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Axial buckling of multi-walled carbon nanotubes and nanopeapods

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ABSTRACT

In this paper, we investigate both pre- and post-buckling behaviors of multi-walled carbon nanotubes and multi-walled carbon nanopeapods by incorporating into the applied forces of a prescribed beam equation both van der Waals interactions between the adjacent walls of the nanotubes and the interactions between the fullerenes and the inner wall of the nanotube. Two beam theories are employed. First, we utilize Donnell's equilibrium equation to derive an axial stability condition for the multi-walled carbon nanotubes and multi-walled carbon nanopeapods. We then determine analytically the critical forces for single-walled and double-walled nanotubes and nanopeapods. Given the outer nanotube of a fixed radius, we observe that the critical force and strain derived from the axial buckling stability criterion decrease as a result of the molecular interactions between the adjacent layers of the nanotubes and the molecular interactions between the embedded fullerenes and the inner carbon nanotube, which is in agreement with existing literature. Next, we utilize an Euler–Bernoulli beam equation incorporating the curvature effect to obtain the post-buckled axial bending displacement for the multi-walled nanotubes and nanopeapods. We find that the interactions between molecules generate an inward force, which tends to resist any applied forces. While the inward force induced by the fullerenes to the inner wall of the nanotube vanishes as we increase the applied force, the inward force induced by the layers increases as the applied force increases. The main contribution of this paper is the incorporation of both van der Waals interactions and the curvature effect into prescribed beam theories to accurately measure the critical forces and the buckled displacements of multi-walled nanotubes and nanopeapods subject to a small external force. Our analysis is relevant to future nano devices, such as biological sensors and measuring devices for small forces arising from electrical charges or Casimir forces.

1. Introduction

The discovery of carbon nanotubes by Iijima (1991) has led to many experimental, theoretical and computational investigations on their unique chemical, electrical and mechanical properties. Owing to the non-polar nature of their molecular bonds, carbon nanotubes are insoluble and stable in water. However, they can be covalently functionalized, i.e. they will respond to certain strong acids and chemical oxidizers. Since they have a large surface to volume ratio, they can be utilized for gas filtration, sensing and energy storage. Furthermore, their electrical properties vary according to their molecular structure. In addition, carbon nanotubes have the largest known axial Young's modulus, which arises due to the sp^2 bond between carbon atoms, resulting in reversible elastic deformations, such as large twisting, kinking and bending deformations.

Continuum mechanics has been widely and successfully applied to the mechanical analysis of carbon nanotubes as an alternative to molecular dynamics simulations. Recently, Govindjee and Sackman (1999) adopt a Benoulli–Euler beam theory to obtain the Young's modulus of multi-walled nanotubes. According to a multiple-elastic beam model, Yoon et al. (2003) examine resonant frequencies and obtain vibrational modes of an individual multi-walled carbon nanotube embedded inside an elastic medium. Li and Chou (2003) also utilize a space truss model to determine the Young and shear moduli of a single-walled carbon nanotube. Moreover, Yakobson et al. (1996) utilize a continuum shell model to predict the buckling of a single-walled carbon nanotube and their results are compared with molecular dynamics simulations. A finite element method (Pantano et al., 2004) and molecular dynamics simulations (Odegard et al., 2002; Sohi and Naghdabadi, 2007; Liew et al., 2004; Zhang et al., 2007) are also utilized to investigate the buckling behavior of nanotubes. Several experimental works have been performed to investigate the deformation of single- and multi-walled nanotubes under high pressure (Thomsen et al., 1999; Elliott et al., 2004).

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In this paper, we investigate the axial buckling of multi-walled nanotubes and nanopeapods, which have a chain of metallofullerenes or fullerenes inside the carbon nanotube (see Fig. 1). Nanopeapods have been experimentally observed by Smith et al. (1998) and Smith and Luzzi (2000) through high-resolution transmission electron microscopy. It is suggested that the encapsulation of C_{60} molecules occurs either through a large opening on the tube wall (Berber et al., 2002) or through the open ends of the nanotube (Ulbricht and Hertel, 2003; Ulbricht et al., 2003). For different possible equilibrium configurations of fullerenes inside a nanotube (e.g. linear, zigzag and spiral patterns), we refer the reader to Baowan et al. (2007) and references therein. Axial buckling may be experimentally demonstrated as a nanoelectromechanical effect on a doubly clamped suspended nanotube or nanopeapod. We assume that a nanotube or a nanopeapod is attached by two electrodes through tunneling contacts, in which Coulomb-blockade effects dominate the transport. The applied gate voltage bends the nanopeapod by an applied external electrical field E_0, which affects both electrical and mechanical properties of the nanostructure, and is generally referred to as a nanoelectromechanical system (Ke et al., 2005a,b; Pugno, 2005; Pugno et al., 2005). Similar to the case of doubly clamped single-walled carbon nanotubes, such hybrid molecular structures as single-walled and double-walled nanopeapods can be utilized as nanotweezers (Kim and Lieber, 1999; Akita et al., 2001), switches in a random access memory device (Rueckes et al., 2000), actuators (Baughman et al., 1999) and nanoelectromechanical switches (Dequesnes et al., 2002; Kinaret et al., 2003). In addition, with natural electronic properties, nanopeapods with embedded metallofullerenes can be utilized as ultra efficient on-and-off gigahertz oscillators (Zheng and Jiang, 2002; Legoas et al., 2003; Cox et al., 2007a,b) using an applied external electric field.

This paper is structured as follows. In Section 2, we derive the linear constants for different layers of the nanotubes (a detailed derivation is given in Appendix A). In addition, the force arising from the Lennard–Jones potential, which comprises both an attractive part (van der Waals) and a repulsive part (Pauli exclusion principle), we simply refer to such force as the van der Waals force for the fullerenes–nanotube interactions and it is derived utilizing a continuous approximation developed by Cox et al. (2007a,b). In Section 3, we introduce Donnell's equation and we determine the critical forces for the single- and double-walled carbon nanotubes and nanopeapods. In Section 4, on assuming a multi-walled carbon nanotube and nanopeapod as a one-dimensional structure, we adopt an Euler–Bernoulli beam theory, derived from a variational principle, to study the doubly clamped suspended single-walled and double-walled nanotubes and nanopeapods under bending. Some conclusions are given in the final section and certain detailed mathematical derivations are presented in the appendices of the paper.

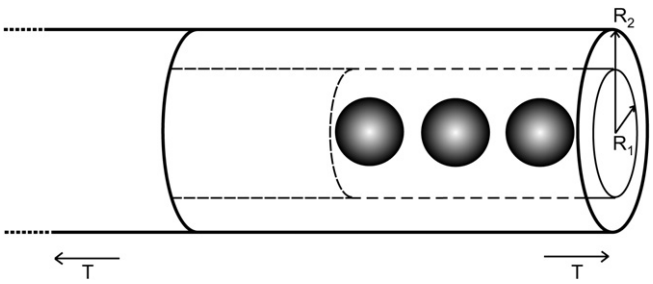

Fig. 1. Nanopeapods.

2. Intermolecular forces

In this section, we derive the linear response constants for the layers of the nanotubes and determine the van der Waals force between fullerenes and the inner wall of a nanotube by utilizing a continuous approximation for which we assume that the carbon atoms are smeared over the surfaces of the fullerenes and the nanotubes. We comment that the results obtained in this section are utilized to correct the critical forces and the post-buckled bending displacements of multi-walled nanotubes and nanopeapods presented in Sections 3 and 4, respectively.

2.1. Intermolecular force between layers

Forces between the layers of carbon nanotubes with different radii (see Fig. 2) must satisfy Newton's third law, i.e. $p_{i,j}R_i = -p_{j,i}R_j$, where $p_{i,j}$ denotes the pressure exerted from the jth layer to the ith layer, R_i denotes the tube radius for the ith layer and where subscripts $i = 1\ldots N$ denotes the ith layer of the carbon nanotube. We assume that the incremental pressure Δp_i of the ith layer arising from an adjacent jth layer to be linear in the displacement difference between the two layers, i.e. $\omega_j - \omega_i$, where ω_i denotes the displacement of the ith layer. From these assumptions we may deduce

$$\begin{aligned}
\Delta p_1 &= p_{1,2} = c_1(\omega_2 - \omega_1),\\
\Delta p_2 &= p_{2,3} + p_{2,1} = c_2\left[(\omega_3 - \omega_2) - \frac{R_1}{R_2}(\omega_2 - \omega_1)\right],\\
&\vdots \quad\quad \vdots\\
\Delta p_N &= p_{N,N-1},
\end{aligned} \tag{1}$$

where c_i denotes the linearity constant for ith layer, which can be found by matching the van der Waals interactions between the nanotube layers and Taylor's expansion around an equilibrium configuration, and which is derived in Appendix A. Assuming that the molecules are at equilibrium, the force per unit length acting on different layers must be equal, which can be written as

$$N_{1z} = R_1 p_1 = N_{2z} = R_2 p_2 = \ldots = N_{Nz} = R_N p_N. \tag{2}$$

Thus, for the total applied force per unit length T, we have

$$\begin{aligned}
T &= R_1 p_1 + R_2 p_2 + \ldots + R_N p_N,\\
&= R_1 p_1 + R_2\left(\frac{R_1}{R_2} p_1\right) + \ldots + R_N\left(\frac{R_1}{R_N} p_N\right) = N R_1 p_1,
\end{aligned}$$

from which we obtain

$$p_1 = \frac{T}{N R_1}, \quad N_{1z} = R_1\left(\frac{T}{N R_1}\right) = \frac{T}{N}, \tag{3}$$

where Eq. (2) is utilized to obtain Eq. (3). Following the same argument as that stated above, we may deduce

$$p_i = \frac{T}{N R_i}, \quad N_{1z} = N_{2z} = \ldots = \frac{T}{N}. \tag{4}$$

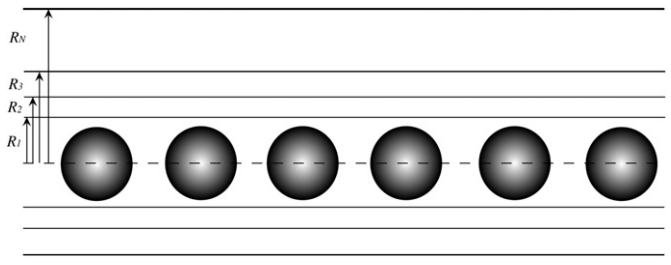

Fig. 2. Schematic of multi-walled nanopeapod.