Fig. 3. The values of the radicand d in formula (1) (fragment)

Based on the calculated values of ¼ of the part of Table (*Zone I*), the remaining fields of Table are filled in according to the following rules (see Fig. 3). Let ***V*** be the calculated value in *Zone I*, then in the table there are three more such values:

1) axis of symmetry I (for ***n=m/2, m=2k,*** where ***k*** is any natural number): values in the table ***đ=kV*** ;

2) axis of symmetry II (for ***m=n***): values in the table ***đ=m=n***;

3) axis of symmetry III (for ***m=n/2***, ***n=2p,*** where ***p*** is any natural number): values in the table ***đ = pV*** ;

4) transition formulas (to search for equivalent cells in Table I, if the values in *Zone I* are calculated):

Zone I → *Zone II* : $m_2 = m_1$, $n_2 = m_1 - n_1$;

Zone I → *Zone III* : $m_3 = m_1 - n_1$, $n_3 = m_1$;

Zone I → *Zone IV* : $m_4 = n_1$, $n_4 = m_1$.

Obviously, all elements of the matrix in Fig. 3 have prime factors, which means that with a **sequential** increase in ***m*** and ***n***, the **diameters** and **lengths** of nanotubes change discretely and unevenly.

In addition, the matrix of diameters has **three symmetry axes** (in Fig. 3 they are marked in red):

- *the diagonal of the table* – relative to it the values are mirror-symmetric;
- "*bisector" of the top part of the table above the diagonal* – relative to it the values of the top part of the table are symmetrical with reflection "from top to bottom";
- *"bisector" of the lower part of the table under the diagonal* – with respect to it the values of the bottom of the table are symmetrical with the reflection "from right to left".

Thus, in order to calculate all possible diameters and lengths of single-layer defect-free nanotubes, **only the ¼ part of all the necessary values** can be calculated by formula (1), and the remaining values are added to the matrix of values according to the calculated values. This will allow us to calculate only those diameters and lengths when n<m/2 (or m<n/2).

III. Application of Nanotubes for Point Doping

In [7, 8], chemical reactions involving carbon were studied, but chemical reactions in carbon nanotubes were not considered in either of these studies. In [9, 10], combustion in a cylinder and a tube was studied, but again, nanotubes were not among the studied structures. Nor were the problems of detonation in nanotubes considered. But in [11, 12], the dependence of the detonation velocity on the ratio of the components of the explosive gas mixture was investigated.

The working hypothesis of the study was as follows. The carbon nanotube is a permeable structure. If we select chemical reagents that, if freely inserted into the tube, can enter into a chemical reaction inside it to form substances whose large molecules can not leave the nanotube through the cells of its walls, then perhaps the pressure of these components inside the nanotube will lead to the fact that they will be forced out of the nanotube outward through the end of the nanotube. If the reaction rate was high, an effect would appear that is similar to the detonation of powder gases in the projectile, which is the reason for the jet propulsion. In this case, there will be a

reactive thrust that will allow the nanotube to move the other end into the surface of the "bombarded" material adjacent to the tube. If this end of the nanotube is "charged" with a given substance, then it will penetrate pointwise into the surface (doping it).

Usually a thermal explosion is an extremely undesirable phenomenon. But for our purposes, it is chosen as a mechanism that provides the reactive thrust of the nanotube for the introduction of impurities into the surface. To study the mechanism of interaction of substances inside a nanotube, let us consider, for example, the ion exchange reaction

$$H_2O + CO \rightleftarrows CO_2 + H_2 .$$

Below 830°C, a stronger reducing agent is CO, and above 830°C – it is a hydrogen. Therefore, the reaction equilibrium to 830°C is shifted to the right, above 830°C to the left. The presence of free nickel (in the form of monatomic molecules) reduces the reaction temperature to 400°C. It is important that atomic nickel freely passes through the cells of the nanotube wall. According to known data, the dimensions of the molecules in this reaction are as follows (see Table I).

TABLE I. DIAMETERS OF MOLECULES

Substance	Diameter of the molecule, nm	Substance	Diameter of the molecule, nm
H_2	0,24	CO	0,32
H_2O	0,30	CO_2	0,33
Ni	0,12		

We obtain that the diameter of nanotubes for our purposes must satisfy the condition ***D>0.30 nm***, which, according to the above procedure of accelerated calculation, gives us the values of chirality indices corresponding to the rows and columns of the table without parameters A, B, 2A and 3A (we denote this ***condition (*)***).

Taking into account that the cell size of the carbon nanotube: $a=2,46A^o$=0,25 nm, we find that in the case of the reaction $CO_2 + H_2 = H_2O + CO$, the reaction products can not leave the tube through its walls, creating in the tube an excessive pressure see Fig. 4). Moreover, due to the known property of the "hydrophobicity" of the carbon nanotube [6], the water molecules will slip out of the tube with the least friction.

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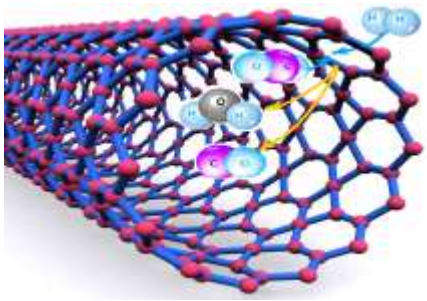

Fig. 4. Model of detonation of gases in a nanotube

If the reaction goes in the opposite direction, then hydrogen has the ability to "leak" through the walls of the nanotube and does not contribute to creating pressure inside the tube.

To calculate the gas pressure inside a nanotube (of a given diameter and length) before and after the reaction, it can be assumed that the molecules are spherical, tightly packed inside the tube, and the tube itself does not exhibit its elastic properties (tensile capacity up to 20% with a simultaneous reduction in diameter).

IV. ALGORITHM OF THE CALCULATION OF THE TRACTION CHARACTERISTICS OF THE NANOTUBES IN THE DETONATION OF GASES IN THEM

Step 1. Find the volume of a nanotube of a given diameter.

Step 2. Find the volume of molecules, like spherical bodies with a known radius.

Step 3. Determine how many molecules of carbon dioxide is placed in the calculated volume of the nanotube, taking into account the ***condition (*)***.

Step 4. Determine the volume of the same pairs of molecules of reaction products, how many CO_2 molecules were obtained in step 3.

Step 5. Find the excess volume of reaction products molecules over the volume of the initial cylinder of the nanotube.

Thus, by specifying the diameter of the tube, one can find the number of CO_2 atoms that will react with H_2 when the system is heated above 830°C (or 400°C with the Ni catalyst).

To determine the number of molecules of CO_2, H_2O and CO, densely placed inside the nanotube should be solved. the task of "packing circles in a circle", the purpose of which is to pack individual circles in the smallest possible circle.

V. ANALYSIS OF THE PROPOSED IMPURITY MECHANISM

The pressure of the emitted substance is the greater, the greater the difference in the volumes of reaction products (H_2O and CO) and the initial component (CO_2). In addition, we must take into account the fact that some of the products in the tube still fit and with respect to this part, we also need to solve the problem of tight packing of circles in a circle. And only then to consider the difference in the volumes of "not placed" products and the initial CO_2. All this is true for a narrow nanotube.

If the nanotube is sufficiently wide, then H_2 does not react with all the CO_2 molecules, and then the products formed will have to be located near the walls of the tube. Given the property of the "hydrophobicity" of a nanotube, one can expect that CO remains inside the tube, and water will be forced out through the free end of the tube. Probably, along the way, it will "wash out" a certain amount of initial CO_2, which will reduce the rate of formation of reaction products and reduce the "traction force".

Most likely, there is some optimal nanotube diameter, above and below which the reactive thrust will be less than at such a diameter (see Fig. 5).

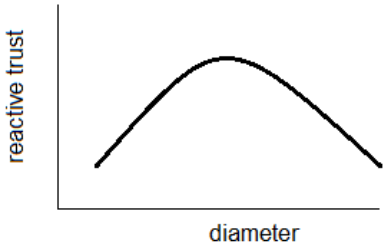

Fig. 5. Dependence of reactive thrust on the diameter of the nanotube

However, it is difficult to make exact corresponding calculations, because there are many other factors that play a big role in creating reactive thrust; and yet we can not accurately assess them. For example, such factors as the rate of the chemical reaction (from which, principally, the possibility of creating the explosive nature of the formation of the reaction products depends), the viscosity of the products obtained, the elasticity of the tube, and other factors.

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