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Influence of temperature change on column buckling of multiwalled carbon nanotubes

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Abstract

Based on theory of thermal elasticity mechanics, an elastic multiple column model is developed for column buckling of MWNTs with large aspect ratios under axial compression coupling with temperature change. In this model, each of the nested concentric tubes is regarded as an individual column and the deflection of all the columns is coupled together through the van der Waals interactions between adjacent tubes. The thermal effect is incorporated in the formulation. Following this model, an explicit expression is derived for the critical buckling strain for a double-walled carbon nanotube. The influence of temperature change on the buckling strain is investigated. It is concluded that the effect of temperature change on the buckling strain is dependent on the temperature changes, the aspect ratios, and the buckling modes of carbon nanotubes.

Keywords: Effect of temperature change; Carbon nanotubes; Column buckling

1. Introduction

Carbon nanotubes (CNTs) have attracted great attention due to their exceptional mechanical, thermal, and electrical properties leading to many potential applications [1–6]. Most potential applications of CNTs are much dependent on a through understanding of their mechanical behavior. For instance, it is shown that electronic properties of CNTs can be changed by mechanical deformations up to several orders of magnitude [7–12]. Thus, mechanical behavior of CNTs has been the subject of numerous recent studies [13–23].

CNTs are cylindrical macromolecules composed of carbon atoms in a periodic hexagonal arrangement. Since CNTs are extremely small, direct measurement of their properties is quite difficult. In view of the experimental difficulties, computational simulations have been regarded as a powerful tool. Molecular-dynamics (MD) method has been highly developed to simulate the properties of nanostructures. However, being very time consuming and computationally expensive for large-sized atomic systems, practical applications of MD method are very limited. To derive theoretical analysis for large-sized atomic systems, it is desirable to develop continuum theories that may overcome the limitations of MD simulation concerning both time and length scales. At present, continuum mechanics models have been regarded as an effective method and widely used to describe the mechanical properties of CNTs [6,18,24–28].

It is known that the phenomenon of buckling often occurs when CNTs are subjected to compressive loads. Thus, buckling of CNTs has become one of the topics of primary interest [25,27,29,30], and many continuum buckling models have been developed [24,31–39]. Yakobson et al. [24] presented a continuum shell model in studying axially compressed buckling of single-walled nanotubes (SWNTs). Ru [31] developed a multiple-elastic beam model to study column buckling of multiwalled carbon nanotubes (MWNTs) embedded within an elastic medium. Based on a multiple-shell model [32], Wang et al. [33] investigated axially compressed buckling of MWNTs under radial pressure. Sudak [34] discussed column buckling of MWNTs on the basis of nonlocal continuum mechanics. Zhang

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et al. [35] studied bending instability characteristics of double-walled carbon nanotubes (DWNTs) of various configurations.

Lately, much research indicates that the mechanical properties of CNTs are related to temperature change. Raravikar et al. [40] studied the temperature dependence of radial breathing mode Raman frequency of SWNTs by using MD simulation and found that the coefficients of thermal expansion are positive in both radial and axial directions as the temperature is varied from 300 to 800 K. Schelling and Keblinski [41] obtained similar results through MD simulation. Pipes and Hubert [42] investigated thermal expansion of helical CNTs arrays, and the effective axial, transverse and shearing coefficients of thermal expansion of the array are determined. Based on the interatomic potential and the local harmonic model, Jiang et al. [43] presented an analytical method to determine the coefficient of thermal expansion for SWNTs. They concluded that all the coefficients of thermal expansion are negative at low and room temperature and become positive at high temperature. Consequently, the investigation of thermal effect on the mechanical properties of CNTs is of great importance and necessity. However, all analyses of buckling for CNTs mentioned above have not accounted for the thermal effect. Very lately, Yao and Han [44] conducted buckling analysis of MWNTs subjected to torsional load under temperature field. Based on a rigorous van der Waals interaction, Wang et al. [45] conducted an investigation on the axially compressed buckling of MWNTs under thermal loads via a continuum shell model.

In this Letter, an elastic multiple column model is developed for the linearized column buckling of MWNTs with large aspect ratios under axial compression coupling with temperature change. The effect of temperature change on the properties of axially column buckling is examined.

2. Multiple column model with thermal effect

The treatment of column buckling which is developed here is on the basis of the Bernoulli–Euler theory. This theory is based upon the assumption that plane cross sections of a beam remain plane during flexure and that the radius of curvature of a bent beam is large compared with the beam's depth. Following the linear form of Hooke's law, the deflection curve of an elastic column subjected to constant axial load and distributed lateral pressure is given by [46]

$$N\frac{\mathrm{d}^2 w}{\mathrm{d}x^2} + p(x) = EI\frac{\mathrm{d}^4 w}{\mathrm{d}x^4}, \tag{1}$$

where x is the axial coordinate, w is the deflection, EI is the bending stiffness of the beam, N is the constant axial force, and $p(x)$ the distributed lateral pressure per unit length (measured positive in the direction of the deflection).

On the basis of the theory of thermal elasticity mechanics, we have the following stress-strain relation [47]:

$$\boldsymbol{\sigma} = \lambda(\mathrm{tr}\,\boldsymbol{\varepsilon})\boldsymbol{\delta} + 2\mu\boldsymbol{\varepsilon} - (3\lambda + 2\mu)\alpha\theta\boldsymbol{\delta}, \tag{2}$$

where $\boldsymbol{\sigma}$ and $\boldsymbol{\varepsilon}$ are, respectively, stress and strain tensors, λ and μ are Lame constants, $\boldsymbol{\delta}$ is the Kroneker delta, symbol "tr" denotes the trace of a tensor, and α and θ are the coefficients of thermal expansion and temperature change, respectively.

Another assumption behind the Bernoulli–Euler beam model is that the beam consists of fibers parallel to the x axis, each in a state of uniaxial tension or compression. For the case of a uniaxial stress state, Eq. (2) reduces to

$$\sigma = E\varepsilon - \frac{E}{1-2v}\alpha_x\theta, \tag{3}$$

where σ is the axial stress, ε is the axial strain, α_x denotes the coefficient of thermal expansion in the direction of the x axis, and E and v are Young's modulus and Poisson's ratio, respectively. It is noted that use is made of the following equations:

$$\lambda = \frac{vE}{(1+v)(1-2v)}, \qquad \mu = \frac{E}{2(1+v)}.$$

For the axial force N, we have

$$N = \sigma A = N_m + N_t, \tag{4}$$

where A is the cross-sectional area of the beam, and

$$N_m = \sigma_m A, \qquad N_t = -\frac{EA}{1-2v}\alpha_x\theta \tag{5}$$

in which σ_m is the axial stress due to the mechanical loading prior to buckling.

Substituting Eq. (4) into Eq. (1), we obtain

$$(N_m + N_t)\frac{\mathrm{d}^2 w}{\mathrm{d}x^2} + p(x) = EI\frac{\mathrm{d}^4 w}{\mathrm{d}x^4}. \tag{6}$$

It is known that MWNTs with large aspect ratios are distinguished from traditional elastic beams by their hollow multilayer structure and associated intertube van der Waals forces. As CNTs have high thermal conductivity, it may be regarded that the change of temperature is uniformly distributed in the CNT. Treacy et al. [48] reported a linear relationship between the mean-square vibration amplitude of the tube's free tip displacement and the tube temperature, which implies that the tube's elastic modulus is temperature independent. Hsieh et al. [49] studied the variation of Young's modulus of SWNTs with temperature, and it was indicated that the Young's modulus of an SWNT is insensitive to temperature change in the tube at temperatures of less than approximately 1100 K, but decreases at higher temperatures. Thus, for the cases of low temperatures and high temperatures (but not very high), the Young's modulus is herein assumed to be temperature independent. In what follows, all nested tubes are supposed to have the same thickness and effective material constants. Applying Eq. (6) to each of the nested carbon nanotubes, we have

$$EI_1\frac{\mathrm{d}^4 w_1}{\mathrm{d}x^4} = p_{12} + (N_{m1} + N_{t1})\frac{\mathrm{d}^2 w_1}{\mathrm{d}x^2},$$

$$EI_2\frac{\mathrm{d}^4 w_2}{\mathrm{d}x^4} = p_{23} - p_{12} + (N_{m2} + N_{t2})\frac{\mathrm{d}^2 w_2}{\mathrm{d}x^2},$$

$$\vdots$$

$$EI_{n-1}\frac{\mathrm{d}^4 w_{n-1}}{\mathrm{d}x^4} = p_{(n-1)n} - p_{(n-2)(n-1)} + (N_{m(n-1)} + N_{t(n-1)})\frac{\mathrm{d}^2 w_{n-1}}{\mathrm{d}x^2},$$