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# ELASTIC MODULI OF CARBON NANOTUBES WITH NEW GEOMETRY BASED ON FEM

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In this paper, the elastic moduli of elliptic single walled carbon nanotubes (ESWCNTs) are described. A three-dimensional finite element (FE) model for such carbon nanotubes is proposed. The covalent bonds are simulated by beam elements in the FE model. The elastic moduli of beam elements are ascertained from a linkage between molecular and continuum mechanics. The deformations of the FE model are subsequently used to predict the elastic moduli of ESWCNTs. In order to demonstrate the FE performance, the influence of length, chirality, diameter and cross sectional aspect ratios on the elastic moduli (Young's modulus and shear modulus) of ESWCNTs is investigated. It is found that the cross sectional aspect ratio of ESWCNTs significantly affects the elastic moduli. With increasing cross sectional aspect ratio, the Young's modulus and shear modulus decrease. As a result, every change in geometry operates as a defect and decreases the elastic moduli. With increasing the length, Young's modulus increases and the shear modulus decreases.

*Key words:* elastic moduli, elliptic single walled carbon nanotubes, length, chirality, cross sectional aspect ratio, finite element model

## 1. Introduction

Since discovery of carbon nanotubes (CNTs) they have attracted considerable attention in scientific communities. This is due to their remarkable mechanical, electrical and thermal properties. In particular, composite materials such as carbon nanotube, nanoparticle-reinforced polymers and metals have shown potentially wide applications (Meo and Rossi, 2007).

The novelty in the field of mechanics includes their greatest Young's modulus and tensiles trength among all known materials (Thostenson *et al.*, 2001). As a consequence, they may provide the ideal reinforcing material for a new class of nanocomposites (Lau and Hui, 2002a,b). Their practical application, however, poses a great challenge to nanotechnology due to their nanoscale size (Zaeri *et al.*, 2010). Recent investigations (Fereidoon *et al.*, 2012b, 2013; Hemmatian *et al.*, 2011; Rajabpour *et al.*, 2012) have shown that CNTs when aligned perpendicular to cracks are able to slow down the crack growth by bridging up the crack path. Although CNTs can be used as conventional carbon fibers to reinforce polymer matrix in order to form advanced nanocomposites, they may be also used to improve the out-of-plane and interlaminar properties of current advanced composite structures (Lau and Hui, 2002a). These composites have attracted a lot of attention due to their high strength-to-weight ratio (Thostenson *et al.*, 2001).

Qian *et al.* (2002) reported on one of the early investigations on nanotube-based composites; it was observed that when nanotubes of about 1% weight are dispersed homogenously into polystyrene matrices, the elastic modulus increases by 36-42% and the tensile strength improves by about 25%. Parl *et al.* (2002) and Smith *et al.* (2002) developed and characterized nanotube polymer composite films for spacecraft applications.

Two main classes of theoretical methods are the atomistic based methods (Yakobson *et al.*, 1996; Lu, 1997; Sanchez-Portal *et al.*, 1999) and the continuum mechanics based ones (Li and Chou, 2003a; Chang and Gao, 2003; Odegard *et al.*, 2002a). 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 (Odegard *et al.*, 2001, 2002b). Li and Chou (2003a, 2004) suggested a linkage between molecular mechanics and structural mechanics in terms of geometric parameters of frame structures.

Some researchers have attempted to characterize CNTs based on the effective bending moduli. Wang *et al.* (2004) 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.* (2004) 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 of steel (Lau *et al.*, 2004; Meo and Rossi, 2006; Qian *et al.*, 2002; Thostenson *et al.*, 2005; Yu, 2004).

Fundamental to Li and Chou (2003a,b) approach was the notion that CNTs are geometrical space-frame structures and therefore, can be analyzed by classical structural mechanics. In this research, based on the concept of Li *et al.* (2003a), three-dimensional (3D) FE models are proposed for investigating ESWCNTs.

## 2. FE modeling

CNTs atoms are bonded together with covalent bonds forming a hexagonal lattice. An elliptic single walled carbon nanotube (ESWCNT) is a kind of nanotube that has oval cross sectional area (Fereidoon *et al.*, 2012a). This kind of CNT may be produced in special states and conditions. The ESWCNT with $a/b = 1$ is known as SWCNT, where $a$ and $b$ are major and minor diameters of ellipse, respectively.

As shown in Fig. 1, these bonds have a characteristic bond length $\alpha_{C-C}$ 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 a 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 of ESWCNTs is proposed to assess the mechanical properties. 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 (from a chemical point of view) and the strain energy of mechanical elements (from a mechanical point of view). Considering a circular beam of length $l$, diameter $d$, Young's modulus $E$, and shear modulus $G$, the model represents the covalent bond between carbon atoms. The properties of this element are given in Table 1 (Li and Chou, 2003a).

The simulation relates the bond length $\alpha_{C-C}$ with the element length $L$ as well as the wall thickness $t$ with the element diameter $d$, as shown in Fig. 1.

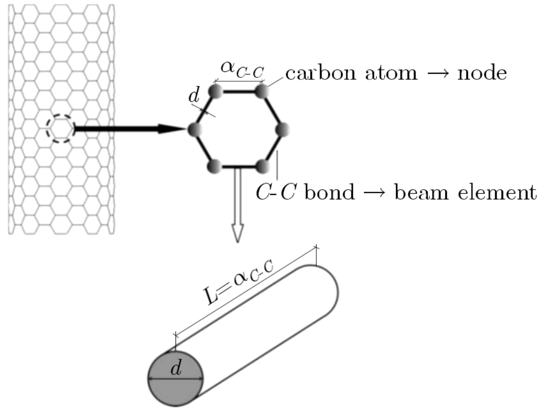


Fig. 1. Simulation of a SWCNT as a space-frame structure

**Table 1.** The properties of beam elements for real carbon nanotube (Li and Chou, 2003a)

| Parameters | Value |
|---|---|
| Nanotube diameter $d$ | 1.466 Å |
| The length of carbon-carbon bond $L$ | 1.421 Å |
| Cross-sectional area $A$ | 1.68794 Å$^2$ |
| Polar inertia momentum $I_{xx}$ | 0.453456 Å$^4$ |
| Inertia momentum $I_{zz} = I_{yy} = I$ | 0.22682 Å$^4$ |
| Young modulus $E$ | $5.188 \cdot 10^{-8}$ N/Å$^2$ |
| Shear modulus $G$ | $8.711 \cdot 10^{-9}$ N/Å$^2$ |

## 3. Calculation of elastic moduli

### 3.1. Young's modulus

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 ESWCNTs is

$$U = \frac{1}{2}\sigma\varepsilon AL \qquad U = \frac{1}{2}E\varepsilon^2 A_0 L \tag{3.1}$$

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

$$E = \frac{2U}{A_0 L\varepsilon^2} \tag{3.2}$$

where $U$ is total strain energy of ESWCNT obtained from summing individual strain energy of all elements of the nanotube, $\varepsilon$ – total applied strain, $A_0$ – cross sectional area and $L$ – initial length. $A_0$ is

$$A_0 = \pi\Big[\Big(a + \frac{t}{2}\Big)\Big(b + \frac{t}{2}\Big) - \Big(a - \frac{t}{2}\Big)\Big(b - \frac{t}{2}\Big)\Big] \tag{3.3}$$

In order to apply the conditions of tension, the nodes of the bottom end of the ESWCNT have been fully built-in (zero displacement and rotation conditions), while the nodes of the upper end are subjected to tension (Jalalahmadi and Naghdabadi, 2007) (Fig. 2a). In this paper, it has been assumed that the wall thickness of the ESWCNT is 0.34 nm.

### 3.2. Shear modulus

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

$$G = \frac{TL}{J\theta} \tag{3.4}$$

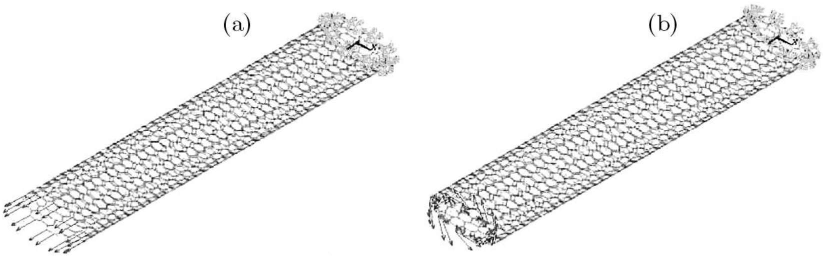


Fig. 2. Isometric view of FE meshes of the $(10, 10)$ elliptic CNT along with the applied boundary conditions: (a) tension, (b) torsion

where $T$ stands for the torque acting at one end of the ESWCNT, $\theta$ for the torsional angle of the tube and $J$ for the polar moment of inertia of the cross-sectional area. For calculating $J$, the ESWCNT is considered as a hollow tube with elliptic cross section. In this case $J$ is

$$J = \frac{\pi}{4}\Big\{\Big(a+\frac{t}{2}\Big)\Big(b+\frac{t}{2}\Big)\Big[\Big(a+\frac{t}{2}\Big)^2+\Big(b+\frac{t}{2}\Big)^2\Big]-\Big(a-\frac{t}{2}\Big)\Big(b-\frac{t}{2}\Big)\Big[\Big(a-\frac{t}{2}\Big)^2+\Big(b-\frac{t}{2}\Big)^2\Big]\Big\} \tag{3.5}$$

The torsional angle $\theta$ is calculated by the FE model. In order to apply the conditions of torsion, the nodes of the bottom end of the ESWCNT have been fully built-in, while the nodes of the upper end, were constrained from moving in the radial direction $(U_R = 0)$ and subjected to tangential forces (Jalalahmadi and Naghdabadi, 2007) (Fig. 2b).

The values of Young's and shear modulus calculated for SWCNTs $(a/b = 1)$ have been compared with the corresponding values from the literature. Table 2 summarizes all calculations and the comparison. As may be seen in Table 2, elastic moduli computed by the present FE model agrees very well with each elastic moduli obtained by the corresponding methods, and the present method is verified.

**Table 2.** Comparison of elastic moduli by different researchers

| Researcher | Element | $E$ [TPa] | $G$ [TPa] |
|---|---|---|---|
| Li and Chou (2003a) | beam | 1.010 | 0.475 |
| Tserpes and Papanikos (2005) | beam | 1.028 | 0.410 |
| Kalamkarov *et al.* (2006) | beam | 0.980 | 0.350 |
| Giannopoulos *et al.* (2008) | spring | 1.307 | 0.383 |
| Shokrieh and Rafiee (2010) | beam | 1.033-1.042 | 0.417 |
| Present work | beam | 1.033-1.035 | 0.46-0.49 |

## 4. Results and discussion

The mechanical properties of ESWCNTs depend on their length, chirality, diameter and cross sectional aspect ratio $(a/b)$. Several works investigating the dependence of elastic moduli of SWCNTs on their diameter and chirality have been reported. In the majority of them, armchair and zig-zag SWCNTs have been only included. In the present work, the FE model is applied to investigate the effect of length, diameter, chirality and cross sectional aspect ratio $(a/b)$ on the elastic moduli of ESWCNTs. All three types of SWCNTs, namely, armchair, zig-zag and chiral are included in the investigation.

The boundary conditions for tension and torsion are shown in Figs. 2a and 2b, respectively. Cross sections of ESWCNTs for different $a/b$ from 1 to 2 are represented in Fig. 3.

Young's and shear modulus of ESWCNTs for some kind of armchair and zig-zag nanotubes with different lengths and cross sectional aspect ratios are calculated. Young's and shear modulus of ESWCNTs with different lengths of 25, 50, 75, 100 Å for armchair nanotubes with chiralites of $(5,5)$, $(10,10)$, $(15,15)$, $(20,20)$ are plotted against the cross sectional aspect ratio $(a/b)$ in Figs. 4-7.

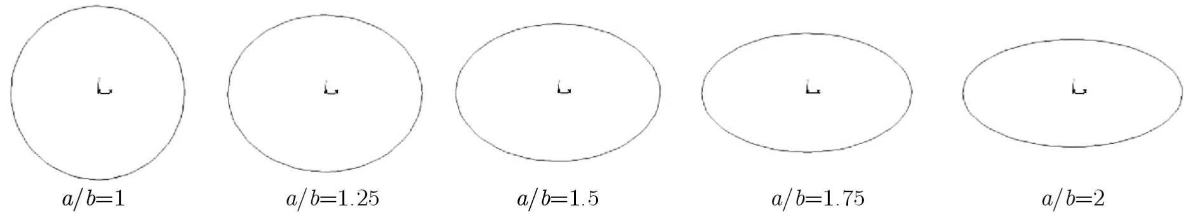


Fig. 3. Cross sections of ESWCNTs for different $a/b$

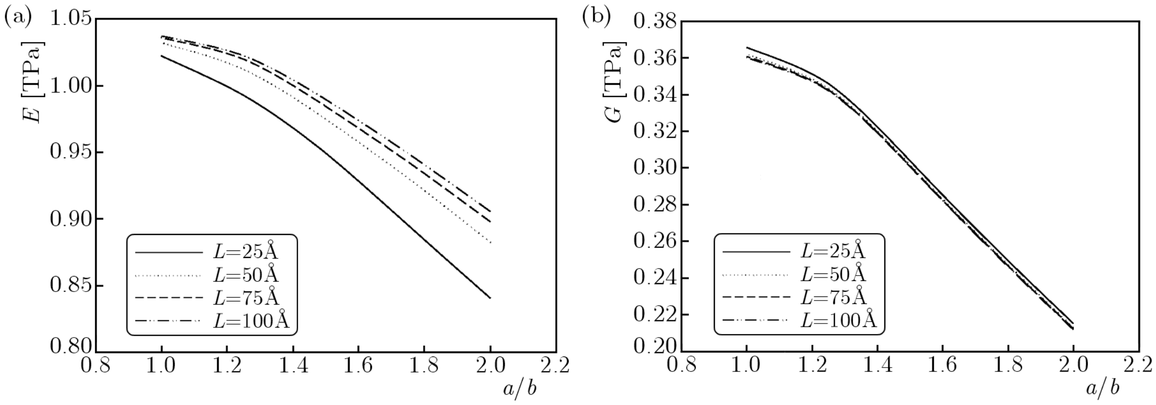


Fig. 4. Variation of Young's modulus (a) and shear modulus (b) of $(5,5)$ with the cross sectional aspect ratio $(a/b)$ for different lengths

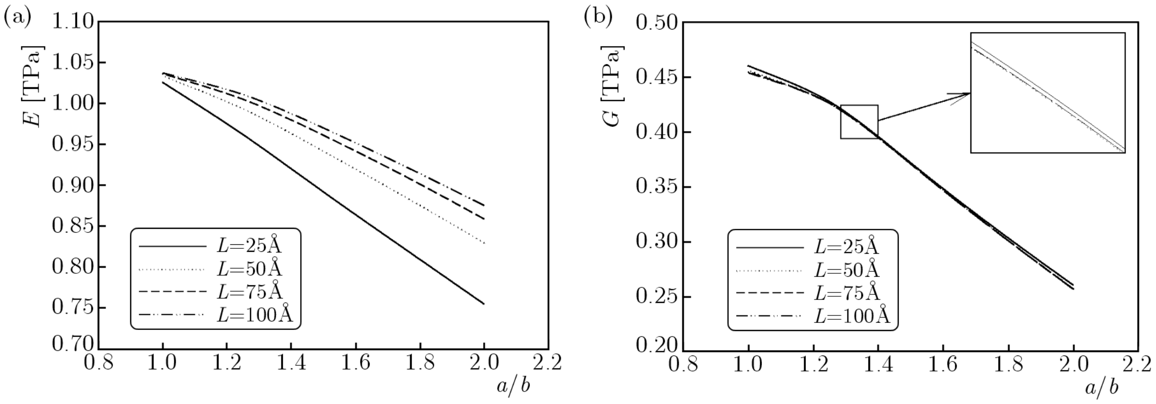


Fig. 5. Variation of Young's modulus (a) and shear modulus (b) of $(10,10)$ with the cross sectional aspect ratio $(a/b)$ for different lengths

Similarly, Figs. 8-11 show the variation of Young's and shear modulus with the cross sectional aspect ratio $(a/b)$ for different lengths of 25, 50, 75, 100 Å for zig-zag nanotubes with chirality of $(5,0)$, $(10,0)$, $(15,0)$, $(20,0)$.

### 4.1. Effects of length and cross sectional aspect ratio $(a/b)$ on the elastic moduli of ESWCNTs

Figures 4-11 show the variation of elastic moduli of armchair, zig-zag ESWCNTs with different length and cross sectional aspect ratio $(a/b)$. It can be observed that there is an evident effect of these parameters on Young's and shear modulus of the armchair and zig-zag ESWCNTs.

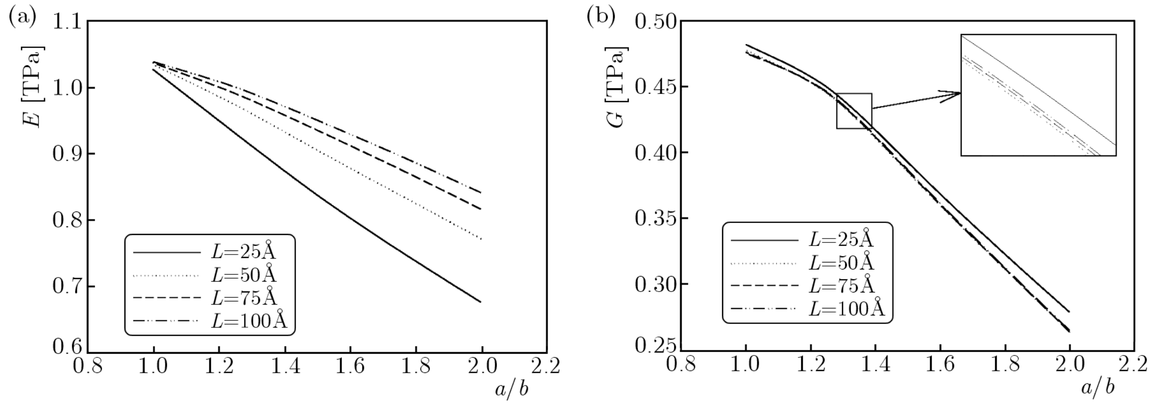


Fig. 6. Variation of Young's modulus (a) and shear modulus (b) of $(15,15)$ with the cross sectional aspect ratio $(a/b)$ for different lengths

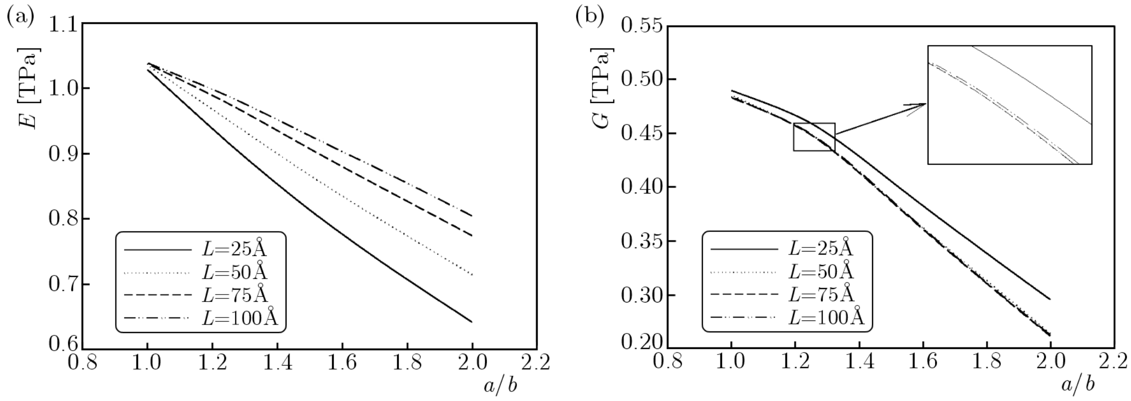


Fig. 7. Variation of Young's modulus (a) and shear modulus (b) of $(20,20)$ with cross sectional aspect ratio $(a/b)$ for different lengths

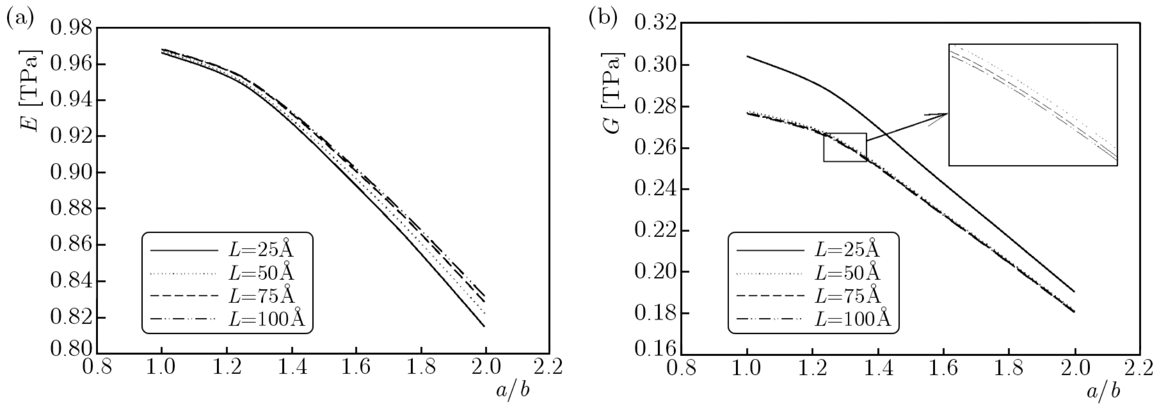


Fig. 8. Variation of Young's modulus (a) and shear modulus (b) of $(5,0)$ with the cross sectional aspect ratio $(a/b)$ for different lengths

As may be seen for all kinds of armchair and zig-zag nanotubes, with increasing the length, Young's modulus increases and the shear modulus decreases. Furthermore, for each length with the increasing cross sectional aspect ratio $(a/b)$, elastic moduli decrease. The figures suggest that the elastic moduli values are inversely proportional to the cross sectional aspect ratio. On the other hand, elastic moduli of ESWCNTs are smaller than SWCNTs (a/b=1). So, by changing geometry of SWCNTs, their elastic moduli decrease. As a result, every change in geometry operates as a defect and decreases the elastic moduli.

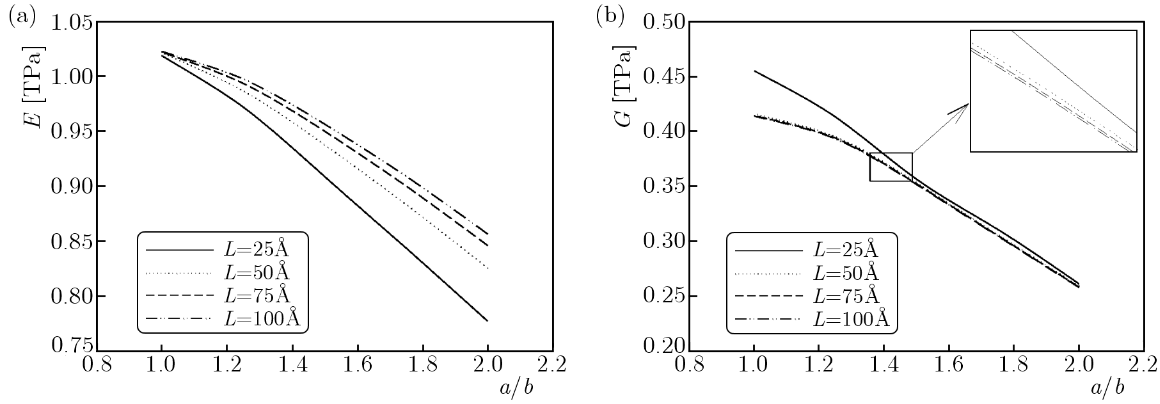


Fig. 9. Variation of Young's modulus (a) and shear modulus (b) of $(10,0)$ with the cross sectional aspect ratio $(a/b)$ for different lengths

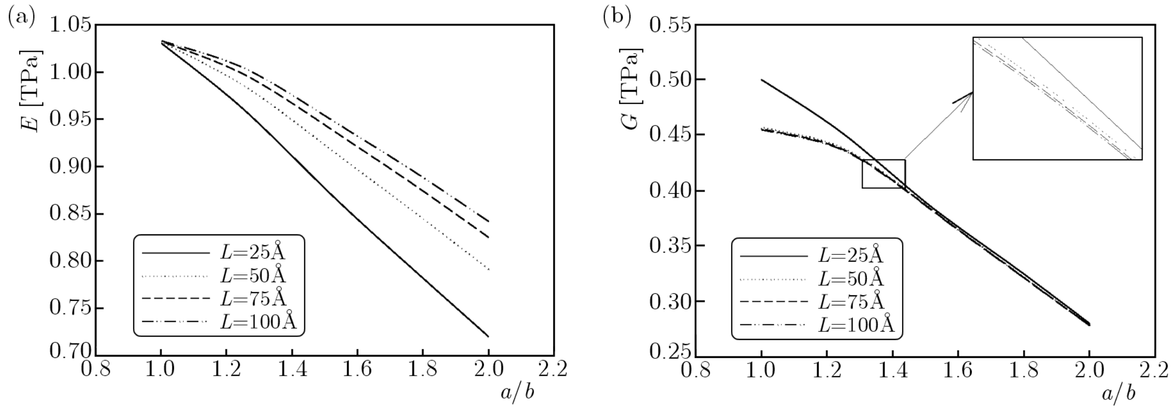


Fig. 10. Variation of Young's modulus (a) and shear modulus (b) of $(15,0)$ with the cross sectional aspect ratio $(a/b)$ for different lengths

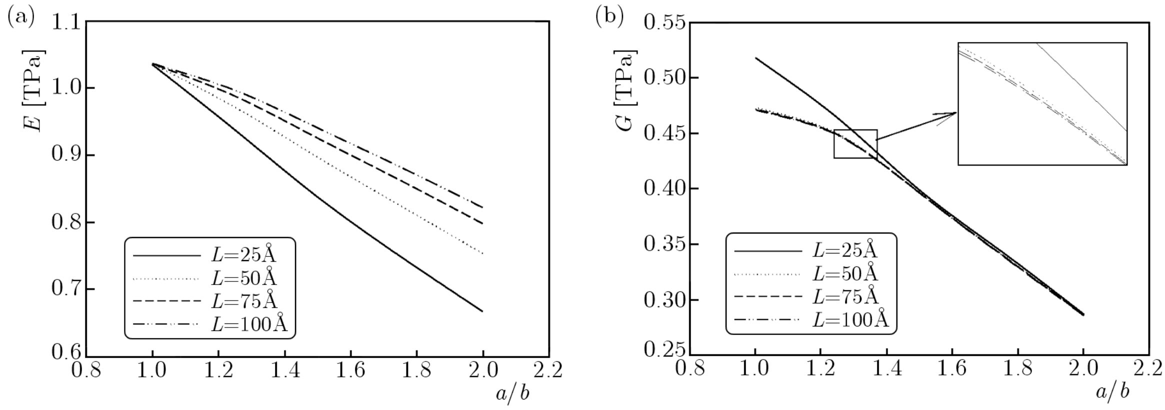


Fig. 11. Variation of Young's modulus (a) and shear modulus (b) of $(20,0)$ with the cross sectional aspect ratio $(a/b)$ for different lengths

### 4.2. Effects of chirality and cross sectional aspect ratio $(a/b)$ on the elastic moduli of ESWCNTs

Figures 12a and 12b indicate the variation of Young's and shear modulus of armchair and zig-zag ESWCNTs as a function of the cross sectional aspect ratio $(a/b)$ with length 50 Å. For armchair and zig-zag nanotubes with increasing chirality, the shear modulus increases, and with increasing cross sectional aspect ratio $(a/b)$, the shear modulus decreases.

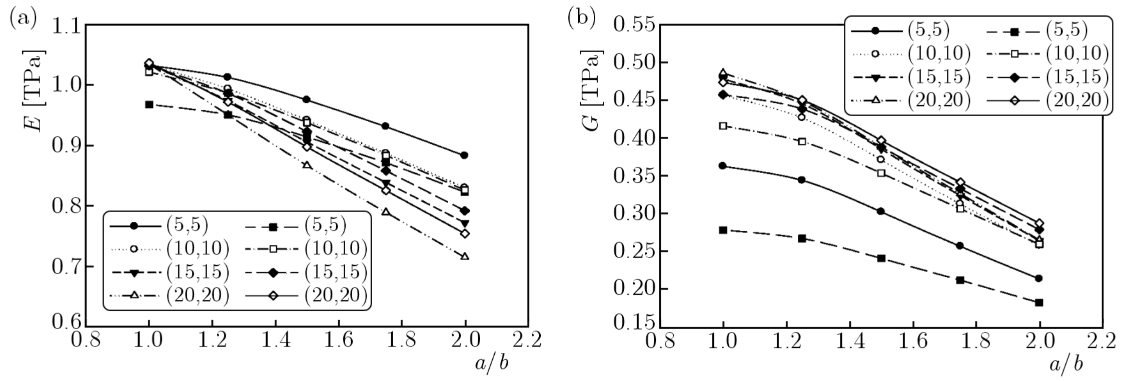


Fig. 12. Variation of Young's modulus (a) and shear modulus (b) with the cross sectional aspect ratio $(a/b)$ and length of 50 Å

Young's modulus of ESWCNTs with armchair and zig-zag chirality increases with the increasing chirality for $a/b = 1$. In the most of other cross sectional aspect ratios $(a/b)$ with increasing chirality, Young's modulus decreases. With the increasing cross sectional aspect ratio $(a/b)$ for each chirality, Young's modulus decreases.

### 4.3. Effects of chirality on the elastic moduli of ESWCNTs

In this section, elastic moduli of eight kinds of armchair, zig-zag and chiral nanotubes with similar lengths and diameters and cross sectional aspect ratio $(a/b)$ equal to 1.5 are calculated. The diameters and lengths of these ESWCNTs are given in Table 3.

**Table 3.** Geometry and mechanical properties of different nanotubes with the same diameter and $a/b = 1.5$

| Chirality | Radius [Å] | $L$ [Å] | $E$ [TPa] | $G$ [TPa] |
|---|---|---|---|---|
| (10, 10) | 6.785 | 49.225 | 0.9415 | 0.3705 |
| (11, 9) | 6.796 | 49.38 | 0.7837 | 0.3087 |
| (12, 8) | 6.830 | 49.55 | 0.9017 | 0.3148 |
| (13, 7) | 6.886 | 49.50 | 0.7844 | 0.3753 |
| (14, 5) | 6.682 | 50.23 | 0.7096 | 0.3613 |
| (15, 4) | 6.796 | 49.75 | 0.8788 | 0.3569 |
| (16, 2) | 6.694 | 49.39 | 0.8314 | 0.3869 |
| (17, 0) | 6.659 | 49.489 | 0.9204 | 0.3968 |

As shown in Fig. 13, the armchair nanotube $(10, 10)$ has the maximum Young's modulus, and the zig-zag nanotube $(17, 0)$ has the maximum shear modulus. The results indicate that the chirality has evident influence on the elastic moduli. In other words, with similar length and diameter and different chirality, the elastic moduli are not equal. Therefore, the elastic moduli of ESWCNTs are sensitive to their atomic arrangement.

## 5. Conclusions

Three-dimensional finite element models for ESWCNTs have been proposed. To create FE models, nodes are placed at the locations of carbon atoms and the bonds between them are modeled using three-dimensional elastic beam elements. As the FE model comprises a small number of elements, it performs under minimal computational time by requiring minimal computational

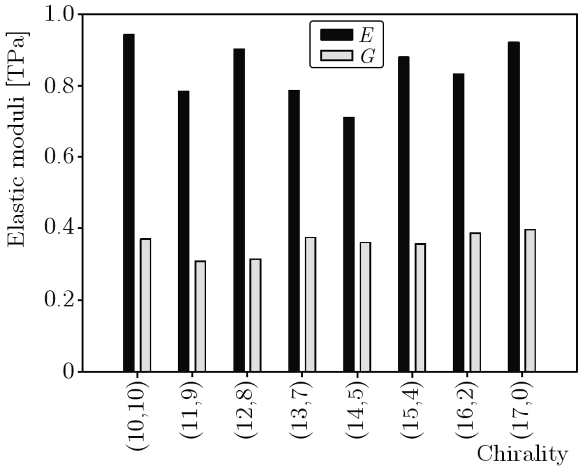


Fig. 13. The elastic moduli versus chirality for ESWCNT with the same diameter and $a/b = 1.5$

power. This advantage, in combination with the modeling abilities of the FE method, extends the model applicability to all kinds of nanotubes with a very large number of atoms. The main conclusions drawn from this study are as follows:

- With increasing the length of ESWCNTs, Young's modulus increases and the shear modulus.
- For each length with the increasing cross sectional aspect ratio $(a/b)$, elastic moduli decrease.
- With increasing chirality, the shear modulus of ESWCNTs increases.
- The elastic moduli of ESWCNTs are sensitive to their atomic arrangement.

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