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Investigation of Elastic Moduli of Twisted Single Wall Carbon Nanotube Based on FEM

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Abstract. In this paper, the Elastic moduli of defected and twisted carbon nanotubes (TCNTs) are described. A three-dimensional finite element (FE) model for this carbon nanotube is proposed. Owing to covalent bonds, the inter-atomic interactions are simulated by beam elements in the FE model. The elastic moduli of beam elements are ascertained from linkage between molecular and continuum mechanics. It is found that the torsional angle of TCNTs significantly affects Young's and shear modulus. Based on the FE model, for TCNTs the values of the Young's modulus have varied from 0.36 to 1.04 TPa and the values of the shear modulus have changed from 0.23 to 0.45 TPa. Also results show that defection in carbon nanotube (CNT) decreased the elastic moduli.

Keywords: elastic moduli, twisted carbon nanotubes, defected carbon nanotubes, finite element model.

1. Introduction

Carbon nanotubes (CNTs), due to their extraordinary mechanical properties, have stimulated great interest and extensive research with regard to the measurement of their exact mechanical properties. The novelty in the field of mechanics includes their greatest Young's modulus and tensile strength among all known materials [1]. Their practical application, however, poses a great challenge to nanotechnology due to their nano scale size [2]. CNTs exhibit exceptionally high stiffness, strength and resilience. As a consequence, they may provide the ideal reinforcing material for a new class of nano-composites [3, 4].

Two main classes of theoretical methods are the atomistic based methods [5, 6] and the continuum mechanics based ones [7, 8]. A few recent publications have proposed the development of structure-property relationships for nanotubes and nanostructured materials through the substitution of the discrete molecular structure with equivalent continuum models [9]. Li and Chou [10, 11] suggested a linkage between molecular mechanics and structural mechanics in terms of geometric parameters of frame structures. Wang et al. [12] studied the relation between bending moment and bending curvature of CNTs to describe the variation of effective bending modulus to Young's modulus ratio with ripples in nanotubes. Another investigation by Wang et al. [13] studied the non-linear bending moment-curvature relationship of CNTs with rippling deformation.

Various theoretical and experimental studies have been carried out to predict and characterize the mechanical properties of CNTs and related materials, all of which generally confirm their superiority. As an example, although the results cover a wide range of 270-5500 GPa for Young's modulus and 290-2300 GPa for shear modulus of different kinds of CNT which are several times greater than those of steel [14-16]. Fundamental to Li and et al. [10, 17] approach was the notion that CNTs are geometrical space-frame structures and therefore, can be analyzed by classical structural mechanics. It seems that deformations and

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defects have considerable effect on mechanical properties. In this paper, based on the concept of Li and et al. [10], three-dimensional (3D) FE models are proposed for TCNTs and defected carbon nanotubes.

2. FE modeling

CNTs atoms are bonded together with covalent bonds forming a hexagonal lattice. These bonds have a characteristic bond length α_{C-C} and bond angle in the 3D space. The displacement of individual atoms under an external force is constrained by the bonds. Therefore, the total deformation of the nanotube is the result of the interactions between the bonds. By considering the bonds as connecting load- carrying elements, and the atoms as joints of the connecting elements, CNTs may be simulated as space-frame structures. In this work, a 3D FE model able to assess the mechanical properties of TCNTs is proposed. The 3D FE model is developed using the ANSYS commercial FE code. For the modeling of the bonds, the 3D elastic BEAM4 element is used. The properties of these elements are obtained by linking the potential energy of bonds and the strain energy of mechanical elements. Considering a circular beam of length l, diameter d, Young's modulus E, and shear modulus G, representing the covalent bond between carbon atoms. The properties of this element are given in Table 1. The simulation relates the bond length α_{C-C} with the element length L as well as the wall thickness t with the element diameter d, as shown in Fig. 1.

Table 1. The properties of beam elements for real carbon nanotube [10]

Nanotube diameter, d	Cross-sectional area, A	The length of carbon-carbon bond	Polar inertia momentum, I_{xx}	Inertia momentum, $I_{zz} = I_{yy} = I$	Young modulus, E	Shear modulus, G
1.466 Å	$1.68794 Å^2$	1.421 Å	$0.453456 Å^4$	$0.22682 Å^4$	$5.488 \frac{N}{Å^2}$	$8.711 \frac{N}{Å^2}$

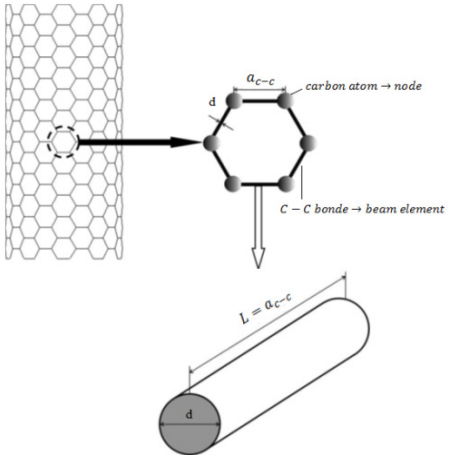


Fig. 1: Simulation of a CNT as a space-frame structure

3. Calculation of elastic moduli

3.1. Young's modulus

The Young's modulus of a material is the ratio of normal stress to normal strain as obtained from a uni-axial tension test ($\sigma = E\varepsilon$) and the strain energy of CNT is

$$U = \frac{1}{2}\sigma\varepsilon AL \tag{1}$$

$$U = \frac{1}{2}E\varepsilon^2 A_0 L \tag{2}$$

Therefore the Young's modulus of CNT is calculated using the following equation

$$E = \frac{2U}{A_0 L\varepsilon^2} \tag{3}$$

where U is total strain energy of CNT and obtained from summing individual strain energy of all elements of nanotube, ε, the total applied strain, A_0, the cross sectional area and L, the initial length. A_0 is equal to πDt, where D is the mean diameter of the tube.

In order to apply the conditions of tension, the nodes of the bottom end of the TCNT have been fully built-in (zero displacement and rotation conditions), while the nodes of the upper end, are subjected to tensile [18] (Fig. 3 (a)). In this paper the wall thickness of CNT is assumed 0.34 nm.

3.2. Shear modulus

For calculating the shear modulus of CNTs, the following relation is used

$$G = \frac{TL}{J\theta} \tag{4}$$

where T stands for the torque acting at the one end of the CNT, θ for the rotational angle of the tube and J for the polar moment of inertia of the cross-sectional area. For calculating J, the CNT is considered as a hollow tube of diameter D and thickness t. In this case

$$J = \left(\frac{\pi}{32}\right)[(D+t)^4 - (D-t)^4] \tag{5}$$

The rotational angle θ is calculated by the FE model. In order to apply the conditions of torsion, the nodes of the bottom end of the CNT have been fully built-in, while the nodes of the upper end, were constrained from moving in radial direction (U_R= 0) and subjected to tangential forces (Fig. 2 (b)).

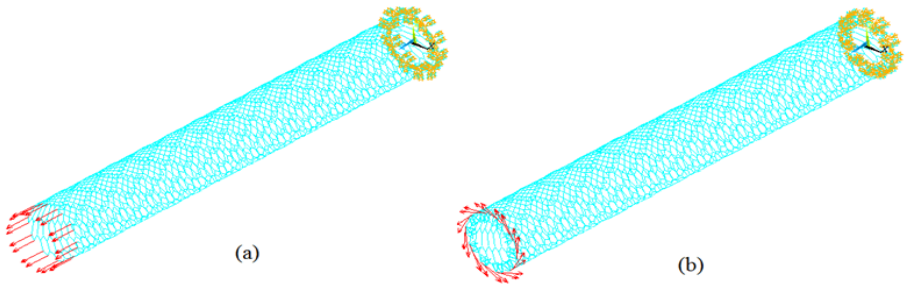


Fig. 2: Iso view of the FE meshes of the (10, 10) twisted nanotube along with the applied boundary conditions (a) tension (b) torsion

4. Results and discussions

4.1. Twisted carbon nanotube

A twisted carbon nanotube is a nanotube that their atoms were rotated respect to nanotube axis with appropriate torsional angle (α). On the other hand, when the atoms of nanotube rotate with appropriate angle, the nanotube changes to twisted nanotube .The boundary conditions for tension and torsion are shown in Fig. 2 a and b, respectively. Young's and shear modulus for chirality of (10, 10) and L=100 Å are given in Table 2. Fig. 3 shows the variations of Young's and shear modulus in term of torsional angle. As illustrated in Fig. 3, with increasing torsional angle, the elastic moduli of twisted nanotube decreased and decreasing rate of Young's modulus was greater than shear modulus.

Table 2. Elastic moduli of TCNT (TPa) for L=100Å

α (degree)	E (TPa)	G (TPa)
0	1.0416 1.025 [19]	0.4539 0.45 [19]
2.5	0.8453	0.4467
5	0.7009	0.4222
7.5	0.5165	0.3394
10	0.3698	0.2339

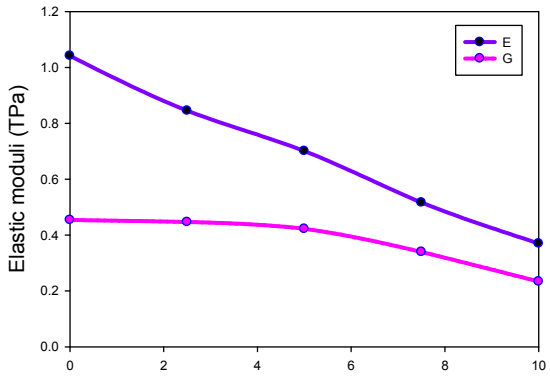
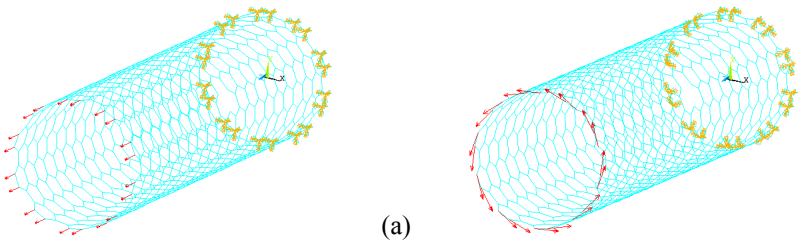


Fig. 3: Elastic moduli of TCNT (TPa) for L=100Å in term of torsional angle α (degree)

4.2. Defected carbon nanotube

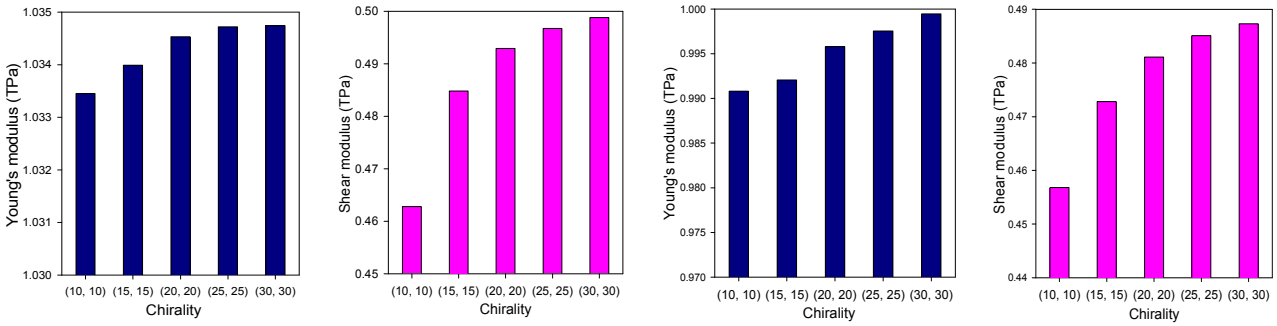
In this section, the FE model is applied to investigate the effect of defect on the elastic moduli of CNTs. For modelling, three bonds and one carbon atom from nanotube is omitted. The boundary conditions for tension and torsion of defected CNT are shown in Fig. 4 (a), and (b), respectively.



(a) (b)

Fig. 4: Boundary conditions of the (10, 10) defected nanotube, (a) tension, (b) torsion

Fig. 5 shows the variations of Young's and shear modulus of CNT and defected nanotube in term of chirality. Results show that with increasing the chirality, the elastic moduli increased weakly. The elastic moduli of defected CNT were lower than nanotube with same chirality.



(a) CNT (b) CNT (c) defected CNT (d) defected CNT

Fig. 5: The elastic moduli of defected nanotube in term of chirality for L=50 Å

5. Conclusions

Three-dimensional finite element models for TCNT and defected CNT have been proposed. As the FE model comprises small number of elements, it performs under minimal computational time by requiring minimal computational power. This advantage, in combination with the modelling abilities of the FE method, extends the model applicability to all kinds of nanotube with very large number of atoms. The results represent that the Young's and shear modulus of TCNT are smaller than CNT. By increasing torsional angle, Young's and shear modulus decreased. So by changing geometry of CNTs, their elastic moduli decreased.

Also results show that defection in carbon nanotube decreased the mechanical properties. As a result, every change in geometry operates as defect and decreased elastic moduli.

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