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Cantilevered single walled boron nitride nanotube based nanomechanical resonators of zigzag and armchair forms

Mitesh B. Panchal *, S.H. Upadhyay

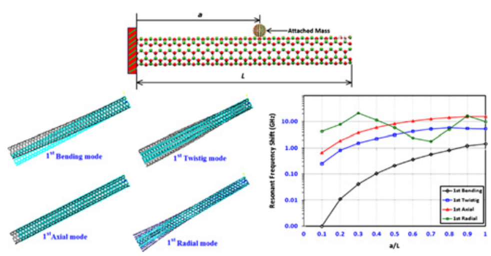
Vibration and Noise Control Laboratory, Mechanical and Industrial Engineering Department, Indian Institute of Technology Roorkee, Roorkee 247667, Uttarakhand, India

HIGHLIGHTS

- ▸ SWBNNT of zigzag and armchair forms are modeled as molecular structural mechanics based FE model.
- ▸ Resonant frequency variations to attached mass is analyzed for mass sensitivity analysis.
- ▸ Higher order modes are explored for detection of added mass and its location identification.
- ▸ Mass sensitivity analysis in terms of different atomic structures of SWBNNT is performed.

GRAPHICAL ABSTRACT

Dynamic response analysis of cantilevered Single Walled Boron Nitride Nanotubes (SWBNNTs), is reported using molecular structural mechanics based 3-dimensional atomistic model for intermediate landing position of the added mass.



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ABSTRACT

In this paper, the dynamic response analysis of single walled boron nitride nanotubes (SWBNNTs) has been done using a finite element method (FEM). To this end, different types of zigzag and armchair layups of SWBNNTs are considered with cantilever configuration to analyze the mass detection application, as a SWBNNT based nanomechanical resonator. Using three dimensional elastic beams and point masses, single walled boron nitride nanotubes are approximated as atomistic finite element models. Implementing the finite element simulation approach, the resonant frequency of cantilevered nanotubes obtained and observed the shifts in it mainly due to an additional nanoscale mass to the nanotube tip. The effect on resonant frequency shift due to dimensional variation in terms of length as well as diameter is explored by considering different aspect ratios of nanotubes. The effect of intermediate landing positions of added mass on resonant frequency shift is also analyzed by considering excitations of different modes of vibration. Also, the effect of chiralities compared for resonant frequency variations to check the effect on sensitivity due to different forms of SWBNNTs. The present approach is found to be effectual in terms of dealing different chiralities, boundary conditions and consideration of added mass to analyze the dynamic behavior of cantilevered SWBNNT based nanomechanical resonators. The simulation results are compared with the analytical results based on continuum mechanics and found in good agreement as one of the toolkits for systematic analysis approach for novel design of SWBNNT based nanomechanical resonators for wide range of applications.

1. Introduction

The atomic resolution characterizations and synthesis of nanoscale one dimensional structures such as carbon nanotubes [1] and boron nitride (BN) nanotubes [2] have actuated great interest, due to their novel properties and potential applications in nanodevices [3–8]. A Boron Nitride Nanotube (BNNT) is a

* Corresponding author. Tel.: +91 1332 285520; fax: +91 1332 285665.
E-mail addresses: miteshbpanchal77@gmail.com, mitesaumya@gmail.com (M.B. Panchal), upadhyaysanjayh@yahoo.com (S.H. Upadhyay).

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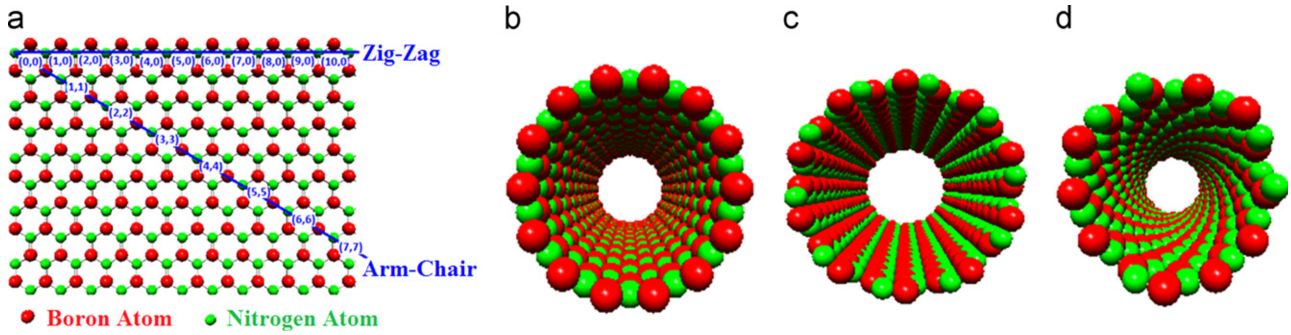

Fig. 1. (a) Plane BN sheet with possible wrapping of zigzag and armchair chiralities and structural models of single walled BNNTs made of a wrapped BN layer: (b) zigzag (c) armchair and (d) chiral.

structural analog of a Carbon Nanotube (CNT) in nature: [1,9] alternating B and N atoms entirely substitute for C atoms in graphitic like sheet with almost no change in atomic spacing (Fig. 1). Similar to carbon nanotubes (CNTs), BNNTs may layups in zigzag, armchair and chiral formation and crystallize in single walled nanotube (SWNT) and multi walled nanotube (MWNT). Such BNNTs possess many of the superior properties of the CNTs [10] such as exceptional elastic properties [11–15], high mechanical strength [16–19], chemical inertness [20] and structural stability [21], high heat conduction and piezoelectricity [22]. In addition, BNNT has a wide band-gap independent of geometrical/atomic configuration. These factors make BNNT particularly suitable for biological applications [23].

Chopra and Zettl, [19] reported mechanical measurement of BNNTs, where the amplitude of thermally induced vibration of a cantilevered BNNT was examined at room temperature inside TEM and the elastic modulus of a single BNNT was estimated to be 1.22 ± 0.24 TPa. Ciofani et al. [24] exploited the use of BNNTs in the nanomedicine field and reported that BNNTs are more suitable for the development of sensors and transducers for the detection of biological entities, due to their chemical stability. In the later study, Ciofani et al. [25] highlighted that BNNT based nanomaterials requires further experiments for the accurate assessment of their biocompatibility.

The past few years have witnessed the growth of nanotechnology that enables the development of nanoscale functional devices designed for specific aims such as nanoscale actuation, sensing and detection [26–28]. Among MEMs/NEMs devices, nanomechanical resonators have been recently highlighted for their unprecedented dynamic characteristics as they can easily reach ultra-high frequency (UHF) and/or very-high frequency (VHF) dynamic behavior up to Giga Hertz regimes [28–31]. The top-drawer performance of nanomechanical resonators for sensing applications is highly correlated with their dynamic characteristics [32–34]. Dynamic response analysis due to additional mass is important as a mass sensor application, but for effective design of nanomechanical resonator it is more significant to consider the weight and landing position of the additional mass along the length of nanotube [35].

Several literatures are available addressing the estimation of mechanical properties of boron nitride nanotubes (BNNTs) considering experimentations and numerical analysis [19,36–39]. Moon and Hwang [40] have investigated the optimized structure of BN nanotubes, based on Universal force field (UFF), and reported structural properties such as bond length (1.432 Å), diameter dilation of smaller nanotubes, buckling of B–N bonds, and strain energy. Chowdhury et al.[41] reported molecular mechanics based model to simulate the optimized structures of SWBNTs and their vibrational behaviors and reported significant impacts on structural instability and electronic properties due to symmetry-breaking. Boldrin et al.[42] reported analytical formulation for the equivalent thickness and in-plane mechanical properties of hexagonal boron nitride (h-BN) nanosheets. Chowdhury and Adhikari [43] use Euler-Bernoulli beam theory to model the bending vibration of single-walled BNNT resonators and validated using the molecular mechanics approach. Jiang and Guo [44] presented an analytical 'stick-spiral' model on the basis of molecular mechanics, for single walled boron nitride nanotubes to investigate their size dependent elastic properties. The present literatures addressing numerical formulations and molecular mechanics approach for the estimation of the mechanical and structural properties of boron nitride nanotubes are not enough considering its wide range of applications. The present work is focused on the atomistic space frame model based analysis of the SWBNNTs. Using this approach different chiralities of SWBNNTs like zig-zag, arm-chair and chiral can be incorporated effectively. Also, different boundary conditions and consideration of added mass in terms of magnitude and location along the length of nanotubes can be efficiently dealt.

Dynamic behavior of cantilevered SWBNNTs based nanomechanical resonators in terms of size of nanotube, atomic structure, and consideration of added mass in terms of magnitude and intermediate position is reported. Two types of nanotubes are considered, namely zig-zag tubes (5,0), (7,0) and (9,0) whose diameter increases from 0.3997 to 0.5596 nm and 0.7195 nm, and arm-chair tubes (5,5), (7,7) and (9,9) where the diameter increases from 0.6923 to 0.9693 nm and 1.2462 nm. The atomistic model is developed by the three dimensional elastic beams and point masses in three dimensional spaces. The elastic properties of beam elements are considered based on mechanical characteristics of the BN bond in hexagonal lattice. The masses of B and N atoms are assumed as point masses at the two nodes of the beam element. FEM simulation approach is implemented to analyze the variation in resonant frequency shift against magnitude of added mass at the free-end of nanotube. Both types of considered chiralities are analyzed for different aspect ratios, the analysis carried out to explore the dynamic behavior of cantilevered SWBNNT based nanomechanical resonators in terms variation in length as well as variation in diameter of nanotubes. The attached mass at the free end of nanotube varies from 10^{-2} zg to 10^{5} zg. The effect on resonant frequency shift for fundamental modes of vibration against intermediate position of attached mass along the length of nanotube is analyzed for armchair (5,5) chairality with aspect ratio of 15 and magnitude of attached mass 100 times the average weight of boron and nitrogen atoms (20.6×10^{-3} zg).

2. Mass–resonant frequency relationship for cantilevered nanomechanical resonators

The Euler–Bernoulli beam model gives equation of motion of a free vibration of a beam in the limit of small amplitude governed