On the Flexural Characteristics of Multi-walled Carbon Nanotubes

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ABSTRACT

We use an analytical solution for bending of coaxial orthotropic cylinders to model the flexural deformation of multi-walled nanotubes with any number of layers. The simulation results show that the bending stiffness of the MWNT increases with the number of nanotube layers. For fixed number of layers, MWNT with larger inner radius has greater bending stiffness. The bending stiffness also increases with out layer radius. For certain outer radius, smaller inner radius results in a larger stiffness. The effective elastic modulus of the MWNT also increases with the number of layers and the outer radius. For the same value of the outer radius, the MWNT with smaller inner radius has a larger effective elastic modulus. As the number of layers increases, the effective modulus approaches the in-plane elastic modulus of graphene. In this work we find that the interface conditions, i.e., perfect bonding or no friction, do not affect the bending stiffness and effective elastic modulus of the MWNT. Furthermore, the cross-section of MWNT does not show any warping under bending, which suggest the classic beam theory is applicable in determining the flexural response of MWNT.

INTRODUCTION

The discovery of carbon nanotubes has led tremendous amount of research in scientific and engineering fields. Carbon nanotubes are anticipated to have elastic modulus of 1 TPa (1000GPa) with the strength around 30 GPa besides other remarkable physical properties. Due to its excellent mechanical properties [1, 2, 3, 4, 5], such as the highest strength and the highest stiffness, it possibly provides us the next generation of super strong, lightweight and highly elastic composite materials.

Fundamental understanding of carbon nanotube mechanical properties at nano-scale is essential for us to fully utilize the potential of nanotubes to reinforce composites. Multiwall nanotubes can be considered as candidates to improve bending rigidity since it has higher stiffness compared to single wall nanotubes. In an earlier publication [6] one of the authors studied the effective properties of single-walled carbon nanotubes and their hexagonal arrays and developed relationships for the effective density and Young's modulus as well as mixing rules for conversion of weight fraction to volume fraction. It was implied in these relationships that in mixtures, the effective engineering properties must account for the entire volume occupied. Since carbon nanotubes may be viewed as hollow cylindrical elements at the nano-scale, the volume occupied by the carbon atoms provides the stiffness and mass for the system. But in computing effective engineering properties the volume contained inside the hollow cylinder must also be considered when computing effective density and modulus. In the present work, the authors develop relationships for prediction of the effective flexural properties of multi-walled carbon nanotubes. Based on the analytical solution for bending of orthotropic coaxial cylinders [7], the solution for the bending response is determined for two inter-tube conditions: perfect bonding and no friction. In addition, the warpage of the cross-section is evaluated for typical nanotube geometries in order to determine the applicability of the Bernoulli-Euler hypothesis in determining the flexural response of multi-walled carbon nanotubes.

ANALYSIS OF MWNT FLEXURE

The equations for flexural deformation of multiwalled carbon tubes are derived similar to the analytical solution of Jolicoeur and Cardou [7] for bending of coaxial orthotropic cylinders. We consider the carbon multiwall nanotube as a set of concentric elastic cylinders. The elastic constants of each cylinder are defined as those of graphene sheet having transversely isotropic symmetry with five independent elastic constants. Let the nanotube axis be along the z-direction and the bending moments applied on the nanotube be M_x and M_y as illustrated in Figure 1. For each layer of the multiwall nanotube, the radial displacement, u_r, tangential displacement, u_θ, and axial displacement, w, can be obtained by integration of the strain tensor that represents the constitutive relation. The results are given as following [7]

$$u_r = -\frac{z^2}{2}(\kappa_x \sin\theta - \kappa_y \cos\theta) + U + u_r' \quad (1a)$$

$$u_\theta = -\frac{z^2}{2}(\kappa_x \cos\theta + \kappa_y \sin\theta) + V + u_\theta' \quad (1b)$$

$$w = z(\kappa_x r \sin\theta - \kappa_y r \cos\theta) + W + w' \quad (1c)$$

where κ_x and κ_y are the curvatures in the plane perpendicular to the x and y directions, u_r', u_θ' and w' are the rigid-body displacements in the three principal directions, and U, V and W represent displacements caused by strains in axial position at $z = 0$ which are functions of r and θ only. Leknitskii's stress functions [2] are used to obtain the partial different equations that represent the problem. Using the method of separating variables, the partial differential equations can be reduced to two Euler-type ordinary different equations. After obtaining the solutions for the stress functions, the expressions for U, V and W can be obtained as

$$U = (\kappa_x \sin\theta - \kappa_y \cos\theta)\left(\sum_{i=1}^{2} K_i U_i' r^{m_i} + U_5' r^2\right) \quad (2a)$$

$$V = (\kappa_x \cos\theta + \kappa_y \sin\theta)\left(\sum_{i=1}^{2} K_i V_i' r^{m_i} + V_5' r^2\right) \quad (2b)$$

$$W = (\kappa_x \cos\theta + \kappa_y \sin\theta)\left(\sum_{i=3}^{4} K_i W_i' r^{m_i} + W_5' r^2\right) \quad (2c)$$

Equations for stresses are obtained as

$$\sigma_r = (\kappa_x \sin\theta - \kappa_y \cos\theta)(K_1 r^{m_1+1} + K_2 r^{m_2+1} + \frac{\mu_1}{2} r^3) \quad (3a)$$

$$\sigma_\theta = (\kappa_x \sin\theta - \kappa_y \cos\theta)(K_1(m_1+1)r^{m_1+1} + K_2 m_2(m_2+1)r^{m_2+1} + 3\mu_1 r) \quad (3b)$$

$$\tau_{r\theta} = (\kappa_x \cos\theta + \kappa_y \sin\theta)(-m_1 K_1 r^{m_1-1} - m_2 K_2 r^{m_2-1} - \mu_1 r) \quad (3c)$$

$$\tau_{rz} = (\kappa_x \cos\theta + \kappa_y \sin\theta)(K_3 r^{m_3-1} - K_4 r^{m_4-1} - \mu_2 r) \quad (3d)$$

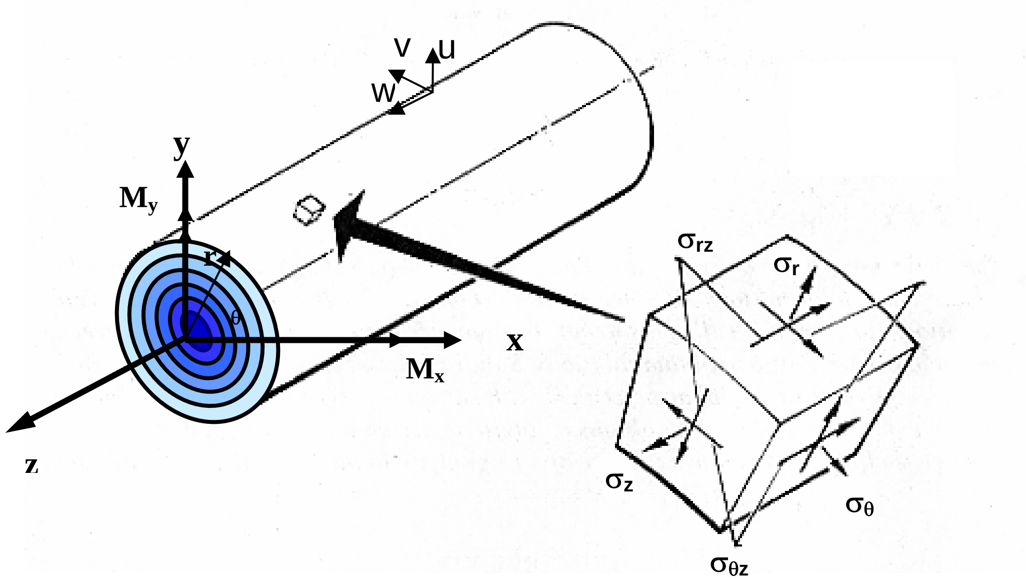


Figure 1 The cylindrical coordinate system.

$$\tau_{\theta z} = -(\kappa_x \sin\theta - \kappa_y \cos\theta)(m_3 K_3 r^{m_3-1} + m_4 K_4 r^{m_4-1} + 2\mu_2 r) \tag{3e}$$

$$\sigma_z = \frac{1}{C_{33}}[\kappa_x r \sin\theta - \kappa_y r \cos\theta - C_{13}\sigma_r - C_{23}\sigma_\theta - C_{34}\tau_{\theta z}] \tag{3f}$$

Where K_i, i = 1 to 4, are constants to be determined by considering proper boundary conditions. Parameters m_i, U_i', V_i', W_i', U_5', V_5', and W_5' are defined for each layer by the elastic constants. The rigid-body displacements u_r', u_θ' and w' are set to insure the compatibility of the deformed cylinders. They are given by

$$u_r' = -\nu\kappa_y \cos\theta + \nu\kappa_x \sin\theta \tag{4}$$

$$u_\theta = \nu\kappa_y \sin\theta + \nu\kappa_y \cos\theta \tag{5}$$

$$w' = 0 \tag{6}$$

where ν is a constant to be determined for each cylinder. For the first layer, ν_1 is set to zero. The values of ν for other layers are to be determined from the boundary and interface conditions. Here we consider t*wo* types of interfacial boundary conditions between the nanotube layers: perfect bonding (no slip) and no friction. For an N-layer multiwall nanotube, we have 5N unknown constants: 4N K_i's and N ν's. There will be $N-1$ interfaces and two free surfaces (inner surface and outer surface). Under the no slip condition, there is continuity of stresses σ_r, $\tau_{r\theta}$, τ_{rz} and displacements u_r, u_θ, w. Under the no friction condition, due to the longitudinal and tangential slip, the displacements u_θ and w will be discontinuous. There is still continuity of σ_r and u_r, and the stresses $\tau_{r\theta}$ and τ_{rz} will have zero values at the interface. In both cases, the $N-1$ interfacial conditions result in $5(N-1)$ equations while the two free-surface conditions yield four more equations. With the known equation $\nu_1 = 0$, we have 5N equations to solve for the 5N unknowns.

By considering the end conditions, the bending rigidity of the MWNT can be obtained.

$$\kappa_x = \frac{M_x}{(EI)_{eff}} \quad \text{and} \quad \kappa_y = \frac{M_y}{(EI)_{eff}} \tag{7}$$

with

$$(EI)_{eff} = \sum_{n=1}^{N} \frac{\pi}{C_{33},n} \left\{ \sum_{i=1}^{2} K_{i,n} m_{i,n} \left[C_{13} + C_{23,n}(m_{i,n}+1) \right] \frac{a_n^{m_{i,n}+2} - b_n^{m_{i,n}+2}}{m_{i,n}+2} + \sum_{3}^{4} K_{i,n} m_{i,n} C_{3,4} \frac{a_n^{m_{i,n}+2} - b_n^{m_{i,n}+2}}{m_{i,n}+2} \right. \\ \left. + \left[\mu_{1,n}\left(C_{13,n} + 3C_{23,n}\right) - 2\mu_{2,n} C_{34,n} - 1 \right] \frac{a_n^4 - b_n^4}{4} \right\} \tag{8}$$

Considering the MWNT as a solid bar, the effective elastic modulus can be defined as

$$E_{eff} = \frac{(EI)_{eff}}{I_{solid}} \tag{9}$$

where $I_{solid} = \pi b_N^4 / 4$ represents the moment of inertia of the solid bar.

MULTI-WALLED CARBON NANOTUBES FLEXURAL PROPERTIES

Two different combinations of multiwall nanotubes are simulated. The first series of MWNT has an inner radius of 9.9669 nm and the second series has an inner radius of 0.339nm. Because the graphene layer is transversely isotropic, the helical angle doest not affect the mechanical properties of the nanotubes. In this work we have chosen the multiwall nanotubes with 30° helix angle for each layer. The first series has the configuration of (147, 147), (152, 152), (157, 157), (162, 162), …, (637, 637), (642, 642). The outer radius of a 100-layer MWNT of this series is 43.995 nm. The second series of multiwalled nanotubes, with a small inner radius, are constructed as the (5n, 5n), with n = 1, 2, …100. The outer radius of a 100-layer MWNT of this series is 34.368 nm. The geometrical data of the two geometries are listed in Table 1 and Table 2. The effective Young’s modulus, bending stiffness, radial displacement, warping and other mechanical properties are determined by the model described above. The elastic constants of graphene sheet [8] are used to define the elastic properties of the nanotube cylinder.

Bending stiffness and effective elastic modulus

In this work, we find out that the interface conditions, i.e., perfect bonding or no friction, do not affect the bending stiffness or the elastic modulus. The bending stiffness for the two geometries are shown in Figure 2. Fig. 2(a) shows the bending stiffness increases with the number of nanotube layers. In this figure we show the results for both interface conditions, but for the following figures, we only show the results for the perfect bonding case. For the same number of layers, the MWNT with

Table 1 Structural parameters of the (147, 147), (152, 152), (157, 157), (162, 162)…(637, 637), (642, 642) multiwall nanotubes series.

n	m	theta	$R_{n\ (nm)}$	R_i (nm)	R_o (nm)
147	147	30	9.9669	9.7959	10.1379
152	152	30	10.3059	10.1349	10.4769
…	…	…	…	…	…
637	637	30	43.1899	43.0189	43.3609
642	642	30	43.5289	43.3579	43.6999

Table 2 Structural parameters of the (5n,5n) series multiwall nanotubes with n=1,2,…100

n	m	theta	$R_{n\ (nm)}$	R_i (nm)	R_o(nm)
5	5	30	0.3390	0.1680	0.5100

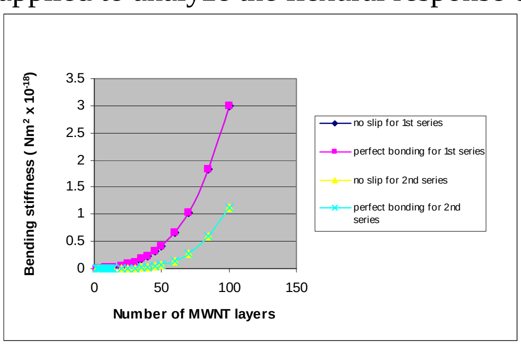
10	10	30	0.6780	0.5070	0.8490
…	…	…	…	…	…
495	495	30	33.8332	33.6622	34.0042
500	500	30	33.9010	33.7300	34.0720

a larger inner radius has greater bending stiffness than the MWNT with a smaller inner radius. Fig. 2(b) shows the bending stiffness increase with the outer radius of the MWNT. For the same value of the outer radius, the MWNT with smaller inner radius has more layers, and thus has greater bending stiffness.

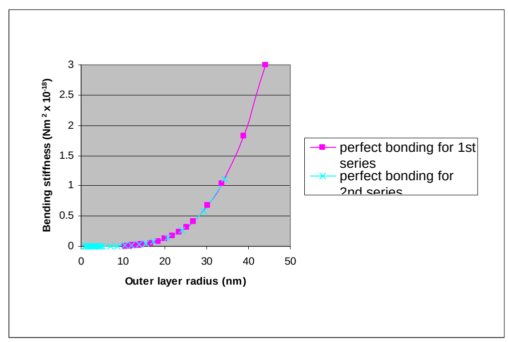
Equation 9 defines the effective elastic modulus for the MWNT. The result is shown in Figure 3. Fig. 3(a) shows the effective Young's modulus increase with the number of the layers. As the number of layers increases, the effective modulus of the MWNT approaches the in-plane elastic modulus of grahpene (1.06 TPa). For fixed number of layers, the MWNT with smaller inner radius has larger effective elastic modulus. Figure 3(b) shows the effective Young's modulus increases with the outer radius. For the same value of the outer radius, the MWNT with smaller inner radius has a larger value of effective elastic modulus. Fig. 3(c) is an enlarge of Fig. 3(b) for the first few inner layers.

Warping:

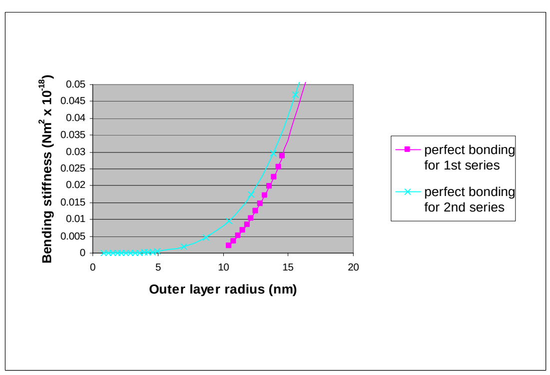
One important result is that for all the cases under two interface conditions: no friction or no slip, there is no warping present. This result indicates that the classic beam theory can be applied to analyze the flexural response of MWNT.



(a)

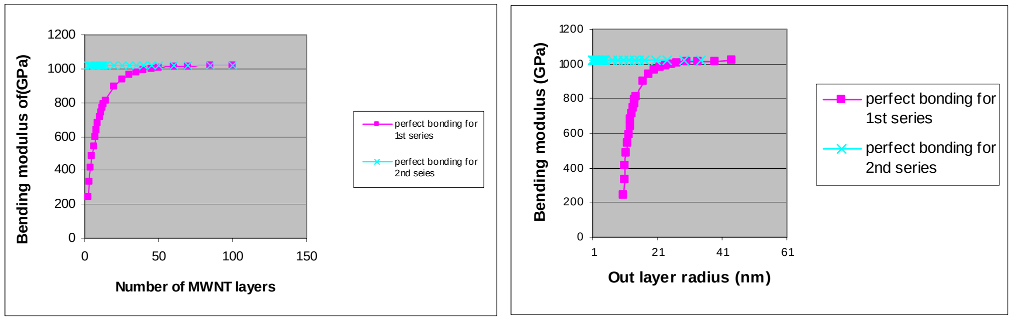


(b)



(c)

Figure 2 Bending stiffness of the two MWNT series. (a) is function as number of layers, (b) is function as out layer radius for whole series and (c) is function as out layer radius for initial few layers.



(a) (b)

Figure 3 The elastic bending modulus of the two MWNT series. (a) is function as number of layers, (b) is function as out layer radius for whole series.

CONCLUSION

The main purpose of the work is to predict the flexural rigidity of multi-walled carbon nanotubes using the analytical solution for coaxial cylinders under bending. The material for each layer is transversely isotropic and the elastic constants are the same as the graphene sheet. The model enables us to predict the flexural rigidity for multi-walled nanotubes with any number of walls. We find that the bending stiffness increases with the number of nanotube layers. The MWNT with larger inner radius has greater bending stiffness than the MWNT with a smaller inner radius when the number of layers is fixed. On the other hand, the effective elastic modulus, when the MWNT is considered as solid bar structure, increases with the outer radius. The MWNT with smaller inner radius has a larger effective elastic modulus. As the number of layers increases, the effective modulus approaches the in-plane elastic modulus of graphene. For fixed number of layers, the MWNT with smaller inner radius has larger effective elastic modulus. In this work the boundary condition does not show any effect on the bending stiffness and effective elastic modulus. It is also found that the cross-section of MWNT does not have any warpage under bending, suggesting the classic beam theory is applicable in determining the flexural response of MWNT

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