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Torsional buckling of multi-walled carbon nanotubes

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Abstract

This paper investigates torsional buckling of an individual multi-walled carbon nanotubes. The multiple shell model is adopted and the effect of van der Waals forces between adjacent nanotubes is taken into account. According to the ratio of radius-to-thickness, multi-walled carbon nanotubes discussed here are classified into three cases: thin, thick, and nearly solid. The critical shear stress and the torsional buckling mode are calculated for various radius-to-thickness ratios. Results carried out show that the buckling mode (m, n) corresponding the critical shear stress is sole, which is obviously different from the axially compressed buckling of an individual multi-walled carbon nanotubes. The investigation on torsional buckling of multi-walled carbon nanotubes in this paper may be used as a useful reference for the designs of nano-oscillators, nano-drive devices and actuators in which multi-walled carbon nanotubes act as basic elements.

Keywords: Multi-walled carbon nanotubes; Torsional buckling; Laminated shells

1. Introduction

Carbon nanotubes discovered by Iijima [1] at the beginning of the last decade, has attracted worldwide attention related to the use of the nanotubes in the fields of chemistry, physics, diverse engineering, materials science, and reinforced composite structures. Carbon nanotubes are made of a highly ordered sheet of carbon atoms rolled into a tube. This uniform structure gives unique properties of this new material, such as strong, light and high toughness fibers for nanocomposite structures, parts of nano-devices, hydrogen storage (high frequency) micromechanical oscillators from Avouris et al. [2], Dresselhaus et al. [3], Yang [4], and Zheng and Jiang [5]. Lau and Hui [6] presented recent developments on the nanotubes and investigations in the applications on nanotube composites, and given much attention on the examination of the mechanical properties such as tensile strength of an individual nanotube or a bundle of nanotube-rope, the buckling properties due to shrinkage of matrices after curing and the bending stiffness of nanotube-composite structures.

Multi-walled carbon nanotubes are composed of concentric layers of single-walled carbon nanotube (SWNT). When multi-walled carbon nanotubes (MWNTs) occur in large strain deformation they bend at large angles and may start to elastically ripple, buckle, and form kink, which induces abrupt changes of physical properties of MWNTs. The investigations on compression, bending or torsional deformations of single- or multi-walled carbon nanotubes has been the subject of numerous experiments and molecular dynamic simulations [7–10]. Generally, there are two theoretical approaches to understand the mechanical behavior of nanostructures: atomistic molecular dynamic simulations and continuum mechanics. The molecular dynamic (MD) simulations have been conducted by several investigators [7,11], and the continuum methods of mechanics such as some analytical methods which is used to investigate diffusive shrinkage of a void within a grain of a stressed polycrystal and to solve stability and shrinkage of a cavity in stressed grain are presented by Wang and Li [12–14]. Yakobson et al. [7] introduced an atomistic model for axially compressed buckling of single-walled nanotube and also compared it with a simple continuum shell model. They found that all changes of buckling patterns displayed by the molecular

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dynamics simulations could be predicted by the continuum shell model. Wang et al. [15–17] constructed different three-dimensional FEM models to obtain an effective bending modulus of CNTs with various rippling deformations.

Recently, considerable attention has turned to mechanical behavior of single- or multi-walled carbon nanotubes embedded in a polymer or metal matrix in Refs. [18–20]. Ru [21] presented an elastic double-shell model for infinitesimal buckling of a double-walled carbon nanotubes embedded in an elastic medium under axial compression. Ru [22] also studied the effect of van der Waals interaction between the inner and outer nanotubes on axial buckling of a double-walled carbon nanotubes, and derived a simple formula for the axially critical strain. Wang and Yang [23] presented the effect of thermal environment on axially critical load of multi-walled CNTs by utilizing a continuum mechanics model. Wang et al. [24] have recently studied elastic buckling of individual MWNTs subjected to radial external pressure based on the laminated shells model from Ru [21,25,26] and their results shown that the predicted critical pressure by using continuum mechanics model is in reasonably good agreement with the some experiment results from Tang et al. [27], which further offers an evidence that the elastic shell model can be used to study buckling behavior of single- or multi-walled carbon nanotubes.

From Arroyo and Belytschko [28], Williams et al. [29], and Fennimore et al. [30], a number of experiments have suggested that multi-walled carbon nanotubes can be used as basic elements of nano-electromechanical systems, such as nano-oscillators, nano-drive devices and actuators, which is subjected to torsional load. Most of previous works on buckling behavior of single- or multi-walled carbon nanotubes have mainly focused on the axially compressed buckling behavior of carbon nanotubes. To our knowledge, few detailed report on the torsional buckling of multi-walled carbon nanotubes is available in the literature. This is apparently due to the fact that experimental research and molecular dynamics simulation for torsional buckling of multi-walled carbon nanotubes remain a formidable task. Because electronic and transport properties of carbon nanotubes could be extremely sensitive to even very small distortion of their otherwise perfect cylindrical geometry [31,32], torsional buckling of multi-walled carbon nanotubes remains an open topic in the literature, which is very significant to design nano-oscillators, nano-drive devices and actuators made by using multi-walled carbon nanotubes.

The present work investigates torsional buckling problems of an individual multi-walled carbon nanotubes (MWNTs), based on multiple-elastic shell model, considering van der Waals interaction force between the inner and outer layers of nanotubes. According to the ratio of radius-to-thickness, multi-walled carbon nanotubes discussed here are classified into three cases: thin, thick, and nearly solid. The critical shear, stress and the torsional buckling mode are calculated for various radius-to-thickness ratios. Results carried out in this paper show that the buckling mode (m, n) corresponding the critical shear stress of an individual multi-wall carbon nanotubes subjected to torsional loading is sole, which is obviously different from the axially compressed buckling of an individual multi-wall carbon nanotubes. This phenomenon gives an important reference valuable for the designs of nano-oscillators, nano-drive devices and actuators in which multi-walled carbon nanotubes are used as basic elements of nano-electromechanical systems.

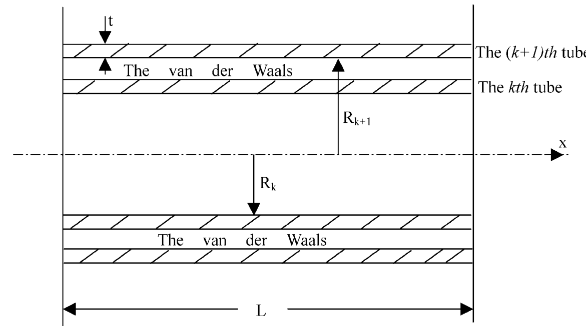

Fig. 1. A multi-walled carbon nanotube.

2. Basic equation for torsional buckling of multi-walled carbon nanotubes

The mechanics properties of single- or multi-walled carbon nanotubes have been effectively studied based on elastic-shell models from Yakobson et al. [7], Falvo et al. [8], and Ru [21,22,25,26]. Motivated by these ideas, MWNTs can be taken as a set of concentric cylindrical shells with van der Waals interaction between adjacent layers, which is shown in Fig. 1. For infinitesimal torsional buckling of a cylindrical shell with radius R, thickness h, Young's modulus E and Poisson's ratio μ, the buckling membrane strains are given by Timoshenko and Gere [33]:

$$\varepsilon_x = \frac{\partial u}{\partial x}, \qquad \varepsilon_y = \frac{\partial v}{\partial y} - \frac{w}{R}, \qquad \varepsilon_{xy} = \frac{1}{2}\left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right) \tag{1}$$

where x and y express the axial and circumferential coordinates of shell, respectively, and $u(x, y)$, $v(x, y)$ and $w(x, y)$ denote the additional displacements of the middle surface due to buckling, along x, y and inward normal directions, respectively. The corresponding membrane forces are expressed as

$$N_x = K(\varepsilon_x + \mu\varepsilon_y), \qquad N_y = K(\varepsilon_y + \mu\varepsilon_x),$$
$$N_{xy} = K(1-\mu)\varepsilon_{xy} \tag{2}$$

where $K = (Eh)/(1 - \mu^2)$.

In the present model, because the interlaminar shear forces between layers of multi-walled carbon nanotubes is negligible from Charlier and Michenaud [34], the additional membrane forces may be expressed by the stress function