Finite element modeling of single-walled carbon nanotubes with introducing a new wall thickness

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Abstract. A three-dimensional finite element (FE) model for armchair, zigzag and chiral single-walled carbon nanotubes (SWCNTs) is proposed. By considering the covalent bonds as connecting elements between carbon atoms, a nanotube is simulated as a space frame-like structure. Here, the carbon atoms act as joints of the connecting elements. To create the FE models, nodes are placed at the locations of carbon atoms and the bonds between them are modeled using three-dimensional elastic beam elements. Using Morse atomic potential, the elastic moduli of beam elements are obtained via considering a linkage between molecular and continuum mechanics. Also, a new wall thickness (=bond diameter) equal to 0.1296 nm is introduced. In order to demonstrate the applicability of FE model and new wall thickness, the influence of tube wall thickness, diameter and chirality on the Young’s modulus of SWCNTs is investigated. It is found that the choice of wall thickness significantly affects the calculation of Young’s modulus. For the values of wall thickness used in the literature, the Young’s moduli are estimated which agree very well with the corresponding theoretical results and experimental measurements. We also investigate the dependence of elastic moduli on diameter and chirality of the nanotube. The larger tube diameter, the higher Young’s modulus of SWCNT. The Young’s modulus of chiral SWCNTs is found to be generally larger than that of armchair and zigzag SWCNTs. The presented results demonstrate that the proposed FE model and wall thickness may provide a valuable tool for studying the mechanical behavior of carbon nanotubes and their application in nano-composites.

1. Introduction

Since the discovery of multi-walled carbon nanotubes in 1991 by Iijima [1], and subsequent synthesis of single-wall carbon nanotubes by others [2,3] there are numerous experimental and theoretical studies of their electronic, chemical, and mechanical properties. Diverse nanoscale device concepts have been proposed to develop nanoscale electronic devices, chemical sensors, and also high strength nanotube composite materials with sensing and actuating capacity. An accurate assessment of the mechanical properties of individual nanotubes maybe is an important first step in guiding the potential development of structural composites.

A variety of outstanding experimental results on the elucidation of the elastic properties of nanotubes is fast appearing. They are mainly based on the techniques of high-resolution transmission microscopy (TEM) and atomic force microscopy (AFM) [4,5]. Yu et al. [6] have demonstrated the use of atomic force microscopy (AFM) to measure the mechanical properties of multi-walled carbon
nanotubes (MWCNTs). They have suggested the tensile strength and modulus range from 11 to 63 GPa and 0.27 to 0.95 TPa, respectively. Wong et al. [7] and Demczyk et al. [8] have estimated the elastic modulus of 1.28 ±0.59 and about 0.9 TPa, respectively. Such results confirm the theoretical predictions that nanostructures like carbon nanotubes have high strength as well as extraordinary flexibility and resilience. Theoretical studies on the mechanical properties of nanostructures are more numerous and advanced than experiments, mainly due to the technological challenges involved in the manipulation of nanometer-sized objects. Two main classes of theoretical methods are the atomistic based methods [9-11] and the continuum mechanics based ones [12-14]. The former is currently limited by the computational complexity with respect to the number of atoms. However, several models in continuum mechanics are used. By comparing different theoretical results concerning the elastic properties of nanotubes, it is found that they vary with the type of technique used.

In this paper, a three-dimensional finite element (FE) model for armchair, zigzag and chiral single-walled carbon nanotubes (SWCNTs) is proposed. Using Morse atomic potential, the elastic moduli of beam elements are obtained via considering a linkage between molecular and continuum mechanics. In order to demonstrate the applicability of FE model and new wall thickness, the influence of tube wall thickness, diameter and chirality on the Young’s modulus of SWCNTs is investigated.

2. Finite element modelling

In this work, a 3D FE model, capable of assessing the mechanical properties of SWCNTs, is proposed. The 3D FE model is developed using the ANSYS commercial FE code. To create the FE models, nodes are placed at the locations of carbon atoms and the covalent bonds between them are modeled using three-dimensional elastic BEAM4 ANSYS elements. This specific element has six degrees of freedom at each node and is defined by two nodes as well as its cross-sectional area, two moments of inertia, two dimensions and the material properties. The simulation leads to the correspondence of the bond length with the element length L as well as the wall thickness t with the element diameter.

To calculate the elastic moduli of beam elements, a linkage between molecular and continuum mechanics is used. There has been a wealth of literature in molecular mechanics devoted to the study of the functional form of the potential energy. Among the earliest ones is Morse exponential pair potential which later has been evolved by adding a bond-angle-bending potential term, as used by Belytschko et al [15]:

\[
E = E_{\text{stretch}} + E_{\text{angle}}
\]

\[
E_{\text{stretch}} = D_e \left\{ \left[ 1 - e^{-\beta (r - r_0)} \right]^2 - 1 \right\}
\]

\[
E_{\text{angle}} = \frac{1}{2} k_\theta \left( \theta - \theta_0 \right)^2 \left[ 1 + k_{\text{sextic}} \left( \theta - \theta_0 \right)^4 \right]
\]

where \( E_{\text{stretch}} \) is the bond energy due to bond stretch, and \( E_{\text{angle}} \) is the bond energy due to bond angle-bending, \( r \) is the length of the bond, and \( \theta \) is the current angle of the adjacent bonds, a standard deformation measure in molecular mechanics. The parameters are:

\[
r_0 = 1.39 \times 10^{-10} \text{ m}, \quad D_e = 6.03105 \times 10^{-10} \text{ N m}, \quad \beta = 2.625 \times 10^{10} \text{ m}^{-1}
\]

\[
\theta_0 = 2.094 \text{ rad}, \quad k_\theta = 0.9 \times 10^{-18} \text{ N m/ rad}^2, \quad k_{\text{sextic}} = 0.754 \text{ rad}^{-4}
\]

This is the usual Morse potential except that the angle-bending energy has been added and the constants are slightly modified so that it corresponds with the Brenner potential for strains below 10%. To obtain the effective stretching and bending stiffness of the bond, first we consider the stiffnesses of the classical beam as follows:

\[
K_{E}^{\text{beam}} = \frac{EA}{l} , \quad K_{M}^{\text{beam}} = \frac{EI}{l}
\]
Where in the above, $E$ is the elastic modulus, $A$ is the cross-sectional area, $I$ is the moment of inertia of the section, and $l$ is the length of the beam. Now, we can differentiate equation (1) to obtain the corresponding stiffness coefficients of the atomic bonds. Consequently, we derive:

$$K_f = 5337.38 \text{ eV/nm}^2 = 854 \text{ nN/nm}$$
$$K_M = 5.617 \text{ eV/rad}^2 = 0.9 \text{ nN.nm/rad}^2$$

Equating equations (3) and (4), the effective stretching and bending stiffness of the equivalent beam element would be obtained as:

$EA = 123.8 \text{nN}$, $EI = 0.13 \text{nN.nm}^2$

Assuming a circular cross-sectional area for the element, we have:

$$d = 0.1296 \text{nm}$$
$$E = 9.382 \text{TPa}$$

3. **Young’s modulus of SWCNTs**

The Young’s modulus of a material is the ratio of normal stress to normal strain as obtained from a uni-axial tension test ($\sigma = E\varepsilon$). Our studies is in the linear regime, so strain energy of SWCNT is

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

Therefore the Young’s modulus of SWCNTs is calculated using the following equation

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

where $U$ is total strain energy of all elements of SWCNT, $\varepsilon$, the total applied strain, $A_0$, the cross-sectional area and $L$, the initial length. $A_0$ is equal to $\pi D t$ where $D$ is the mean diameter of the tube. $U$ is obtained from summing individual strain energy of all elements of SWCNT.

![Figure 1](image.png)

Figure 1. The FE meshes of the (a) (7,7), (b) (12,0) and (c) (5,9) SWCNTs along with the applied boundary conditions.
In order to apply the conditions of tension, the nodes of the bottom end of the SWCNT have been fully built-in (zero displacement and rotation conditions), while the nodes of the upper end, are subjected to tensile strains. Figure 1 shows the FE meshes of the three different types of SWCNTs along with the applied boundary conditions.

### Table 1. Comparison of Young’s modulus for different values of wall thickness

| Investigators                  | Method                                     | Wall Thickness (nm) | Young’s modulus (TPa) | Present FE model (TPa) |
|-------------------------------|--------------------------------------------|---------------------|-----------------------|------------------------|
| Yakobson et al. [9]           | Molecular Dynamics                          | 0.066               | 5.5                   | 6.474 6.504 6.902     |
| Zhou et al. [16]              | Tight-binding model                         | 0.074               | 5.1                   | 5.774 5.801 6.156     |
| Tu and Ou-Yang [17]           | Local Density approximation model           | 0.075               | 4.7                   | 5.697 5.724 6.074     |
| Pantano et al. [18]           | Continuum shell modeling                    | 0.075               | 4.84                  | 5.697 5.724 6.074     |
| Kudin et al. [19]             | Ab initio computations                      | 0.089               | 3.859                 | 4.801 4.823 5.118     |
| Li and Chou [12]              | Structural mechanics:stiffness matrix method | 0.34                | 1.01                  | 1.257 1.263 1.340     |
| Lu [20]                      | Molecular Dynamics                          | 0.34                | 0.974                 | 1.257 1.263 1.340     |
| Hernandez et al. [21]         | Tight-binding molecular Dynamics            | 0.34                | 1.24                  | 1.257 1.263 1.340     |
| Jin and Yuan [22]             | Molecular Dynamics                          | 0.34                | 1.238                 | 1.257 1.263 1.340     |
| Odegard et al. [14]           | Equivalent-continuum modeling               | 0.69                | -                     | 0.619 0.639 0.660     |
| Present work                  | Finite Element Method                       | 0.1296              | -                     | 3.296 3.312 3.514     |

3.1. Effect of wall thickness on Young’s modulus of SWCNTs

In contrary to bond length, for which the experimentally observed value of 0.1421 nm has been accepted as the exact value, the wall thickness t of CNTs has not yet clearly specified. Several values ranging from 0.064 to 0.69 nm have been adopted for the CNT wall thickness. In the current work, energy equivalence between molecular and structural mechanics provides a wall thickness of 0.1296 nm. The uncertainty of the exact value of CNT wall thickness as well as the wide scatter of the values used for it in the literature, originate the need to perform a parametric study. By using the FE model and equation (5), the Young’s modulus of (7,7), (12,0) and (5,9) SWCNTs are calculated for different values of t=d found in the literature. The values of Young’s modulus calculated for each t have been compared with the corresponding values from the literature. Table 1 summarizes all calculations and comparisons. Three SWCNTs have been selected in order for the effect of chirality to be present also. They were chosen such as to have contiguous diameters (9.519, 9.422 and 9.62 Å, respectively).

![Figure 2. Variation of Young’s modulus of armchair, zigzag and chiral SWCNTs with wall thickness.](image)

From the results it is clear that the wall thickness of CNTs significantly affects the calculation of Young’s modulus of SWCNTs. The larger the wall thickness, the smaller the Young’s modulus
calculated. Concerning the effect of chirality, no definite conclusions can be made since the small
difference between the Young’s moduli calculated for the three nanotubes might depend on the
difference in their diameters. As seen in table 1, for all t the Young’s modulus computed by the
present FE model agree very well with each Young’s modulus obtained by the corresponding method.
The agreement with the aggregation of the methods verifies the ability of the FE model to accurately
calculate the deformation of SWCNTs. The results of table 1 are shown schematically in figure 2 for
three SWCNTs. The figure suggests that the Young’s modulus values obtained with the FE model are
inversely proportional to the wall thickness. Same dependence of Young’s modulus to t has been
obtained by the finite deformation continuum model of Gao and Li [23] and the equivalent-continuum
model of Odegard et al. [14], who correctly stated that the Young’s modulus of CNTs should be
inversely proportional to their cross-sectional area A.

3.2. Effect of diameter and chirality on Young’s modulus of SWCNTs
In this section, the FE model is applied to investigate the effect of both diameter and chirality on the
elastic moduli of SWCNTs. All three types of SWCNTs, namely, armchair, zigzag and chiral are
included in the investigation. Figure 3 shows the variation of Young’s modulus of armchair, zigzag
and two series of chiral SWCNTs with tube diameter D. It can be seen that there is an evident effect of
diameter on the Young’s modulus of armchair and zigzag SWCNTs, especially for small diameters.
The Young’s modulus of chiral SWCNTs is also affected but not significantly. With increasing tube
diameter, the Young’s modulus of SWCNTs increases but not with the same trend for all SWCNTs.
As pointed out by Li and Chou [12], the increase is due to the effect of nanotube curvature. The
smaller the nanotube diameter, the higher the curvature, resulting in large distortion of the carbon–
carbon (C–C) bonds and therefore, in large elongation of the nanotube.

The findings described above are verified by two recent theoretical studies. Li and Chou [12] found
a similar variation of Young’s modulus of zigzag SWCNTs with their diameter. Jin and Yuan [22]
found that the Young’s modulus of armchair SWCNTs with diameters ranging from 0.814 to 2.714 nm
have an almost constant Young’s modulus showing small variation only for small diameters, as shown
in the present study. In figure 3, it is also clear, that in general, a larger Young’s modulus is calculated
for both series of chiral SWCNTs than for armchair and zigzag SWCNTs. This finding verifies the
finding of Table 1 and ascertains that the difference in the calculated Young’s moduli is due not only
to the difference of diameters. Between the two series of chiral SWCNTs, the same trend of variation
of Young’s modulus is obtained.

4. Conclusions
A three-dimensional finite element (FE) model for armchair, zigzag and chiral single-walled carbon
nanotubes has been proposed. To create the FE models, nodes are placed at the locations of carbon
atoms and the bonds between them are modeled using three-dimensional elastic beam elements. Using
Morse atomic potential, the elastic moduli of beam elements are obtained via considering a linkage between molecular and continuum mechanics. Also, a new wall thickness (=bond diameter) equal to 0.1296 nm has been introduced. 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 modeling abilities of the FE method, extends the model applicability to SWCNTs with very large number of atoms as well as to MWCNTs, other carbon-related nano-structures and moreover, to CNT-based nano-composites.

In order to demonstrate the applicability of FE model and new wall thickness, the influence of tube wall thickness, diameter and chirality on the Young’s modulus of SWCNTs has been investigated. Armchair, zigzag and two series of chiral SWCNTs have been included in the investigation. It is found that the choice of wall thickness significantly affects the calculation of Young’s modulus. For the values of wall thickness used in the literature, the Young’s moduli are estimated which agree very well with the corresponding theoretical results and experimental measurements. The FE model results suggest that Young’s modulus is inversely proportional to the wall thickness. We also examine dependence of elastic moduli to diameter and chirality of the nanotubes. With increasing tube diameter, the Young’s modulus of SWCNTs increases but not with the same trend for all SWCNTs. The Young’s modulus of chiral SWCNTs is found to be generally larger than that of armchair and zigzag SWCNTs. The presented results demonstrate that the proposed FE model and new wall thickness may provide a valuable tool for studying the mechanical behavior of carbon nanotubes and their applications, particularly in nano-composites.

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