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Investigating the influence of surface deviations in double walled carbon nanotube based nanomechanical sensors

Ajay M. Patel, Anand Y. Joshi *

Mechatronics Engineering Department, G.H. Patel College of Engineering & Technology, Vallabh Vidyanagar, Gujarat, India

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ABSTRACT

This manuscript investigates the influence of surface deviations, i.e. curvature in double walled carbon nanotube based nano sensors. A number of papers have been published regarding the sensing characteristics of carbon nanotubes particularly single walled carbon nanotubes. The effect of waviness or curvature has been considered and modeled in single walled carbon nanotubes when used as mass or other types of sensors but very little information is available regarding the deviations in double walled carbon nanotubes and the use of such tubes as sensors. It has been found from the experimental images that double walled carbon nanotubes are not straight and that they have a significant amount of surface deviation associated with them. It is also observed that CNTs do not possess the same wavy thickness throughout their length. Hence a constant curvature or radius model may give uniform thickness in terms of curvature throughout the length which may lead to some what inaccurate results. To model the actual curvature ratio a half sine wave model has been selected which better represents the non-uniform thickness. In this paper resonant frequency of double walled carbon nanotubes (DWCNT) with deviations along it is axis and different boundary conditions namely cantilever and bridged have been investigated. The nonlinear equations of motion of the double-walled carbon nanotubes are derived by using Euler beam theory and Hamilton principle, with considering the nonlinear van der Waals forces. The sensitivity of the apparently deviated double walled carbon nanotubes, different masses (attached to the end of outer tube tip on DWCNT and center outer tube tip of the bridged DWCNT) and different lengths has been explored and presented. The dynamic response of sensors has been explained using orbit plot. The system is seen to be exhibiting an onset of periodic and quasi periodic behavior with the change in the surface deviations. The presented results clearly suggest that change in the stiffness associated with the backed out modulus leads to a frequency shift which is considered as a measure of change in mass. The results obtained have been validated with the published experimental literature as well as shell model and are found in good agreement.

1. Introduction

Carbon nanotubes discovered by Iijima [1], has engrossed worldwide attention related to the use of nanotubes in the field of material science, chemistry, physics, diverse engineering, reinforced composite structure and mass sensors. Emerging trade applications include nano electromechanical oscillators, nano scale clocks, parametric amplifiers, and charge detection devices [2]. In carbon nanotubes vibration, bending and buckling behavior has been a subject of interest for theoretical researchers. Aydogdu and Ece [3] studied the buckling of in-plane loaded double-walled CNTs. It has been observed that sensors based on frequency shift offer a great deal of potential of reuniting the high-performance requirement of many sensing applications, including metal deposition monitors, chemical reaction monitors, biomedical sensors, mass detector, etc. [4–7]. This frequency shift principle has been used by many researchers in quantifying the variable which needs to be measure at frequent intervals.

Considering the computational approach, molecular structural mechanics is based on observed similarities between the molecular structure of a nanotube and that of a frame structure and the combination of the methods of classical structural mechanics and molecular mechanics to study to mechanical behavior of CNTs. Using this approach, Li and Chou [8,9] studied the possible use of CNTs as nanoresonators and used the combined molecular structural mechanics and stiffness matrix methods to calculate the

* Corresponding author. Tel.: +91 09879145910.
E-mail addresses: ajaympatel2003@yahoo.com (A.M. Patel), anandyjoshi@gmail.com (A.Y. Joshi).

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fundamental frequencies of CNTs for both cantilevered and bridged boundary conditions. Li and Chou also used this approach to demonstrate the possible use of CNT-based nanomechanical resonators for mass detection [10]. Natsuki et al. [11] applied wave propagation approach to vibration analysis of simply supported doubled-walled carbon nanotubes. DWCNTs are considered as a two-shell model coupled together the van der Waals interaction between two adjacent nanotubes. Wang et al. [12] studied the group velocities of longitudinal and flexural wave propagations in single- and multi-walled carbon nanotubes in the frame of continuum mechanics. Zhang et al. [13] applied the wave propagation approach to analyze the vibration frequencies of cylindrical shells filled with fluid.

Recent literature shows an increased use of modeling methods based on elastic continuum as well as nonlocal mechanics theories for studying the vibration of carbon nanotubes. Berhan et al. [14] presented that the waviness plays an important role in stiffness of these materials when the theoretical limits were investigated on achievable modulus in nanotube materials by stiffening of bonds. Yazdchi and Salehi [15] analyzed the effects of CNTs waviness on interfacial stress transfer characteristics of CNT/polymer composites. Ouakad and Younis [16] adopted a 2D nonlinear curved beam model to study the natural frequencies and mode shapes of simply supported CNTs subjected to electric excitation. Moreover, Mayoof and Hawwa [17] used a model of curved elastic beam to investigate the nonlinear vibration of doubly clamped CNTs subjected to harmonic excitation.

In modeling the dynamic behavior of carbon nanotubes, a number of investigators have adopted different theories. Continuum beam and shell models were explored by Harik [18]. Barkaline et al. [19] studied the properties of ordering carbon nanotube arrays in sensory systems based on molecular dynamics and finite element method. The mechanical and acoustic properties of such arrays, elastic modulus and density dependence on oxygen adsorption value are calculated. Pradhan et al. [20] analyzed the vibration of orthotropic nanoplates by using nonlocal elasticity theory. To examine the small scale effect of nanoplate, nonlocal elasticity theory was used. Mir et al. [21] used a finite element model with beam elements as building blocks to study the vibration response of a single walled carbon nanotube. Wang et al. [22] analyzed nonlocal elastic beam and shell models are developed and applied to investigate the small scale effect on buckling analysis of carbon nanotubes (CNTs) under compression. Patel and Joshi [23] analyzed vibrational characteristics of double walled carbon nanotube (DWCNT) modeled using spring elements and lumped masses. The inner and outer walls of carbon nanotube were modeled as two individual elastic beams interacting each other by van der Waals forces. To simulate the interlayer interactions and describe the van der Waals potentials between carbon atoms on different layers appropriate spring elements are utilized [23]. Moreover, Joshi et al. [24] have reported that SWCNT based mass sensors exhibit super harmonic and sub harmonic response with different level of the mass. In recent times it has been shown that a doubly clamp wavy SWCNT with and without attached mass shows periodic and different nonlinear behaviors as mass is attached at different positions along the length [25].

In the review paper by Gibson et al. [26], it has been indicated that different researchers have assumed, carbon nanotubes to be behaving as perfectly straight beams or straight cylindrical shells.

However, as per the Scanning Electron Micrograph [27] it is pretty clear that CNTs do possess some amount of surface deviations along its length. These tiny structures are not straight, but have certain degree of surface deviation or waviness with varying thickness along the length. The curved characteristic can be attributed to the manufacturing process used, in addition to mechanical properties such as low bending stiffness and large aspect ratio. A no. of papers have been found which study the vibration characteristics of double walled carbon nanotubes, but very little information is available pertaining to the curvatures in DWCNT which is quite clear from Fig. 1 [27]. Simple analytical formulas are developed for CNT-based nanoresonators with attached mass and simple linear approximation of the nonlinear sensor equation has been investigated by Chowdhury et al. [28]. Two types of sensor configurations, namely, cantilevered and bridged, have been used. Explicit closed-form expressions of the sensitivities of the BNNT sensors have been resulting using the continuum-beam theory [29].

This paper deals with modeling the surface deviations in the double wall carbon nanotubes when used as a mass sensing device considering a cantilever and bridged elastic beam and analyzing the vibration responses of straight and curved DWCNT with attached masses. The surface characteristic of the carbon nanotubes is modeled as a sinusoidal curvature with small rise function. Apparently, Fig. 2 shows the experimental results of Zhang et al. [13] from which it is quite clear that CNTs do not possess the same wavy thickness throughout their length. Hence a constant curvature or radius model may give uniform thickness in terms of curvature throughout the length which may lead to some what inaccurate results. To model the actual curvature ratio a half sine wave model was selected which better represents the non-uniform thickness. The results showed the sensitivity of the DWCNTs having different curvature to mass (attached to tip of cantilever and center of bridged DWCNTs) and different length.

2. Modeling a DWCNT based nano resonator with surface deviation

It is difficult to model an actual experimental size DWCNT along with the curvature with varying thickness using a space frame model because of the huge number of elements and nodes required, but the Finite Element (FE) continuum model, if benchmarked properly, can solve that problem. The FE continuum model treats the DWCNT as a solid, continuous two thin-walled cylinder. Elemental level properties used in the FE models are the effective continuum properties, and depend upon the type of FE model used for benchmarking. While benchmarking against the results of Li and Chou's molecular structural mechanics approach [30], effective continuum properties $E = 1.1$ TPa, $t = 0.3$ nm, and $\rho = 1.3$ g/cm^3 are used. Effective continuum properties used for other standard cases have been extracted from Joshi et al. [25].

For utilizing the finite element procedure potential energy is used to evaluate linear spring stiffness. The total force is the sum

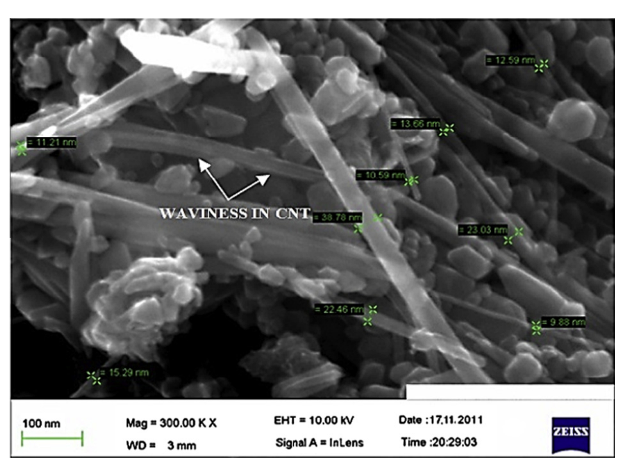

Fig. 1. Scanning Electron Microscope images of CNT indicating the waviness [27].