

CALCULATION OF YUNG'S MODULUS OF CARBON NANOTUBES

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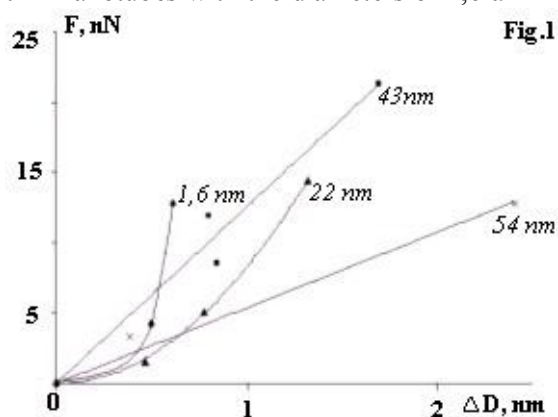
Introduction

The Investigation of the carbon nanotubes, as an independent scientific direction has entered relatively fast and easily to the list of national scientific priorities of the leading countries of the world. The explanation of this is the fundamental meaning of the science about nanotubes, natural objects that take the bordering position between separate atoms and a solid state. The discoveries of the extraordinary forms of carbon made during the last decades faces us to make a new glance on fundamental processes that take place along with a participation of carbon in an alive and non-alive nature. At the same time the experience of the world science witnesses that fundamental features of the new class of objects often opens the absolutely unexpected possibilities for practice use. To create the sets based on semiconductor nanotubes the knowledge of physical parameters is necessary. In this work the theoretical and computer calculations on the flexibility coefficient. Where determined, as well as the dependence of the radial deformation of the layers of carbon nanotubes of stress force. Using experimental data the Yung's modulus were calculated.

Results and discussions

In this mechanical features of 1-, 5-, 10-, and 30 layers nanotubes with corresponding outward diameters of 1,6; 43; 22; and 54 nm when pressed perpendicular to their axes were researched by methods of atomic – force microscopy (AFM) and transmission electronic microscopy (TEM). At present, there is no completed theory of ACM of interrupted contact, which would correlate the quantities of cantilever's tip oscillations amplitude with the intensity of its influence upon the example. Because of that, a semi-quantitative analysis of elastic features of different diameters nanotubes with different wall thickness was conducted. Methodical peculiarities of Yung's module definition in radial direction as for both a separate single-layer nanotubes with diameter of 40-50 nm.

The dependence of inter-atomic force (F) on the value of absolute deformation (ΔD) for all the considered nanotubes was received (fig.1). The graph shows the Guk's law doesn't act on the most thin nanotubes with the diameters of 1,6 and 22 nm.



It means that non-lasting Born's repelling forces, acting among some of the carbonic atoms, dominate at small distances in single-layer nanotubes.

Using the data on inter-atomic force, depending on the value of absolute deformations, Yung's modulus of 1-, 5-, 10-, and 30 layer carbon nanotubes with diameter 1,6; 43; 22; and 54 nm are calculated.

To calculate the Yung's modulus the theory of contact deformation is proposed. It's assumed that the contact surface of carbon nanotubes and probe of cantilever is ellipse with the square of contact $S = \pi \cdot a \cdot b$, where a , b are the axis of ellipse. The tensors of curvature A and B , characterizing the curvature of the surface, are :

$$A = \frac{1}{2} \left(\frac{1}{r} + \frac{1}{r'} \right), \quad B = \frac{1}{2r} \quad (1)$$

In our case $A > B$ and $a < b$. The distance between probe and carbon nanotubes can be estimated using the following equation:

$$h = (C + 1) \frac{2FD}{\pi b} \quad (2)$$

C , D are non-dimensional parameters. C depend of ellipse's axis and equal 2. For an ellipse the axis are:

$$a = \left(\frac{4}{\pi^2 C} \right)^{1/6} (FD)^{1/3} \left(\frac{B}{A^3} \right)^{1/6} \quad (3)$$

$$b = \left(\frac{2C}{\pi} \right)^{1/3} (FD)^{1/3} \left(\frac{1}{B} \right)^{1/3} \quad (4)$$

From the (3), (4) equations the dependence between a and b can be obtained from:

$$a/b = \sqrt{\frac{B}{CA}} \quad (5)$$

D depend of the Yung's modulus of carbon nanotubes (E) and of the Yung's modulus of cantilever's probe (E').

$$D = \frac{3}{4} \left(\frac{1 - \sigma^2}{E} + \frac{1 - \sigma'^2}{E'} \right) \quad (6)$$

For an ideal material σ is constant and equal 0,5. Than D are

$$D = 0,56 \frac{E + E'}{EE'} \quad (7)$$

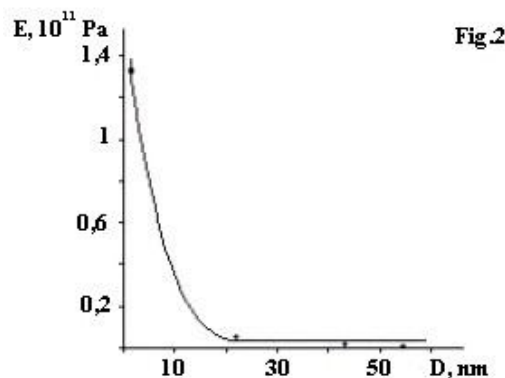
Assuming $E' = 1,5 \cdot 10^{11}$ Pa, the Yung's modulus of carbon nanotubes can be found.

The result of calculations of the Yung's modulus are shown at Fig.2. On the picture we can see that the highest Yung's module's value corresponds one-layer of SWNT, and the number of layers are reduced because of diameter of nanotubes is increasing.

Conclusions

1. The radial deformations of carbon nanotubes are measured in a mode of periodic contact of the AFM.

2. The dependences of inter-atomic force (F) on the value of absolute deformation (ΔD) are investigated: linear dependence according to the Guk's law for nanotube in diameter of 43 and



54 nanometers; square-law ($F \sim \Delta D^2$) for nanotube in diameter of 22 nanometers and for the most thin single-layered in diameter 1,6 nanometers $F \sim \Delta D^5$.

3. It means that non-lasting Born's repelling forces, acting among some of the carbonic atoms, dominate at small distances in single-layer nanotubes.

4. The Yung's modulus of 1-, 5-, 10-, and 30 layer carbon nanotubes are calculated. The carbon nanotubes in the diameter 1,6 nm are calculated $E = 1,32 \cdot 10^{11}$ Pa; 22 nm – $5 \cdot 10^9$ Pa; 43 nm – $2,15 \cdot 10^9$ Pa и 54 nm – $0,63 \cdot 10^9$ Pa.

Reference

1. Landau L.D. Theory of elasticity. (1987). Krishnan A., Dujardin E., Ebbesen T.W., Yianilos P.N., and Treacy M.J. Phys. Rev. B 58, 1401390 (1998).