MECHANICAL PROPERTIES OF «ZIGZAG» AND MULTI-WALLED CARBON NANOTUBES

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A carbon nanotube (which is the most popular nanotube type at the moment) is a cylinder with a wall of single graphite atoms. Its diameter is exactly one nanometer. Carbon nanotubes (CNTs) attract growing interest due to their exceptional mechanical, thermal, and electrical properties.

They were discovered in 1991 by the Japanese electron microscopist Simio Iijima who was studying the material deposited on the cathode

during the arc-evaporation synthesis of fullerenes.

Nanotubes are categorized as single-walled nanotubes (SWNTs) and

multi-walled nanotubes (MWNTs).

Most single-walled nanotubes (SWNT) have a diameter close to 1 nanometer, with a tube length that can be many millions of times longer. The way of wrapping the graphene sheet is represented by a pair of indices (n, m) called the chiral vector. If m = 0, the nanotubes are called "zigzag". If n = m, the nanotubes are called "armchair". Otherwise, they are called "chiral".

Single-walled nanotubes are an important variety of carbon nanotube because they exhibit electric properties that are not shared by the multi-

walled carbon nanotube (MWNT) variants.

Multi-walled nanotubes (MWNT) consist of multiple rolled layers (concentric tubes) of graphite. There are two models which can be used to describe the structures of multi-walled nanotubes: the Russian Doll model and the Parchment.

Nanotubes can be metals or semiconductors, and because of their strong chemical bonds and satisfied valences, the materials boast high thermal, mechanical, and chemical stability. In addition, carbon nanotubes can be efficient conductors due to their tiny diameters, long lengths, and defect-free structures that make them ideal one-dimensional systems.

The radius of nanotube "zigzag" can be determined by bending

a graphite sheet:

$$Q_n = \frac{\sqrt{3}b}{2\pi}\sqrt{n^2 + m^2 + mn},$$

where b — internuclear distance (0,142 nm).

Taking the effective thickness of the walls of SWNTs (t) as 0,074 nm, the effective radius Q_{na} find as:

$$Q_{na} = \frac{\sqrt{3}b}{2\pi} \sqrt{(n^2 + m^2 + mn)} + \frac{t}{2}.$$
 (2)

To calculate the modulus of elasticity of single-layer nanotubes (SWNTs) «zigzag» following relationship was obtained:

$$E = \frac{\lambda K^{\theta} K^{Q}}{3b^{2} K^{Q} + 9\lambda K^{\theta}} \left(\frac{8\sqrt{3}Q_{n}}{Q_{n\theta}^{2}} \right). \tag{3}$$

where $\lambda = \frac{8-2\cos^2\gamma}{4-3\cos^2\gamma}$.

The angle associated with the effect of curvature and is equal $\frac{\pi}{2n}$.

With the change in the number of layers of the nanotube a modulus of elasticity for the MWNT is expressed by the formula:

$$E_{m} = \frac{8\sqrt{3}N}{[(N-1)h+1]} \frac{K^{\theta}K^{Q}}{b^{2}K^{Q}+18K^{\theta}}, \ 1 < N \le 1+2Q_{0}/h, \tag{4}$$

where h — distance between the layers of multilayer nanotubes, equal to 0.34 nm. $K^Q/2 = 46\,900\,\text{kkal/mol/nm}^2$, $K^\theta/2 = 63\,\text{kkal/mol/rad}^2$. There are a permanent forces of tension and constriction.

As a result, we see that with decreasing radius of a single-layer nanotubes «zigzag» and, as a consequence, a decrease of chirality, the modulus of elasticity increases. The modulus of elasticity for multilayer nanotubes depends of the diameter of the nanotube and becomes less sensitive to an increase in the number of layers when $(N \ge 8)$.

REFERENCES

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BANK

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A bank is a financial institution licensed by a government. Its primary activities include borrowing and lending money.

The first state deposit bank, Banco di San Giorgio (Bank of St.

George), was founded in 1407 at Genoa, Italy.