THE ANALYSIS OF THE ELASTIC PROPERTIES OF ARMCHAIR AND ZIGZAG SINGLE-WALLED CARBON NANOTUBES

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ABSTRACT

Computational simulation is a powerful tool for predicting the mechanical properties of carbon nanotubes. In this paper we present analytical molecular mechanics models of elastic properties of armchair and zigzag single-walled nanotubes. The aim of this work is investigation and comparison of Young's modulus, shear modulus and Poisson's ratio variations of armchair and zigzag tubes as functions of diameter. We obtained a set of concise, closed-form expressions for the size-dependent elastic modulus, shear modulus and Poisson's ratio of armchair (n, n) and zigzag (n, 0) nanotubes, which are basic for constructing mathematical models of elastic properties of SWNTs. We investigated armchair nanotubes with chirality (3, 3)–(40, 40) and zigzag (3, 0)–(40, 0) with diameters 4,2–54,2 Å and 2,4–31,3 Å respectively. We calculated Young's modulus to be 0,26–2,95 TPa for armchair and 0,5–3,7 TPa for zigzag nanotubes. The shear modulus calculated for armchair nanotube appeared to be in the range of 0,2–2,0 TPa and for zigzag one in the range of 0,2–2,7 TPa. Specifically, it was inverse dependences of Young's modulus and shear modulus on diameter. The Poisson's ratio was in range from 0,28 to 0,42 and from 0,27 to 0,39, respectively. Results of this research can be used for design, analysis and evaluating of nanotubes functioning and creating new materials based on CNTs.

Key words: carbon nanotubes, Young's modulus, shear modulus, Poisson's ratio

INTRODUCTION

The advancement of science and technology has evolved into the era of nanotechnology. Carbon nanotubes (CNTs) have stimulated great interest and extensive research with regard to the measurement of their exact mechanical properties [1, 2] and the search for potential structural applications [1] ever since their discovery by Iijima [3].

Specific characteristics, such as the exceptionally high stiffness and strength, which are in the range of TPa, the extreme resilience, the ability to sustain large elastic strain as well as the high aspect ratio and low density [1, 4], make CNTs the ideal reinforcing material for a new class of superstrong nanocomposites. That is why the accurate assessment of the mechanical properties

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of the nanotubes is an important first step towards the potential development of the structural composites. Investigation of the properties of those structures has a lot of experimental difficulties arising from their nanoscale, necessity for complicated and expensive equipment and apparatus with large resolution. Computational simulation is a powerful tool relative to the experimental difficulties. In this paper we present two mathematical models, based on classical mechanics and molecular mechanics approach, for investigating the difference between properties of armchair and zigzag single-walled CNTs (SWNTs).

METHODS OF INVESTIGATION

The methods of molecular dynamics (MD) and molecular mechanics (MM) based on the molecular nature of nanotube structure are often used for simulation [4-6] of their mechanical properties. In this work we used MM approach based on modern continuum mechanics and elasticity theory. It allows to calculate the geometry of the frame with sufficient accuracy and to model some physical processes in nanotubes under influence of external factors: the deforming forces, external electromagnetic fields, etc.

We used some basics of molecular mechanics [4, 5] which is based on the concept of molecular force field for this investigation. This approach was based on a link between molecular and solid mechanics. Using the harmonic energy functions the nanotube was modeled as a frame structure and a closed-form elastic solution was obtained.

Let a_1 and a_2 be unit vectors of the two-dimensional graphene sheet, (n, m) be a pair of integers that indexes the atomic structure of CNT uniquely determining the size of the SWNT. Then a pair (n, m) corresponds to a lattice vector $C_h = na_1 + ma_2$ on the graphite plane. If $m = 0$, then such a tube is called zigzag, and when $n = m$ it is an armchair tube. Based on rolling graphene sheer model the diameter D of nanotube can be determined as follows:

$$D = \frac{\sqrt{3}b}{\pi}\sqrt{\left(n^2 + m^2 + mn\right)}, \qquad (1)$$

where b is the carbon-to-carbon bond length. This parameter was taken as 0,66 Å [4].

For armchair and zigzag tubes diameter is equal to D_1 and D_2 respectively:

$$D_1 = \frac{3bn^2}{\pi}, \; D_2 = \frac{\sqrt{3}bn}{\pi}. \qquad (2)$$

Given the effective wall thickness t of SWNTs which corresponds to the thickness of the graphene layer, the effective diameter D_{eff} is equal to $D_{eff} = D_i + t$, where the parameter D_i $(i = 1, 2)$ is taken by D_1 for an armchair tube, and D_2 for a zigzag tube. Effective thickness t was taken as 0,66 Å [4].

We have analyzed the forces and geometrical relations for an armchair tube. Also we have used the assumption that all atomic interactions in a molecular structure of nanotubes satisfy the potential laws, so they can be described by using molecular mechanics. Regarding aforementioned we have build the following relations which comprise our model.

Young's modulus of armchair and zigzag nanotubes is expressed as follows:

$$E = \frac{\lambda_i K^\theta K^\rho}{3b^2 K^\rho + 9\lambda K^\theta}\left(\frac{16\sqrt{3}D_i}{D_{eff\,i}^2}\right), \tag{3}$$

where parameters λ_i, D_i, $D_{eff\ i}$ ($i = 1, 2$) are taken by λ_1, D_1, $D_{eff\ 1}$ for an armchair tube, and λ_2, D_2, $D_{eff\ 2}$ for a zigzag tube; λ_i is the elongation, equaled to the ratio of total nanotubes elongation δl to its length l_0 before deformation:

$$\lambda_1 = \frac{16 + 2\cos^2\gamma}{4 - \cos^2\gamma},\ \lambda_2 = \frac{18 - 2\cos^2\gamma}{4 - 3\cos^2\gamma}, \tag{4}$$

where K_ρ, K_θ are force constants, which depend on the force field. K_ρ = 97800 kcal/mole/nm2, K_θ = 126 kcal/mole/rad2, $\gamma = \pi/2n$ is the angle, related to the curvature effect.

Shear modulus is given by

$$G = \frac{D_{eff_i}^4 - 16\left(\frac{D_{eff_i}}{2} - t\right)^4}{tD_{eff_i}^4}\left(\frac{\sqrt{3}}{3}\frac{\lambda_i K^\theta K^\rho}{b^2 K^\rho + \lambda K^\theta}\right). \tag{5}$$

Poisson's ratio is defined as:

$$\nu = \frac{b^2 K^\rho - \lambda_i K^\theta}{b^2 K^\rho + 3\lambda_i K^\theta}. \tag{6}$$

Mathematical models of elastic properties of armchair and zigzag tubes have been obtained in the form of equations (2), (3), (5) and (6) with taken $i = 1$ for an armchair tube, and $i = 2$ for a zigzag tube.

RESULTS AND DISCUSSION

The elastic properties of two main types of CNT — armchair and zigzag – were investigated and discussed in this paper. We can say that calculated values of elastic properties largely depend on the assumption of the wall thickness t of SWNT. There are other information about different wall thickness such as 6,9 Å, 5,7 and 3,4 Å [4-6]. In this investigation t was taken as 0,66 Å [4].

It was build application for investigation elastic properties using software Delphi 7 and mathematical models of SWNTs. It makes possible to estimate Young's modulus E, shear modulus G and Poisson's ratio v of armchair (n, n) or zigzag (n, 0) tubes with any specified diameter D.

For example, we investigated armchair tubes with chirality from (3, 3) to (40, 40) and zigzag tubes from (3, 0) to (40, 0). Those armchair tubes had diameter from 4,2 to 54,2 Å and zigzag tubes – from 2,4 to 31,3 Å. The values of Young's modulus ranged from 0,26 to 2,95 TPa for armchair and from 0,5 to 3,7 for zigzag nanotubes. We calculated that shear modulus of armchair nanotubes was in the range of 0,2–2,0 TPa and of zigzag was in the range of 0,2–2,7 TPa. Young's and shear moduli have shown inverse chirality and diameter dependences. The Poisson's ratio was ranging from 0,28 to 0,42 and from 0,27 to 0,39 for an armchair and zigzag tubes, respectively. Those results agree well with reported results in literature [3, 4, 6].

CONCLUSIONS

In this paper we present the approach for investigation the elastic properties of SWNTs, based on molecular mechanics. The mathematical models for simulation Young's modulus, shear modulus and Poisson's ratio of armchair and zigzag tubes were built. Those parameters were investigated as functions of the nanotube size and structure. According to the presented models we calculated values of Young's modulus, shear modulus and Poisson's ratio for armchair and zigzag CNTs. It can be seen that predicted values of Young's and shear modulus for zigzag tube are larger than for armchair tube, especially for smaller tubes, but they both decrease rapidly while the diameter increases. With diameter increasing Young and shear modulus of the both type of tubes begin to have the same value. As for Poisson's ratio, we can say that zigzag tube is more sensitive to the diameter than that of the armchair tube.

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