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Composites: Part B 35 (2004) 95–101
composites Part B: engineering
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On the effective elastic moduli of carbon nanotubes for nanocomposite structures

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Received 3 June 2003; accepted 11 August 2003

Abstract

A critical review on the validity of different experimental and theoretical approaches to the mechanical properties of carbon nanotubes for advanced composite structures is presented. Most research has been recently conducted to study the properties of single-walled and multi-walled carbon nanotubes. Special attention has been paid to the measurement and modeling of tensile modulus, tensile strength, and torsional stiffness. Theoretical approaches such as molecular dynamic (MD) simulations, finite element analysis, and classical elastic shell theory were frequently used to analyze and interpret the mechanical features of carbon nanotubes. Due to the use of different fundamental assumptions and boundary conditions, inconsistent results were reported. MD simulation is a well-known technique that simulates accurately the chemical and physical properties of structures at atomic-scale level. However, it is limited by the time step, which is of the order of 10^{-15} s. The use of finite element modeling combined with MD simulation can further decrease the processing time for calculating the mechanical properties of nanotubes. Since the aspect ratio of nanotubes is very large, the elastic rod or beam models can be adequately used to simulate their overall mechanical deformation. Although many theoretical studies reported that the tensile modulus of multi-walled nanotubes may reach 1 TPa, this value, however, cannot be directly used to estimate the mechanical properties of multi-walled nanotube/polymer composites due to the discontinuous stress transfer inside the nanotubes.

Keywords: A. Nanostructures; B. Mechanical properties; Carbon nanotubes

1. Introduction

Since the discovery of carbon nanotubes in 1991 [1], much research has been focused on their mechanical and electrical properties. A single-walled nanotube is a hollow structure formed by covalently bonded carbon atoms. It can be imagined as a rectangular graphene sheet rolled from one side of its longest edge to form a cylindrical tube. Hemispherical caps seal both ends of the tube as shown in Fig. 1. For multi-walled nanotubes, a number of graphene layers are co-axially rolled together to form a cylindrical tube. The spacing between graphene layers is about 0.34 nm. Theoretically, the tensile modulus and strength of a graphene layer reach up to 1 TPa and 200 GPa, respectively. These values have been widely used to interpret the mechanical properties of single-walled and multi-walled nanotubes. The size, mechanical strength, and electrical properties of nanotubes are highly dependent on their atomic architectures. Armchair nanotubes exhibit better ductility and electrical conductivity than zigzag nanotubes [2,3]. In recent years, carbon nanotubes have been utilized as nano-fillers to enhance the mechanical strength of polymeric matrices. An important increase of the tensile modulus and yield strength of polymers has been reported [4,5] after the random dispersion of single-walled or multi-walled nanotubes. For example, the hardness of epoxy is increased after the dispersion of multi-walled nanotubes [6]. However, the pull out of nanotubes that reflects a poor bonding strength between nanotubes and matrix was reported in fractured samples [6].

Typically, there are two types of interactions in a nanotube/polymer system: chemical bonding and mechanical interlocking of atoms. Many theoretical, experimental,

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doi:10.1016/j.compositesb.2003.08.008

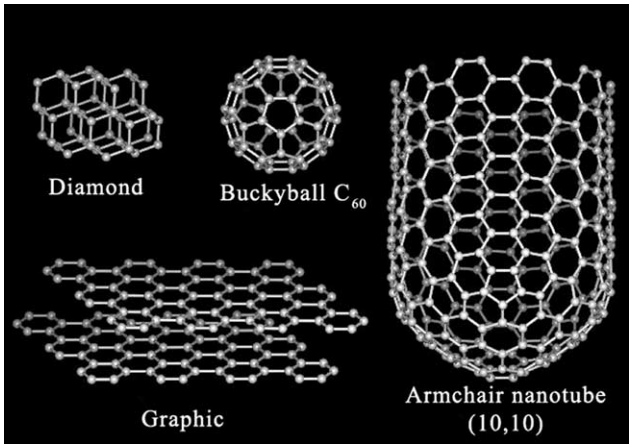

Fig. 1. Different forms of carbon-based materials.

and computational studies have been conducted to isolate the intrinsic contribution of the interfacial bond between the nanotubes and the polymeric matrix in composites [7–11]. Experimental results showed that the interfacial shear strength is strongly dependent on the size and strength of nanotubes. While the composites are subjected to a tensile load [11], increasing the modulus of nanotubes results in inducing a higher shear stress at the interface. A precise estimation of the tensile modulus of nanotubes is required to accurately estimate the mechanical properties of nanotube/polymer composites. The first mechanical studies on nanotubes [12,13] was done using Atomic Force Microscopy (AFM). The tensile test was carried out through the tip of AFM. In this experiment, it was found that an outmost layer of the nanotubes was firstly broken followed by sliding. Tensile moduli ranging from 270 to 950 GPa [13] were measured during the experiment. However, as the binding forces between individual layers (van der Waals), is very weak, the amount of stress transfer from the outermost layer to the innermost is doubtful.

This paper aims to review recent developments in the calculations of tensile modulus of carbon nanotubes and their validity for advanced composite structures. Different methods such as molecular dynamic (MD) simulations, continuum methods of mechanics, elastic shell theory, and finite element analysis will be reviewed in this paper.

2. Molecular dynamic simulations

In the early stage, empirical-force-potential MD simulations have been used to estimate the Young's modulus of a single-walled nanotube. It has been calculated that the modulus of carbon nanotubes is four times larger than that of diamond. However, these calculations were solely based on the properties of the graphene sheet. MD simulations predict with high accuracy the mechanical properties of materials for most structural and physical problems at atomic scale. The details of atomic arrangements have to be clearly known to simulate the mechanical properties of nanotube structures. In general, there are three types of nanotube structures: Zigzag $(n,0)$, armchair (n,n), and chiral $(n,m$ where $n \neq m)$ nanotubes. Lau and Hui [14] have given a comprehensive review on the structures of the nanotubes. To investigate the mechanical properties of materials at atomic scale by using MD simulations, the interactions between neighboring atoms have to be accurately calculated.

Two common approaches based on quantum mechanics and molecular mechanics are used to simulate these interactions. Both approaches attempt to capture the variation of system energy associated with the change in atomic positions by following the Newton's second law, $F = ma$. In carbon nanotubes, the mutual interactions are described by force potentials from both bonding and non-bonding interactions. The non-bonding interactions are either due to the van der Waals force (that can be an attractive or repulsive depending on the distance between atoms), or to electrostatic interactions. The van der Waals force F_{VDW} is most often modeled using the Lennard-Jones potential function [15], originally derived for inert gases. The general form of this potential is

$$\Phi(r) = \frac{\lambda_n}{r^n} - \frac{\lambda_m}{r^m} \tag{1}$$

For van der Waals forces arising from dipole–dipole interactions, the attractive part corresponds to $m = 6$. The most common form of this potential is the so called (6–12) form:

$$\Phi(r) = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right] \tag{2}$$

The minim of $\Phi(r)$ is determined by equating to zero the first order derivative of $\Phi(r)$ versus r. The van der Waals force between two carbon atoms can be estimated from:

$$F_{\mathrm{VDW}} = -\frac{\mathrm{d}\phi}{\mathrm{d}r} = \frac{24\varepsilon}{r}\left[2\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right] \tag{3}$$

The two parameters, σ and ε can be estimated from experimental data such as the equilibrium bond length (lattice parameters at equilibrium), equilibrium bond energy (cohesive energy), and bulk modulus at equilibrium. The bonding energy (E_{bond}) is the sum of four different interactions among atoms, namely bond stretching (U_ρ), angle variation (U_θ), inversion (U_ω) and torsion (U_τ) [16].

$$E_{\mathrm{Bond}} = U_\rho + U_\theta + U_\omega + U_\tau \tag{4}$$

A schematic illustration of each energy term and corresponding bond structure for a graphene cell is shown in Fig. 2. The most commonly used functional forms are:

$$U_\rho = \frac{1}{2}\sum_i K_i(\mathrm{d}R_i)^2 \tag{5a}$$

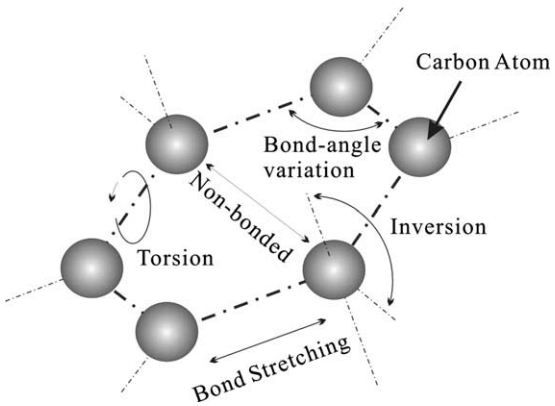

Fig. 2. Bond structures and corresponding energy terms of a graphene cell.

$$U_\theta = \frac{1}{2}\sum_i C_j(\mathrm{d}\theta_j)^2 \tag{5b}$$

$$U_\omega = \frac{1}{2}\sum_k B_k(\mathrm{d}\omega_k)^2; \text{ and} \tag{5c}$$

$$U_\tau = \frac{1}{2}\sum_i A_i[1+\cos(n_i\tau_i - \phi_i)] \tag{5d}$$

Where $\mathrm{d}R_i$ is the elongation of the bond identified by the label i, K_i is the force constant associated with the stretching of the i bond, $\mathrm{d}\theta_j$ and $\mathrm{d}\omega_k$ are the variance of bond angle j and inversion angle k, respectively. C_j and B_k are force constants associated with angle variance and inversion, respectively. A_i is the 'barrier' height to rotation of the bond i; n_i is multiplicity which gives the number of minims as the bond is rotated through 2π [16].

To determine the tensile modulus of a single-walled nanotube subjected to uniaxial loadings it is useful to observe that at small strains the torsion, the inversion, the van der Waals, and the electrostatic interactions energy terms are small compared with the bond stretching and the angle variation terms. Thus, the total energy of the single-walled nanotube can be reduced to:

$$E_{\text{Total}} = \frac{1}{2}\sum_i K_i(\mathrm{d}R_i)^2 + \frac{1}{2}\sum_j C_j(\mathrm{d}\theta_j)^2 \tag{6}$$

The force constants K_i and C_i can be obtained from quantum mechanics (ab initio). The average macroscopic elastic modulus and Poisson's ratio were estimated to be about 1.347 and 0.261 TPa, respectively [16]. Such calculations may be performed either using the force or the energy approach, by measuring the mechanical forces developed between carbon atoms in nanotubes with different chiral arrangements. Lu [17] has used the empirical-force potential MD simulation to investigate the properties of nanotubes. The structure of the nanotubes was obtained by the conformational mapping of a graphene sheet onto a cylindrical surface. The nanotube radius was estimated by using the relation:

$$R = \frac{a_0\sqrt{3(n^2+m^2+nm)}}{2\pi} \tag{7}$$

where $a_0 = 0.142$ nm is the carbon–carbon distance. The interlayer spacing d between individual layers of multi-walled nanotubes is 0.34 nm. The average estimated tensile modulus of single-walled and multi-walled nanotubes is about 1 TPa. The elastic properties are the same for all nanotubes with a radius larger than 1 nm. Zhou et al. [18] have used the first principles cluster model within the local density approximation to evaluate the mechanical properties of a single-walled nanotube. The estimated values for tensile modulus, tensile strength and Poisson's ratio were 0.764 TPa, 6.248 and 0.32 GPa [18] respectively. The binding energy of the nanotube is less than that of graphite due to the curvature effect. Lier et al. [19] calculated the tensile modulus of zigzag and armchair single-walled nanotubes using the ab initio multiplicative integral approach (MIA), which is based on the energy of elongation of nanotubes in a simple tension (that is not constrained laterally or in any other way). They found that the modulus of single or multi-walled nanotubes was larger than that of a graphene sheet. The MD simulations show that the fracture behavior of zigzag nanotubes is more brittle than the fracture behavior of armchair nanotubes [2]. The formation of a local Stone-Wales defect (5-7-7-5) in the deformed armchair nanotube induced ductile deformation.

3. Continuum methods of mechanics and elastic shell theory

Although MD simulation is a well-known technique to simulate the chemical and physical properties of structures at atomic-scale level, the time step is usually of the order of femto-seconds. Recent research has reported that elastic rods and beams can be used to simulate the overall mechanical deformation of nanotubes provided the aspect ratio of the nanotubes is greater than 10^3. Krishnan et al. [20] derived Young's modulus of single-walled nanotubes from the measurement of the vibration amplitude of a cantilever nanotube by using the classical vibration theory for elastic rods. In their study, the vibration amplitude of the cantilevered nanotubes described by Eq. (8) was assumed small:

$$y = \cos(c\alpha^2 t)[B\cos(\alpha x) + C\sin(\alpha x) + D\cosh(\alpha x) + E\sinh(\alpha x)] \tag{8}$$

where

$$c^2 = \frac{E_{\text{SWNT}} I}{\rho A} \tag{9}$$

where α is the wave number. By appropriately applying the boundary conditions to a cantilever beam system, the Young's modulus of nanotubes can be determined by measuring directly their diameter;

$$E_{\mathrm{SWNT}} = 0.8486\frac{L^3E_n}{\sigma^2 2Rd((2R)^2+d^2)} \tag{10}$$

Where L, R, d, E_n and σ^2 denote the length of the nanotube, the outer radius of the nanotube, the interlayer spacing, the total energy contained in the vibration mode, and standard deviations of measurement, respectively. An average value of 1.25 ± 0.45 TPa was reported. The cross-sectional area A and the second moment of inertia I of the nanotube were determined by assuming that the wall of the nanotube is a solid shell, i.e. $A = \pi(r_o^2 - r_i^2)$ and $I = \pi(r_o^4 - r_i^4)/4$. The thickness of the wall was equivalent to the graphene sheet thickness (3.4 Å). Sohlbery et al. [21] also used classical vibration theory within the continuum mechanics approximation to investigate the structural rigidity of nanotubes. Different vibration modes were considered in their study: longitudinal stretching, circumferential breathing, torsional twist and transverse flex, odd number of nodes, and even number of nodes.

Ru [22–24] has used the elastic shell theory to study the mechanical properties and buckling behavior of nanotubes. He found that the actual stiffness of a single-walled nanotube was much lower than that predicted by the elastic shell when the graphene sheet thickness is used. He also pointed out that the bending rigidity D as predicted by the classical elastic theory cannot exploited to describe the bending properties of the nanotubes unless an equivalent wall thickness t, very small compared with the interlayer spacing d of the graphene sheet, is utilized. If the aspect ratio of the nanotubes is small, or local deformations are present, the elastic shell model leads to accurate results. Wang et al. [25] have found that the thin multi-walled nanotube with the radius-to-thickness ratio larger than 5 can be modeled as a single layer elastic shell. However, due to the existence of interlayer spacing, the bending curvature of each layer of multi-walled nanotubes might be different. Hence, the use of general elastic parameters to interpret the flexural properties of the nanotubes may not be appropriate unless the fraction barrier is so high that interlayer slips between adjacent nanotubes are prohibited.

Recently, Tu and Ou-yang [26] have theoretically studied the elastic properties of single and multi-walled nanotubes using the local density approximation model combined with a classical elastic shell theory. Their estimate of the Young's modulus of a single-walled nanotube (E_{SWNT}) was about 4.7 TPa. They reported that the Young's modulus of the multi-walled nanotube (E_{MWNT}) is decreased as the number of wall layers increases (see Fig. 3):

$$E_{\mathrm{MWNT}} = \frac{N}{N-1+\xi}\xi E_{\mathrm{SWNT}} \tag{11}$$

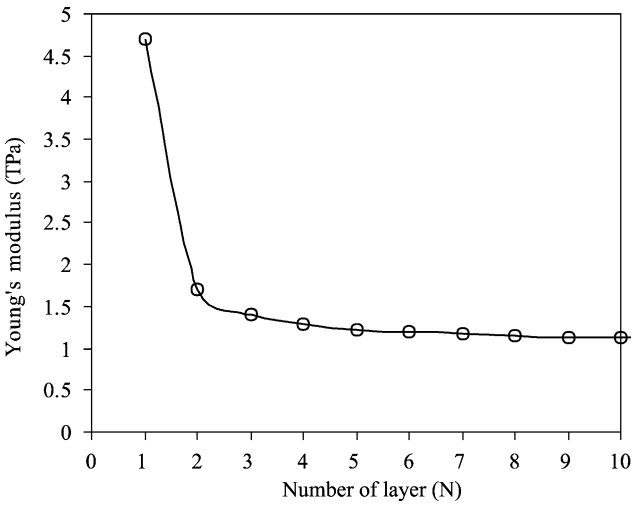

Fig. 3. Estimated Young's modulus of multi-walled carbon nanotubes [26].

where ξ denotes the thickness-to-interlayer spacing (t/d) ratio. The Young's modulus of multi-walled nanotube is dependent on the number of tube layers (N) within a wide range of values (A 64% reduction of the Young's modulus is expected as the number of tube layers is enhanced from $N = 1$ to 2).

4. Finite element modeling

In the past few years, the demand for the development of faster methods to compute the mechanical properties of nanostructures has been increasing. The classical shell theory has been judged as too simple and less accurate because it is limited by some unrealistic boundary conditions. Finite element modeling (FEM) method associated with MD or equivalent-continuum (EC) model has been recently adopted to calculate the mechanical properties of nanotubes. Odegard et al. [27] have developed an EC tube model to determine the effective geometry and effective bending rigidity of a graphene structure. Molecular mechanics considerations (see Eqs. (4) and (5)) were firstly used to determine linking forces between individual carbon atoms. This molecular force field was simulated by using a pin-joint truss model, i.e. each truss member represents the force between two atoms as shown in Fig. 4. Therefore, the truss model allows the accurate simulation of the mechanical behavior of nanotubes in terms of atoms displacements. As the nanotube was subjected only to an uniaxial load [27], solely the bonding stretching and bond-angle variation energies (see Eq. (6)) have been considered. The strain energy of the whole system was used in the FEM computation to estimate the effective thickness of the nanotube layer. It was found that the effective thickness of the nanotubes (0.69 and 0.57 Å) was significantly larger than the inter-layer spacing of graphite, estimated to about ~0.34 Å.

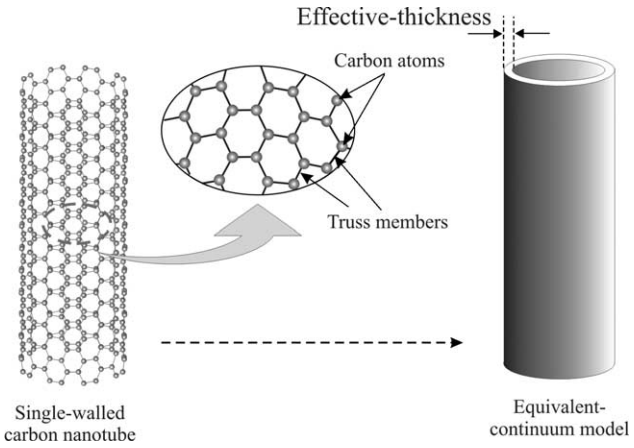

Fig. 4. Truss model of carbon nanotube's structure.

Li and Chou [28,29] have worked out the contributions of van der Waals interactions between individual carbon atoms within nanotubes within FEM truss model. The relationships between the structural mechanics parameters EA, EI and GJ and the molecular mechanics parameters K_ρ, C_θ and A_τ as shown in Eqs. (5a, b and d) for each truss member:

$$\frac{EA}{L} = K_\rho; \quad \frac{EI}{L} = C_\theta \text{ and } \frac{GJ}{L} = A_\tau \tag{12}$$

In Fig. 5, the dependence of the van der Waals force versus the distance between two carbon atoms is plotted. Non-linear truss elements were used in simulations, as the force between two carbon atoms is also non-linear. An uniaxial load was applied uniformly at the end of the nanotubes [28,29]; the effects due to end caps were neglected. It was found that the Young's modulus of the nanotubes increases as the nanotubes' diameter is increased. The Young's and shear moduli of multi-walled nanotubes are in the range of 1.05 ± 0.05 and 0.4 ± 0.05 TPa, respectively. For single-walled nanotubes, the Young's modulus is almost constant when the nanotubes' diameters are larger than 1.0 nm. The average Young's modulus of the zigzag nanotubes is slightly higher than the armchair type.

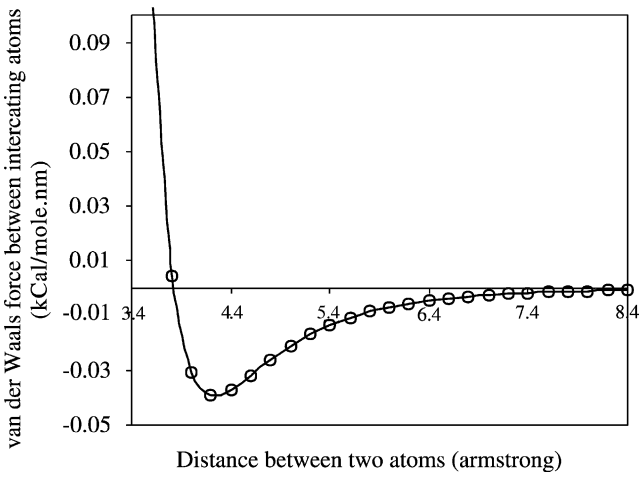

Fig. 5. Van der forces versus the distance between two carbon atoms.

Besides, the Young's modulus of multi-walled nanotubes is generally higher (~7%) than those of single-walled nanotubes.

5. Discussion

In the previous sections, a review of recent works focused on the Young's modulus of carbon nanotubes based on MD simulations, classical elastic shell theory, and finite element modeling was presented. However, there is no direct experimental testing method to measure the real tensile properties of the nanotubes. Realistic tensile tests of multi-walled nanotube were conducted by mounting the nanotube across opposing AFM tips, and followed by application of tensile load [12]. Elastic tensile moduli ranging from 270 to 950 GPa were measured. In site observations show that the outermost layer of the nanotubes took almost all the applied load [12]. Pulling out of the outermost layer was reported. Demczyk et al. [30] also conducted pulling out and bending tests of multi-walled nanotubes in a microscope. However, in several instance tubes 'telescoping' with straining was seen. This phenomenon might be due to a weak bonding strength between individual tubes. This scenario was experimentally demonstrated and very low static and dynamic friction forces (of about 6.6×10^{-15} and 4.3×10^{-15} N/Å, respectively) were measured [31]. Table 1 shows the value of Young's moduli as estimated by theoretical, numerical predictions, and experimental measurements. The diversity of the experimental results might be due to the differences in bulk materials and to sample purification.

Lau and Shi [32] investigated the fracture behavior of nanotube/polymer composites. They found that the nanotubes were pulled out after a flexural property test on nanotube/epoxy composites (see Fig. 6). They also mentioned that the use of multi-walled nanotubes may not be appropriate for advanced composite structures since only the outermost layer of the nanotubes takes all applied loads. This conclusion is supported by MD simulation [33]. Wei et al. [33] have reported that for strains larger than 2%,

Table 1
Comparison of the Young's moduli of carbon nanotubes estimated by previous studies

Authors	E (TPa)	ν	Year	Method	Reference
Yakobson	5.5	0.19	1996	MD	[35]
Zhou et al.	0.77	0.32	2001	Theoretical	[18]
Lu	1.0	0.28	1997	MD	[17]
Tu	4.7	0.34	2002	Theoretical	[26]
Chang and Gao	1.325	0.26	2003	MD	[16]
Krishnan et al.	1.25	-	1998	Theoretical	[20]
Li and Chou	1.05	-	2003	FEM	[29]
Yu et al.	0.27-0.95	-	2000	Experimental	[12]
Li et al.	0.79	-	2000	Experimental	[34]
Demczyk et al.	0.9	–	2002	Experimental	[30]

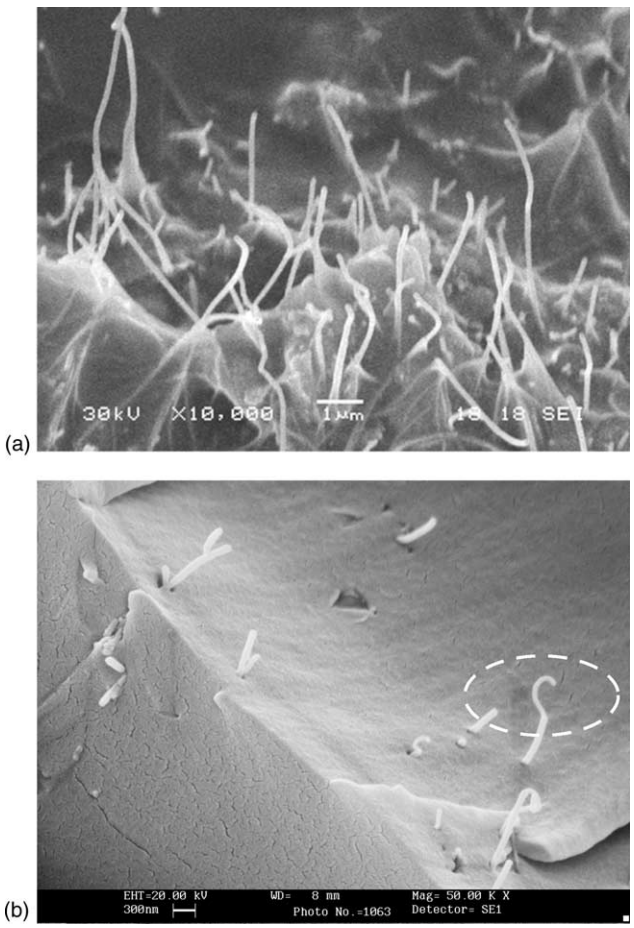

Fig. 6. Pull out of (a) the multi-walled carbon nanotubes and (b) an outermost layer of the nanotubes (right hand side).

the load transfer from the outermost layer to the inner tubes begins to cease, which suggests that the van der Waals forces between the layers is not strong enough to hold additional interfacial tensile stress. The simulation also shows that all tensile loads were applied only to the outermost layer of the nanotubes.

Due to the fact the interfacial bonding strength between the interlayer of the nanotubes is very weak, the load transferability from the outer layer to the inner tubes is doubtful. The successful use of multi-walled nanotubes in advanced composite structures is highly relied on the amount of load taken by the nanotubes. If only an outermost layer of the nanotubes takes all applied load, and the stress and strain in individual layers of the nanotubes are different, the Young's modulus estimated by the previous theoretical and molecular simulations, which assumed that the force is applied uniformly to the ends of all tubes without considering the end caps' effects, are invalid. In general, multi-walled nanotubes with end caps were entirely embedded into the matrix of the composites. The bonding strength between the matrix and the end caps of the nanotubes is still unknown. The Young's modulus estimated

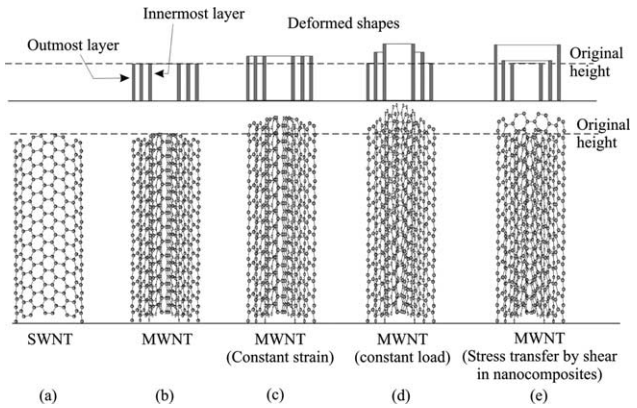

Fig. 7. Schematic illustration of the deformation shapes of nanotubes subjected to different load applications.

by the assumption of the uniform load applied to the end of each layer of the nanotubes cannot be used to predict the global tensile modulus of nanotube/polymer composites. Fig. 7 schematically shows the movement of each individual nanotubes at different load applied conditions. Realistically, for embedded multi-walled nanotubes in an elongated nanocomposite structure, only the outermost layer is deformed while all inner layers may not be affected because the friction forces between the individual layers are not high enough to transfer the load to these layers (see Fig. 7e). All previous studies have been mainly focused on the mechanical strength of the nanotubes. However, due to their unique structural properties, the estimated properties, particularly the Young's modulus and strength of multi-walled nanotubes, may not be suitable for the estimation of mechanical properties of nanotube/polymer composites. Based on the results from previous theoretical and numerical studies and on the observation of telescoping phenomena inside multi-walled nanotubes when multi-walled nanotube/polymer composites are subjected to straining, it is reasonable to assume that only an outmost layer of the nanotubes takes all applied loads. The Young's modulus of multi-walled nanotubes used in polymer composites can then be estimated by treating these nanotubes as a single-walled type with the same outermost diameter as shown in Fig. 8.

$$E_{\mathrm{MWNT}}|_{d_0} = E_{\mathrm{SWNT}}|_{d} \tag{13}$$

Where d_o and d represent the diameters of the outmost layer of the multi-walled and single-walled nanotubes, respectively. The Young's modulus of the single-walled nanotubes based on the diameter described in Eq. (13) can be determined using the MD simulation [19]. Besides, the interfacial bonding characteristics between the nanotubes and matrix is also an open question. The successful use of nanotubes for advanced composite requires an accurate estimation of the Young's modulus of nanotubes and a better understanding of interfacial bonding properties of nanocomposites.

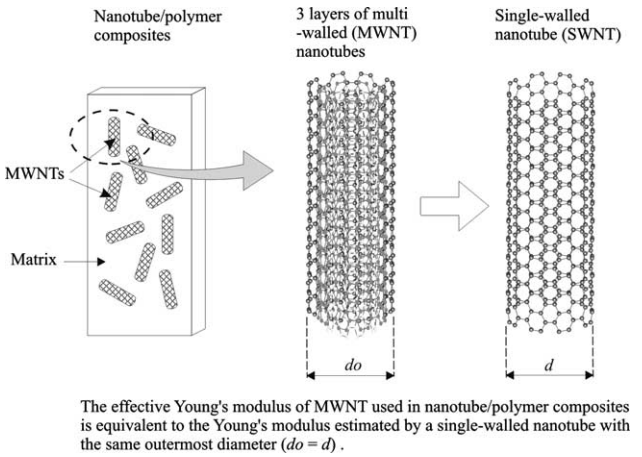

Fig. 8. An equivalent model for the anticipation of the Young's modulus of multi-walled nanotubes.

Acknowledgements

This project was supported by the Hong Kong Polytechnic University Grants (G-T 684 and G-T 861), Graduate Enhancement Fund from University of New Orleans, and Indiana University.

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