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## Predicting the Young's Modulus of Single-Walled Carbon Nanotubes using Finite Element Modeling

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**Abstract:** A finite element simulation technique for estimating the mechanical properties of Single-Walled Carbon Nanotube (SWCNT), polymer composites is developed. In the present modeling work, individual carbon nanotube is simulated as a frame-like structure and the primary bonds between two nearest-neighbor atoms are treated as 3D beam elements. The beam element nonlinear properties are determined via the concept of energy equivalence between molecular dynamics and structural mechanics using Modified Morse potential. Young's modulus of SWCNTs is estimated to illustrate the accuracy of this simulation technique. Results show that the obtained mechanical properties of nanotubes by the present method are in good agreement with their comparable results.

**Key words:** Single Walled Carbon Nanotube (SWCNT), Finite Element Model, morse potential functions, continuum mechanics, young's modulus

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### INTRODUCTION

The discovery of carbon nanotubes (CNTs) has stimulated considerable experimental and theoretical studies. Various promising applications have been proposed based on their unique geometrical and mechanical properties Li and Chou (2004). The potential use of CNTs as reinforcing materials in nano-composites has originated the need to explore their mechanical properties.

Due to these difficulties in experimental investigation of CNTs, FE modeling techniques have been also developed to estimate physical properties of nanotubes. Carbon nanotubes were simulated extensively using molecular dynamics and continuum mechanics. The atomistic approaches include classical molecular dynamics, tight-bonding molecular dynamics and density functional theory Tserpesa and Papanikos (2005). Despite the fact that these approaches can be used for any problem associated with molecular or atomic motions, their huge computational tasks restricted their application to small number of molecules or atoms Shokrieh and Rafiee (2010a).

The continuum mechanics approaches, on the other hand, mainly involve classical continuum mechanics and continuum shell modeling Tserpesa and Papanikos (2005). Since a nanotube can be well described as a continuum solid beam or shell subjected to tension, bending or torsional forces, it is reasonable to model nanotube as a

frame-or shell-like structure, then the mechanical properties of such structure can be obtained by classical continuum mechanics for finite element method.

However, due to the uncertainty of the nanotubes characteristics for both of the above modeling techniques, the obtained mechanical properties of nanotubes are widely scattered. The predicted Young's modulus of CNTs yields a widespread range of about 1.0 to 5.5 TPa (Selmi *et al.*, 2007). Experimentally determined Young's modulus of SWCNTs also scattered in a relatively large interval of 2.8-3.6 TPa (Selmi *et al.*, 2007; Thostensona *et al.*, 2001).

The main objective of this article is to develop finite element model of single-walled CNTs (SWCNTs) and investigate the Young's modulus of SWCNTs based on nanoscale continuum modeling. By employing frame elements to simulate carbon-to-carbon bonds, a finite element model is presented for simulating of elastic modulus of SWCNTs. Furthermore, the effect of nanotube diameter and structure is also studied in this work.

**Carbon nanotube simulation:** There are several ways to view a SWCNT. The most widely used is by reference to rolling up grapheme sheet to form a hollow cylinder with end caps. The cylinder is composed of hexagonal carbon rings, while the end caps of pentagonal rings. The atomic structure of nanotubes depends on tube chirality, which is defined by the chiral vector and the chiral angle (Thostensona *et al.*, 2001). The hexagonal pattern is

repeated periodically leading to binding of each carbon atom to three neighboring atoms with covalent bonds. This covalent bond is a very strong chemical bond and plays significant role to the impressive mechanical properties of graphitic and as a consequence, of all carbon-related nano-structures (Thostensona *et al.*, 2001; Lau *et al.*, 2006).

These bonds have a characteristic bond length  $a_{C-C}$  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 Tserpesa and Papanikos (2005). In Fig. 1, a typical nanotube in the form of a 3D frame structure illustrated.

As mentioned above, by treating CNTs as space-frame structures, their mechanical behavior can be analyzed using classical structural mechanics methods. In this work, a 3D FE model able to assess the mechanical properties of SWCNTs is proposed. The 3D FE model is developed using ANSYS commercial FE code. For the modeling of the C-C bonds, 3D elastic BEAM4 element is used Fig. 2. The specific element is a uni-axial element with tension, compression, torsion and bending capabilities. It has six degrees of freedom at each node: Translations in the nodal x, y and z directions and rotations about the nodal x, y and z-axes. The element is defined by two or three nodes as well as its cross-sectional area, two moments of inertia, two dimensions and the material properties.

To calculate the elastic modulus of beam elements, a linkage between molecular and continuum mechanics is used. In its general formula, the potential energy is described as Shokrieh and Rafiee (2010a),

$$V = \sum V_r + \sum V_\theta + \sum V_\phi + \sum V_\psi + \sum V_{vdw} + \sum V_{el} \quad (1)$$

where,  $V_r$ ,  $V_\theta$ ,  $V_\phi$ ,  $V_\psi$ ,  $V_{vdw}$ ,  $V_{el}$  are bond stretching, bond angle bending, dihedral angle torsion, inversion terms, van der Walls interaction and electrostatic interaction, respectively. Various functional forms may be used for these potential energy terms depending on the particular material and loading conditions considered. In some papers, the effects of  $V_\theta$ ,  $V_\psi$ ,  $V_{vdw}$ , are neglected under the uniaxial loading and small strain (Shokrieh and Rafiee, 2010a; Tserpesa and Papanikos, 2005; Fan *et al.*, 2009). In addition, in most cases where continuum methods have been used to

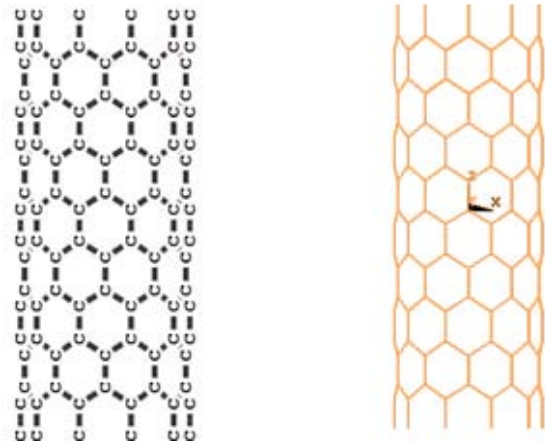


Fig. 1: The hexagonal structure of a typical CNT

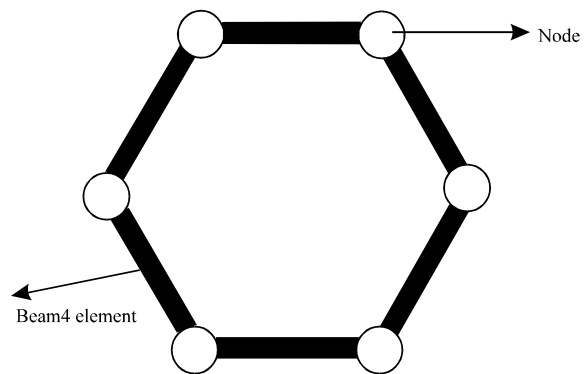


Fig. 2: Finite element modeling concept of the hexagonal structure of a CNT

analyze carbon nanotubes embedded in an elastic Figure medium, a linear behavior of the reinforcements has been assumed such as reported in Fan *et al.* (2009) and Shokrieh and Rafiee (2010b) works. This assumption leads to accurate predictions only in cases where very small nanotube deformations take place. Consequently, all these methods cannot be used for modeling the mechanical behavior of the composites. Therefore, in the present work, the tensile behavior of the isolated carbon nanotubes is simulated using the progressive fracture model developed by Tserpes *et al.* (2008).

To model the bond stretching, a simple analytical Morse function is used to represent the experimentally determined bond energy curves of diatomic molecules, which can be written as Shokrieh and Rafiee (2010a),

$$V_r = D_{ij}^e [e^{-2\Delta r_{ij}} - e^{-\Delta r_{ij}} - 2e^{-2\Delta r_{ij}}] \quad (2)$$

where,  $D_{ij}^e$  represent the energy required to stretch the bond  $r_{ij}$  from its equilibrium distance to infinity,  $r_{ij}$  is the bond length variation and  $a_{ij}$  is equal to  $(k_c/D_{ij}^e)^{1/2}$  where,  $K_c$  is the force constant at the minimum of the well. For a Nanotube system the modified potential energy is expressed as (Shokrieh and Rafiee, 2010a; Tserpes *et al.*, 2008):

$$E = E_{stretch} + E_{angle} \quad (3)$$

$$E_{stretch} = D_e \left[ 1 - e^{-\beta \Delta r} \right] - 1 \quad (4)$$

$$E_{angle} = \frac{1}{2} K_\theta (\Delta\theta)^2 \left[ 1 + K_{sezi} \Delta\theta^4 \right] \quad (5)$$

where,  $E_{stretch}$  is the bond energy due to bond stretching and  $E_{angle}$  is the bond energy due to bond angle-bending,  $r$  is the current bond length and  $\theta$  is the current angle of the adjacent bond. The other parameters of the potential are (Tserpes *et al.*, 2008):

- $r_0 = 1.421 \ 1010 \text{ m}$
- $D_e = 6.03105 \ 1019 \text{ Nm}$
- $\beta = 2.625 \ 1010 \text{ m}^{-1}$
- $\theta_0 = 2.094 \text{ rad}$
- $K_\theta = 0.9 \ 10^{-18} \text{ Nm rad}^{-2}$
- $K_{sezi} = 0.754 \text{ rad}^4$

For strains above 10%, as bond stretching dominates nanotube fracture and the effect of angle-bending potential is very small, only the bond stretching potential is considered. By differentiating the stretching energy term in (4), the stretching force of atomic bonds is obtained in the molecular forcefield as

$$F = 2\beta D_e \left[ 1 - e^{-\beta \Delta r} \right] e^{-\beta \Delta r} \quad (6)$$

The relationship between stress  $\sigma$  and bond strain for the C-C bonds could be calculated using the element's cross-sectional area equal to  $1.6910^{-20} \text{ m}^2$  for C-C bond as shown in Fig. 3. The strain of the bond is defined by  $\epsilon$ . As may be seen, the stress-strain relation is highly non-linear especially at large strains and the inflection point (peak force) occurs at about 19% strain.

The initial stiffness is set at 6.5 TPa, according to initial slope of the C-C bond stress-strain curve Fig. 3. The nanotube is loaded by an incremental force at one end while the other end being fully constrained. Zero transverse displacement is applied to the

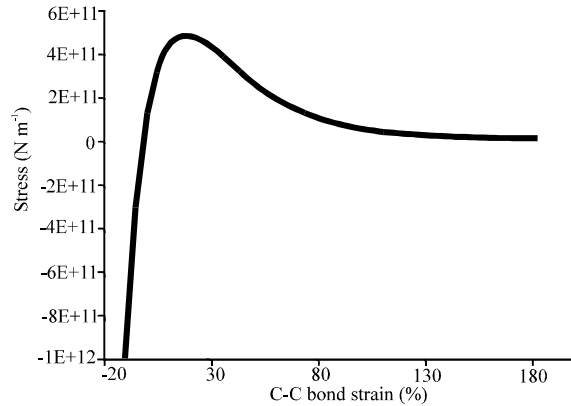


Fig. 3: The stress-strain curve of the modified Morse potential

loading end in order to prevent nanotube buckling at high loads (Fig. 4).

It should be noted that before we feed in the input data of the BEAM4 element properties, the dimensions of the parameters stated above were further adjusted to avoid possible digits of overflow/underflow error during the computation performed by ANSYS as suggested by Fan *et al.* (2009).

## RESULTS AND DISCUSSION

In this section, we will use the finite element results to compute the axial Young's modulus of carbon nanotubes of various types and sizes. In addition, comparison of these results to those found in the literature will be given. We also discuss the influence of tube size and type on the mechanical properties we obtained.

To compute the axial Young's modulus from the numerical results, following equation was used:

$$E = \frac{\sigma}{\epsilon} = \frac{FL_n}{A\Delta L_n} \quad (7)$$

where,  $E$  is the axial Young's modulus,  $\sigma$  and  $\epsilon$  are the axial stress and strain respectively,  $F$  is the total force applied on one end of the tube,  $A$  is the cross section area of the nanotube, which is defined as  $A = \pi D_n t_n$  (where  $D_n$ =nanotube diameter, thickness  $t_n=0.34 \text{ nm}$  is the interlayer graphite distance) Shokrieh and Rafiee (2010a). Nanotube radius was estimated by using Selmi *et al.* (2007).

$$R = \frac{a_0 \sqrt{3(n^2 + m^2 + nm)}}{2\pi} \quad (8)$$

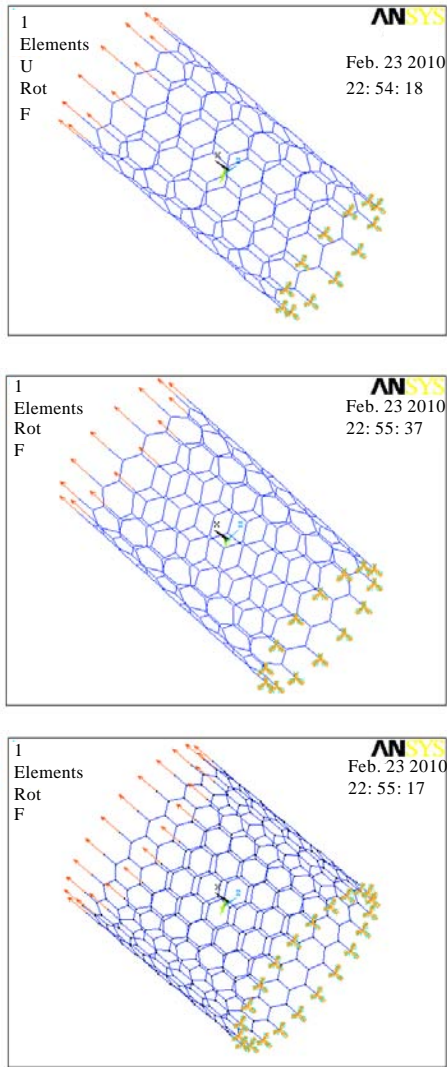


Fig. 4: Iso view of the FE meshes of the (a) (12,0), (b) (14,0) and (c) (22,0) SWCNTs along with the applied boundary conditions

Table 1: Axial Young's modulus of single-walled carbon nanotubes

Tube type	Axial Young's modulus (Tpa)	Nanotube Diameter (nm)
Zingzag (6,0)	1.19500	0.469732
Zingzag (8,0)	1.21700	0.62631
Zingzag (10,0)	1.22700	0.782887
Zingzag (12,0)	1.22898	0.939464
Zingzag (14,0)	1.23160	1.096042
Zingzag (22,0)	1.23280	1.722351

Table 2: Comparison between Young's modulus of carbon nanotube reported by developed methods and experimental observations in literature

Investigators	Method	CNT type	Young's modulus (Tpa)	CNT thickness (nm)
Georgantzinos <i>et al.</i> (2009)	FE method	SWNTs	0.936GPa	0.34
Wong <i>et al.</i> (2009)	Experimental	MWNTs	1.28	-
Fan <i>et al.</i> (2009)	FE method	SWCNTs	1.033	0.34
Tserpes and Papanikos (2005)	FE method	SWCNTs	1.029	0.34
Jin and Yuan (2003)	Molecular dynamics	SWCNTs	1.238	0.34

where,  $a_n = 0.142$  nm is the C-C bond length and  $n, m$  are chirality index of nanotubes.

Six zigzag type single walled carbon nanotubes of different sizes are simulated and their axial Young's modulus calculated by (7) are listed in Table 1 and depicted in Fig. 5.

Form the results it could be seen that the axial Young's moduli whose values are about 1.2 Tpa for all cases increase slightly with increasing diameter. From Fig. 5, the effect of tube diameter on the Young's modulus is also clearly observed. For smaller tubes, for example, diameter less than 1.0 nm, the Young's modulus exhibits a strong dependence on the tube diameter.

However, for tube diameters larger than 1.0 nm, this dependence becomes very weak. The general tendency is that the Young's modulus increases with increasing tube diameter. The lower Young's modulus at smaller nanotube diameter could be attributed to the higher curvature, which results in a more significant distortion of C-C bonds. As the nanotube diameter increases, the effect of curvature diminishes gradually Li and Chou (2003).

Our computational results are comparable to those obtained from experiments and theoretical studies. The obtained results for CNT are in a good agreement with experimental results which was reported by Wong *et al.* (1997). He pinned MWCNTs at one end to molybdenum disulfide surfaces and measured the bending force versus displacement along the unpinned lengths.

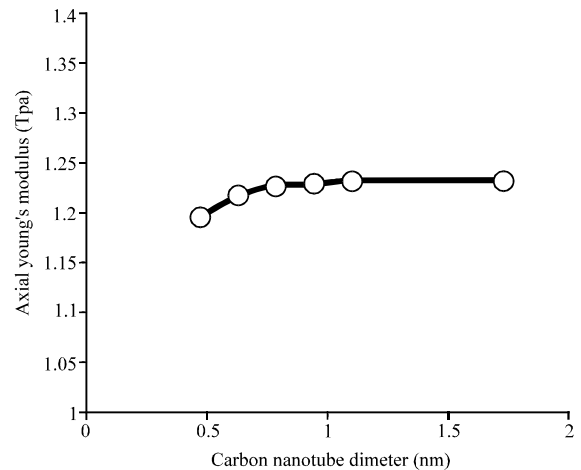


Fig. 5: The relation between the axial Young's modulus and diameter of carbon nanotubes

Numerical results which were reported by Jin and Yuan (2003) using Molecular dynamics are also comparable to present work. Comparison between reported data for nanotube Young's modulus in literature and obtained results in this study is presented in Table 2.

### CONCLUSION

A finite element simulation technique for SWNTs has been developed which can be easily performed by commercial code ANSYS. The key modeling concept is that simulating molecular bonds are presented as beam elements. We propose and verified a simplifying method to model non-linear nature of covalent bond between to carbon atoms in the nanotube wall. This method can significantly save the modeling and computing effort when finite element analysis is performed. Numerical results for axial Young's modulus are presented to illustrate the accuracy of the established finite element models. In addition, the relations between these mechanical properties and the nanotube size are also investigated to give a better understanding of the variation of mechanical properties of nanotubes. From the above results and the outstanding advantage that the present modeling concept can be easily extended to cases of MWNTs with higher number of layers, this method will be an effective and convenient tool in studying the mechanical behavior of MWNTs.

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