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Effects of initial stress on non-coaxial resonance of multi-wall carbon nanotubes

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Abstract

This paper reports an investigation of the influence of initial stress on the flexural vibration of an individual multi-wall carbon nanotube with simply supported ends, based on a laminated elastic beam model considering the van der Waals force interaction between two adjacent nanotubes. The results obtained show that the influence of initial stress in carbon nanotubes on their natural frequency is obvious, but the influence of initial stress in carbon nanotubes on the intertube resonant frequency of multi-wall carbon nanotubes is not obvious, especially for large aspect ratios. The influence of initial stress in carbon nanotubes on their flexural vibration modes is dependent on the tension or compression forms of the initial stress. This investigation on the influences of initial stress in multi-wall carbon nanotubes on natural frequency and intertube resonant frequency may be used as a useful reference for the application and design of nano-oscillators, nano-drive devices, nano-sensors and actuators in which multi-wall carbon nanotubes act as basic elements.

Keywords: Dynamic phenomena; Carbon and graphite; Deformation structure

1. Introduction

Since the discovery of carbon nanotubes (CNTs) at the beginning of the 1990s [1], extensive research related to nanotubes in the fields of chemistry, physics, materials science and engineering, and electric engineering has been reported [2–4]. Single- and multi-wall CNTs hold substantial promise for use as super-stiff and strong nano-fibers, as catalysts, and as components of novel electronic and micro-drive devices [5–7]. Yakobson et al. [8] introduced an atomistic model for axially compressed buckling of single-wall nanotubes and also compared it with a simple continuum shell model. They found that all the changes of buckling patterns displayed by molecular dynamics simulations could be predicted by the continuum shell model. Wang et al. [9–11] constructed different three-dimensional finite element models to obtain an effective bending modulus of CNTs with various rippling deformations. Wang and Yang [12] studied the effect of thermal environment on axially critical load of multi-wall CNTs by utilizing a continuum mechanics model. Shen [13] investigated the postbuckling behavior of double-wall carbon nanotubes under hydrostatic pressure. Despite the potential impact of carbon nanotubes in many areas of science and industry, a robust understanding of their dynamic behavior is lacking, thus limiting the design and optimization of nano-electronic and nano-drive devices and (high-frequency) micromechanical oscillators [7,14,15].

The study of vibration and wave propagation in CNTs is of great current interest, which can be used to understand further the dynamic behavior of CNTs. The dynamic behavior of CNTs has been the subject of numerous experimental, molecular dynamics, and elastic continuum modeling studies. Since controlled experiments at nanoscales are difficult [16–19], and molecular dynamics simulations are limited to systems with a maximum number of atoms of about 10^9 by the scale and cost of computation, elastic

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continuum models have been widely used to study vibration [20,21] in CNTs. In the literature [15,20], multi-wall CNTs (MWNTs) have been modeled as single elastic beams, which neglected van der Waals force interactions between adjacent nanotubes [22,23]. Recently, the role of van der Waals force interaction between two adjacent nanotubes in non-coaxial resonance in MWNTs using the multiple Euler beam model has been studied [24–27]. Results in the literature [24–26] show that non-coaxial intertube vibration and transverse waves of MWNTs will be excited at ultrahigh frequencies. In view of the growing interest in terahertz vibrations and wave propagation of nanoscale materials and devices [28–32], it is interesting to study systematically the terahertz vibrations of an individual MWNT.

Recently, much research has been focused on the vibration characteristics of carbon nanotubes that are used in electro-active polymers to enhance their actuation and sensing properties, ultrahigh-frequency resonators, electron emission devices, high-frequency oscillators, and various electric, optical, chemical, and mechanical sensors [33,34]. The carbon nanotubes acting as basic elements of these nanostructures can often occur with initial stresses due to thermal stress, mismatch between different materials, or initial external axial loads. However, in early investigations on the dynamic characteristics of MWNTs, the effects of initial stress in the MWNTs on their vibration frequency and vibration modes were not reported.

Based a molecular structural mechanics method, Zhao et al. [35] investigated vibration behaviors of MWNTs used as nanomechanical resonators, and reported that double-wall nanotubes show a non-coaxial vibration phenomenon at the third-order resonant frequency. Utilizing molecular dynamics simulations, Li and Chou [36] investigated energy dissipation mechanisms in CNT oscillators, and pointed out that a non-coaxial rocking motion between the inner nanotube and the outer nanotube is responsible for friction in the oscillators. Because the dynamic characteristics of nanostructures based on MWNTs are sensitive to their non-coaxial vibration frequencies and modes, it is very important for practical nano-engineering applications to study the effect of initial stress on the non-coaxial resonance characteristics of MWNTs.

The main aim of this paper is to study the effect of initial stress in CNTs on the flexural vibration and non-coaxial resonant vibration of an individual MWNT. The analysis is based on a laminated beam model, which considers van der Waals force interactions between two adjacent nanotubes. Example calculations show that flexural vibration modes of CNTs are dependent on initial stresses in the nanotubes; the natural frequency of CNTs is sensitive to initial stress; and when the initial strain is close to a critical strain the natural frequency decreases sharply, and once the initial strain is larger than the critical strain the natural frequency disappears leaving only the intertube resonant frequency. Because electronic and transport properties of CNTs are extremely sensitive to even very small distortions of their otherwise perfect geometry, it is very important to study the effects of initial stresses on the non-coaxial resonance of CNTs.

2. Laminated beam model considering initial stress

A laminated beam model considering van der Waals interactions is used to study flexural vibrations of MWNTs with initial stress. Each of the nested, initially concentric nanotubes of a MWNT is represented by an individual elastic beam, and the deflections of all nested tubes are coupled through the van der Waals interaction between any two adjacent tubes [26]. The van der Waals interaction potential, as a function of the interlayer spacing between two adjacent tubes, can be estimated using the Lennard-Jones model from Girifalco and Lad [37] and Girifalco [38]. Since the innermost radius of a MWNT is usually much larger than 0.5 nm [39], the interlayer interaction potential between two adjacent tubes can be simply approximated by the potential obtained for two flat graphite monolayers, denoted by $g(\delta)$, where δ is the interlayer spacing [40]. This model has previously been shown to provide good agreement with experimental results [41]. For the present infinitesimal buckling analysis, the van der Waals pressure $p_V(x, \theta)$ at any point between two adjacent tubes should be a linear function of the deflection jump at that point, so we have

$$p_V = \left[\frac{dg(\delta)}{d\delta}\right]_{\delta=t} + c(\Delta w) \tag{1a}$$

where

$$c = \left.\frac{d^2 g}{d\delta^2}\right|_{\delta=t} \tag{1b}$$

and t is the initial interlayer spacing prior to deformation, which is equal or very close to the representative thickness of a CNT, (Δw) expresses the deflection jump due to deformation, and c is the van der Waals interaction coefficient. Because the initial interlayer spacing is very close to the equilibrium interlayer spacing at which $dg(\delta)/d\delta = 0$ described by Girifalco and Lad [37] and Girifalco [38], the first term of Eq. (1a) is negligible, reflecting the fact that all initial interlayer pressures vanish. Here, the interaction coefficient c is calculated at the initial interlayer spacing (about 0.34 nm). The van der Waals interaction coefficients c_j $(j = 1, 2, \ldots, N-1)$ based on a laminated beam model are approximately expressed as [27]

$$c_j = \frac{320 \times (2R_i)\ \text{erg/cm}^2}{0.16 d^2} \quad (d = 1.42 \times 10^{-8}\ \text{cm},\ j = 1, 2, \ldots, N-1) \tag{1c}$$

For small-amplitude vibrations, the van der Waals pressure should be a linear function of the difference of the deflections of the two adjacent layers at the point as follows:

$$p_{12} = c_1[w_2 - w_1],\ p_{23} = c_2[w_3 - w_2], \ldots, \quad p_{(N-1)N} = c_{N-1}[w_N - w_{N-1}] \tag{2}$$