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ESTIMATION OF MATERIAL PROPERTIES OF CARBON NANOTUBES USING FINITE ELEMENT METHOD

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Abstract: The paper deals with estimation of material properties of single-walled carbon nanotubes (SWCNTs). The SWCNTs are simulated as frames, where carbon atoms are replaced by nodes and interatomic interactions are replaced by beams. The tension and torsion loading is applied on SWCNTs for determining the elastic modulus, Poisson's ratio, shear modulus and membrane stiffness of SWCNTs. The simulations for obtaining elongations and torsion angles of SWCNTs are accomplished by the finite element method.

KEYWORDS: beam element; carbon nanotube; FEM; material characteristics

1 Introduction

Carbon nanotubes are structures of nanoscale, which were discovered by Iijima in 1991. The publication of Iijima scientific paper [7] started extensive research of carbon nanotubes. This paper has revealed a new sphere of research in the field of material science and started investigation of different properties of multi-walled and later single-walled carbon nanotubes from different point of views, different ways using different theories. The attention of many researchers and engineers to nanotubes is attracting by interesting electrical and mechanical characteristics of such materials. Between the important mechanical properties belong the high tensile strength and Young's modulus.

The mechanical behaviour of CNTs are investigated using two basic methods: the atomistic-based modelling and the continuum approach. The atomistic-based modelling includes the different types of molecular dynamic simulations. The molecular dynamic simulation was used in [2]. The authors studied elastic properties of SWCNTs with various boundary conditions. In [11] the authors investigated the buckling behaviour of axially compressed carbon nanotubes with different number of walls. The other applications of atomistic-based modelling are listed in [6, 18, 22]. This approach is very time consuming, for this reason is mostly used only for CNTs consisting of one wall and small numbers of atoms. The classical treatment based on continuum mechanics approach can include the standard continuum as well as shell mechanics. In classical continuum mechanics linear and nonlinear elements (truss, beam and spring elements) are used for representation interatomic covalent and non-covalent interactions. In [10] the authors presented structural mechanics procedure for modelling of graphite and CNTs. The authors analysed the material characteristics, e.g. elastic moduli of SWNCTs. They established junction between two treatments - structural and molecular mechanics and used the beam elements for modelling of graphite and SWCNTs. The beam elements for modelling of carbon nanotubes are used in [16, 19, 20] as well. The spring elements for computation of Young's modulus were used in [4, 14]. The authors used three-dimensional nonlinear spring elements, where behaviour of these elements is deduced using the Morse potential energy function. In publications [3, 5, 10, 23] shell elements were used for modelling carbon nanotubes. The advantage of shell elements is that they can be used for prediction static,

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dynamic and buckling behaviours of carbon nanotubes. Other applications of nanotubes or composites are listed in the publications [1, 9, 13, 17].

In this paper the material properties (elastic and shear modulus, Poisson's ratio and membrane stiffness) of all three chirality types of CNTs with one wall are analysed using the finite element method (FEM).

1.1 Carbon nanotubes

The CNTs are made by the rolling graphene sheets. The graphene sheets can be rolled in three directions (Fig. 1) defined by chiral vector

$$\mathbf{C}_h = n\mathbf{a}_1 + m\mathbf{a}_2 \tag{1}$$

Here, the unit vectors $\mathbf{a}_1$ and $\mathbf{a}_2$ and numbers (n, m) represent the chirality of CNT. For the armchair, zigzag and chiral nanotubes (Fig. 2) are $n = m$, $m = 0$ and $n \neq m$, respectively.

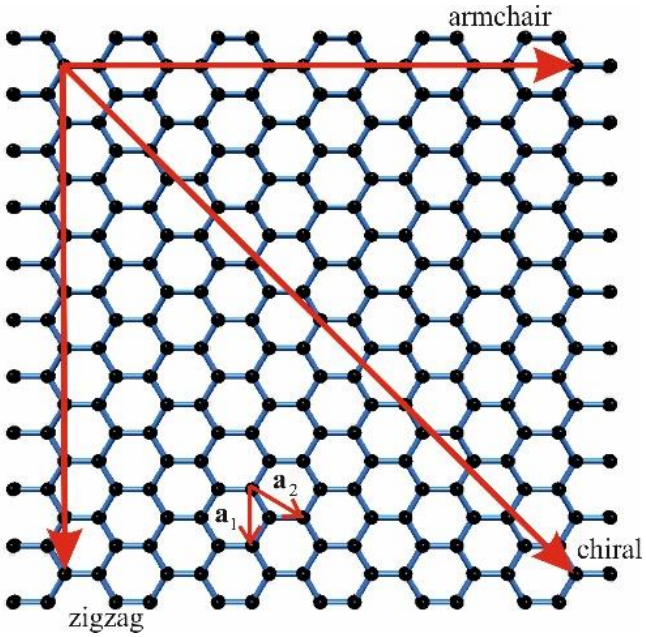

Fig. 1 Graphene sheet with unit vectors and directions of rolling

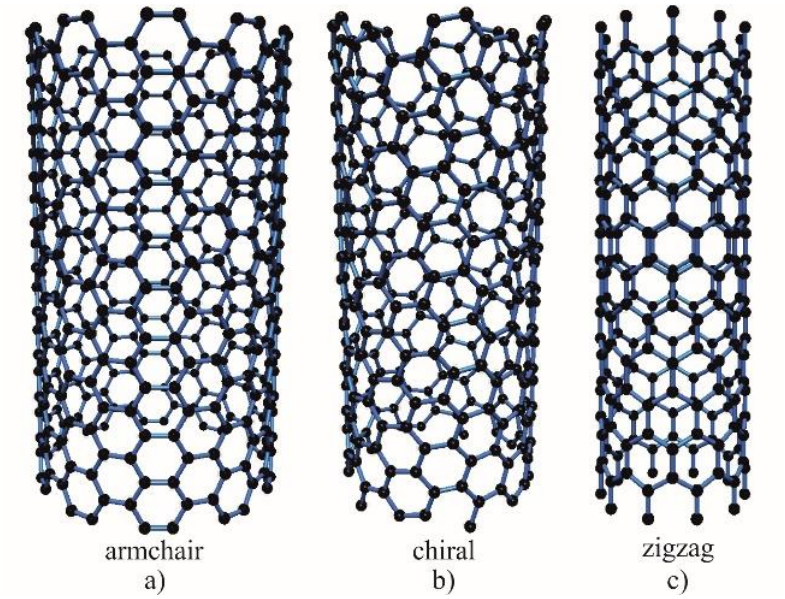

Fig. 2 Scheme of CNT a) armchair b) chiral, c) zigzag

The SWCNTs are analysed as frame structures, where atoms of carbon are modelled by nodes and interatomic interactions are simulated by beam structural members. The input parameters of these structural members are obtained from establishing of the junction of two areas of mechanics - continuum and molecular [19]. The following junctions relating constants in the molecular mechanics k_r, k_θ, k_τ and constants in the continuum mechanics *EA*, *EI*, *GJ* were derived using this connection

$$k_r = \frac{EA}{L}, \qquad k_\theta = \frac{EI}{L}, \qquad k_\tau = \frac{GJ}{L}, \tag{2}$$

where k_r, k_θ, k_τ are bond parameters dependent on stretching, bending and torsional rigidity, respectively, and E, G, L, A, I, J are elastic modulus, shear modulus, length, cross-sectional area, moment of inertia and polar moment of inertia of cross-section, respectively.

The Eq. (2) represents the elementary dependencies for using of continuum mechanics for simulating of carbon nanotubes. Considering a beam with circular cross-section with diameter d and corresponding parameters $A = \pi d^2/4,\ I = \pi d^4/64$ and $A = \pi d^4/32$ then Eq. (2) gives

$$d = \sqrt[4]{\frac{k_\theta}{k_r}}, \qquad E = \frac{k_r^2}{4\pi k_\theta}, \qquad G = \frac{k_r^2 k_\tau L}{4\pi k_\theta^2}. \tag{3}$$

Here, the parameters are given according to [8, 16]: $k_r = 6.52 \times 10^{-7}$ Nnm^{-1}, $k_\theta = 8.76 \times 10^{-10}$ Nnmrad^{-2}, $k_\tau = 2.78 \times 10^{-10}$ Nnmrad^{-2}, $L = a_{C-C} = 0.1421$ nm. From this connection the characteristics of beam structural members are: diameter of beam element $d = 0.1466$ nm, length of beam element $L = a_{C-C} = 0.1421$ nm, elastic modulus $E = 5.49$ MPa and shear modulus $G = 0.871$ MPa.

2 Mechanical properties of SWCNTs

The simulations of two loading types (tension and torsion) are made for obtaining the material properties of SWCNTs. The elongations and torsion angles are obtained from the simulations. The boundary conditions used to calculate the elastic modulus E of the one wall CNTs are defined as follows: one boundary of SWCNT is fixed, the force F is acting on the second boundary (Fig. 3a). The elastic modulus of SWCNT is obtained from relation

$$E = \frac{\sigma}{\epsilon} = \frac{\frac{F}{A}}{\frac{\Delta L}{L}}. \tag{4}$$

Here, *F* is the applied tension force, *A* is the cross-sectional area of CNT and *L* is the total length of CNT. The cross-sectional area is expressed as

$$A = \pi D h. \tag{5}$$

Here, *D* is the mean diameter and *h* is the CNT thickness.

The boundary conditions used to determine SWCNTs shear modulus *G* are defined as follows: one boundary of SWCNT is fixed, the torsion moment *M* about longitudinal axis of CNT is acting on the second boundary (Fig. 3b). From the simulation the angle of twist θ is obtained and then the shear modulus is given as

$$G = \frac{ML}{\theta J}, \tag{6}$$

where *J* is the moment of inertia. For the one wall carbon nanotube the second moment of inertia can be expressed as

$$J = \frac{\pi}{32}[(D+h)^4 - (D-h)^4]. \tag{7}$$

The Poisson's ratio μ is determined using the results of simulations to compute elastic and shear moduli according to equation

$$\mu = \frac{E}{2G} - 1. \tag{8}$$

Finally, the membrane stiffness C is computed as follows

$$C = Eh = \frac{\sigma}{\varepsilon}h = \frac{\frac{F}{A}}{\frac{\Delta L}{L}}h = \frac{\frac{F}{\pi D h}}{\frac{\Delta L}{L}}h = \frac{FL}{\pi D \Delta L}. \tag{9}$$

From Eq. (9) it can be seen, that the membrane stiffness C is independent of the wall thickness h of CNT.

The all simulations are made for four CNTs with armchair chirality ($n = m$), for four CNTs with zigzag chirality ($m = 0$) and for five CNTs with chiral chirality ($n \neq m$). The computed magnitudes of elastic modulus E, Poisson's ratio μ and shear modulus G for wall thickness h = 0.1466 nm are given in Fig. 4 – Fig. 6. The computed magnitudes of membrane stiffness C are shown in Fig. 7.

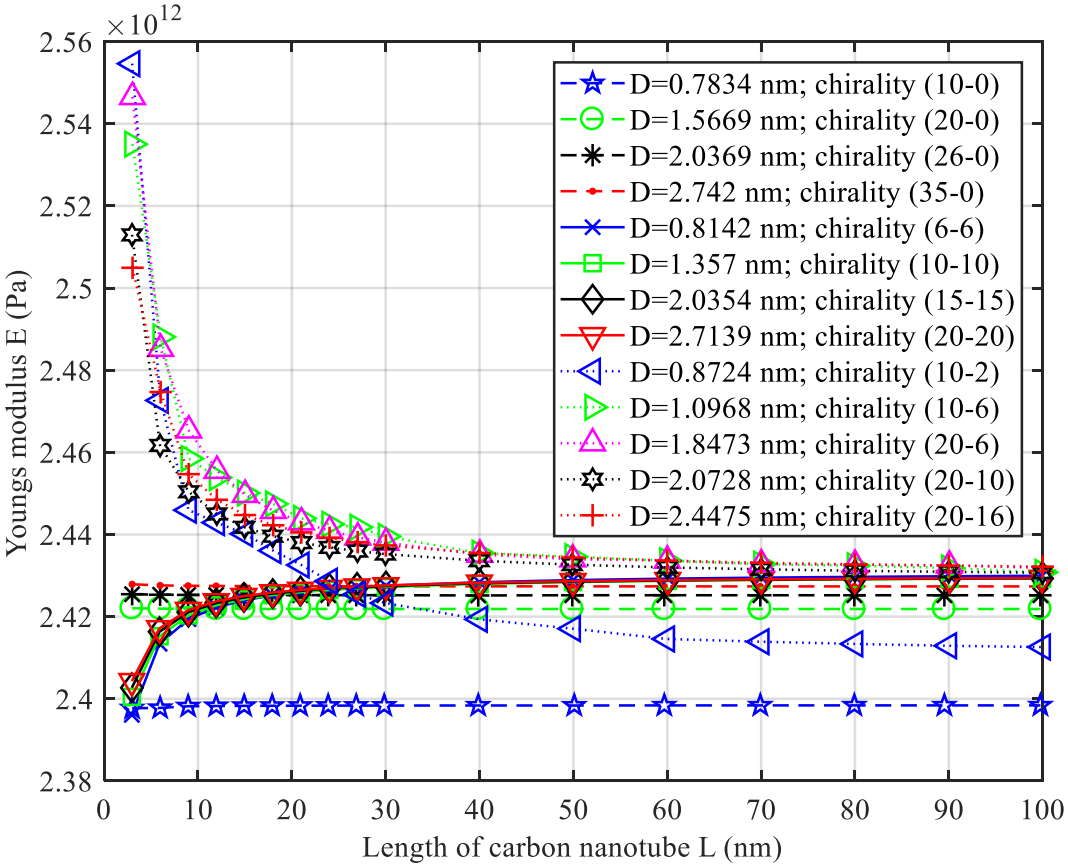

Fig. 4 The elastic modulus E of single-walled carbon nanotubes

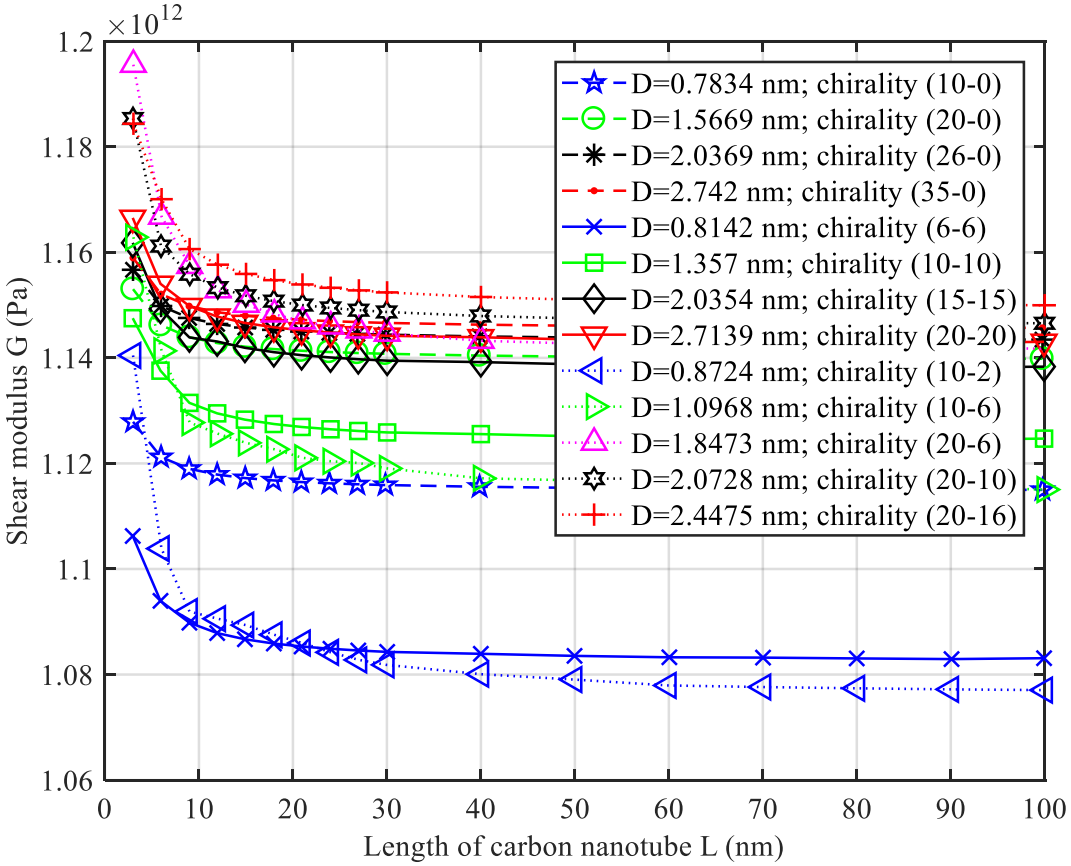

Fig. 5 Shear modulus *G* of single-walled carbon nanotubes

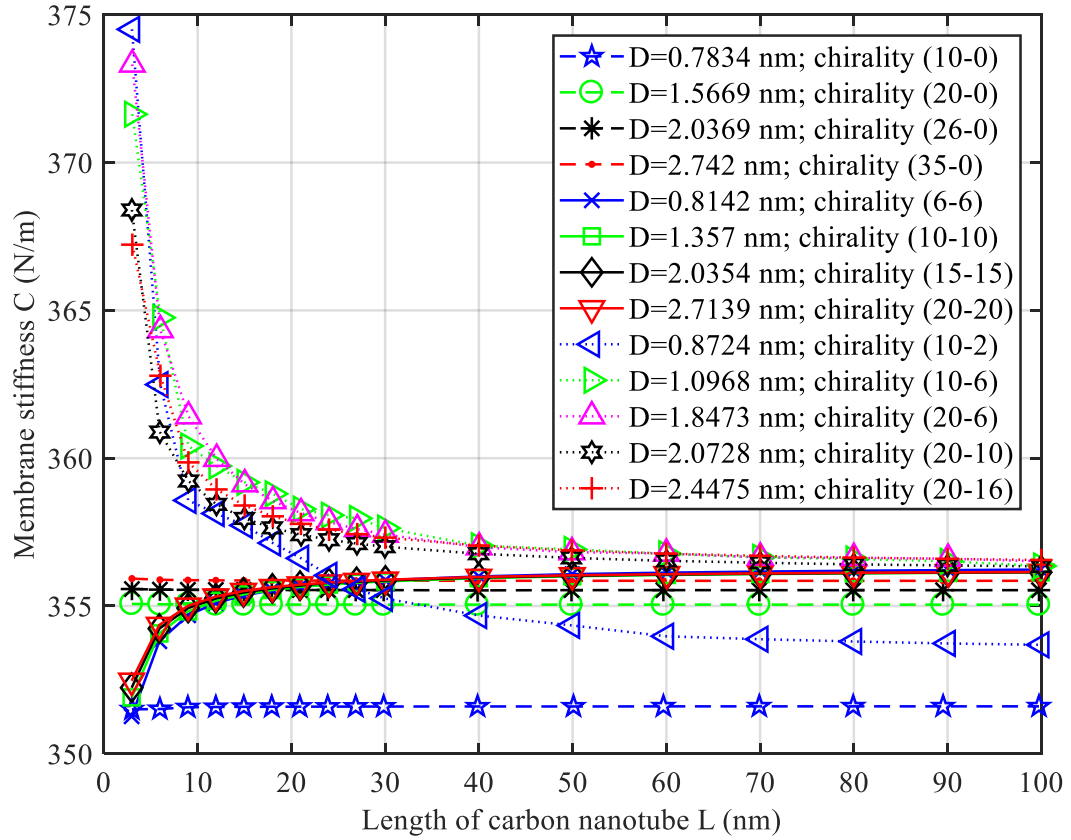

Fig. 6 Poisson's ratio μ of single-walled carbon nanotubes

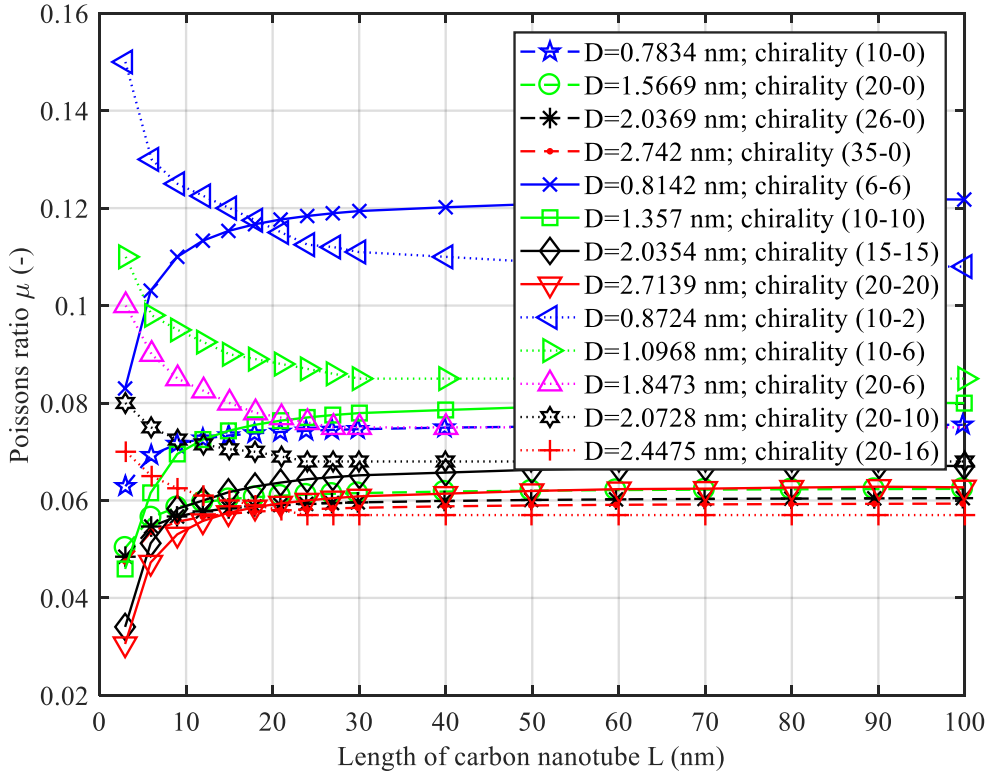

Fig. 7 Membrane stiffness *C* of single-walled carbon nanotubes

Table 1 Elastic modulus for different thickness of SWCNTs

Researchers	Research method	Wall thickness (nm)	Elastic modulus (TPa)	Elastic modulus present method (TPa)
Yakobson et al. [22]	Molecular dynamics	0.066	5,5	5,39
Xin et al. [21]	Tight-binding model	0.074	5,1	4,82
Pantano et al. [15]	Continuum shell method	0.075	4,84	4,74
Kudin et al. [8]	Ab initio computations	0.089	3,86	3,9
Tserpes and Papanikos [20]	Structural mechanics: FE method	0.147	2,38	2,42
Li and Chou [10]	Structural mechanics: stiffness matrix method	0.34	1,01	1,045
Lu [12]	Molecular dynamics	0.34	0,974	1,045
Hemandez et al. [6]	Molecular dynamics	0.34	1,24	1,045
Present work	Structural mechanics: FE method	0.1466	2,43	2,43

From the results it is clear that all investigated parameters depend on chirality and diameter size of SWCNTs. The differences obtained for small length of SWCNTs are caused by boundary conditions in FEM. The wall thickness of SWCNTs h = 0.1466 nm was used for all the numerical computation, but nowadays there is a problem with exact determination of wall thickness. For this reason, the comparison of elastic modulus with different thickness of wall is presented in Tab. 1).

CONCLUSION

The material characteristics as elastic and shear moduli, Poisson's ratio and membrane stiffness of single-walled CNTs were analysed using the finite element method. The all three chirality types of SWCNTs were modelled as the frame structures. The atoms of carbon were modelled using nodes and covalent and non-covalent interactions in atoms were represented by beam structural members. The input properties for these members were obtained establishing connection of two areas of mechanics - continuum and molecular. The tension and torsion loading was applied to obtain the elongations and torsion angles of SWCNTs. These values were used for the numerical computation of mechanical properties. The results of this paper show that:

1) All the material characteristics of SWCNTs are depending on the chirality types. The values of mechanical properties for the small lengths of zigzag and chiral SWCNTs are affected by boundary conditions, but for the enough length of SWCNTs they are linear.

2) The smaller diameter of SWCNTs influences the material properties more than the bigger one.

3) Very important parameter for the determination of SWCNTs material properties values is the SWCNTs's wall thickness. The elastic modulus decreases with increasing wall thickness.

4) The computed membrane stiffness of SWCNTs is independent on the wall thickness. For this reason, the membrane stiffness is better tool of comparing of diverse methods of computation than the elastic modulus.

This method is appropriate for the estimating material properties of SWCNTs and for the other applications in multi-walled carbon nanotubes and modelling complex structures. The results are in good agreement with published data based on atom modelling, the continuum approach and the experimental measurements [8, 10, 12, 15, 22].

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