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Efficient FEM simulation of static and free vibration behavior of single walled boron nitride nanotubes

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ABSTRACT

This paper describes the static and free vibration behavior of single walled boron nitride nanotubes using a structural mechanics based finite element method. First, depending on the type of nanotube under investigation, its three dimensional nanostructure is developed according to the well-known corresponding positions of boron and nitride atoms as well as boron nitride bonds. Then, appropriate point masses are assigned to the atomic positions of the developed space frame. Next, these point masses are suitably interconnected with two-noded, linear, spring-like, finite elements. In order to simulate effectively the interactions observed between boron and nitride atoms within the nanotube, appropriate potential energy functions are introduced for these finite elements. In this manner, various atomistic models for both armchair and zigzag nanotubes with different aspect ratios are numerically analyzed and their effective elastic modulus as well as their natural frequencies and corresponding mode shapes are obtained. Regarding the free vibration analysis, the computed results reveal bending, breathing and axial modes of vibration depending on the nanotube size and chirality as well as the applied boundary support conditions. The longitudinal stiffness of the boron nitride nanotubes is found also sensitive to their geometric characteristics.

1. Introduction

Boron nitride nanotubes (BNNTs) are similar to carbon nanotubes (CNTs) since they present an equivalent nanostructure. They are hollow cylinders formed by boron (B) and nitrogen (N) atoms, covalently bonded together in hexagonal shapes [1]. In contrast to CNTs, BNNTs have more consistent electrical properties since independently of their type, may be used as semiconductors [2]. Furthermore, BNNTs are almost as strong as CNTs [3] and, thus, their potential use in composites is currently being investigated [4]. It is evident that such strong composites may be useful in aeronautics and other engineering application in which lightweight materials are required.

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There has been a lot of effort in characterizing the mechanical behavior of BNNTs via theoretical studies based on density functional theory (DFT) [5], tight-binding approximation [6], molecular dynamics (MD) [7], continuum mechanics (CM) [8,9] and molecular mechanics (MM) [10]. In addition, several experimental attempts concerning the mechanical characterization of BNNTs may be found in the literature [11–14].

Several interesting and more focused attempts have been made the last few years concerning the study of the vibrational behavior of BNNTs, mainly by using theoretical approaches. Panchal et al. [15]. have investigated the vibration response analysis of single walled BNNTs (SWBNNTs) treated as thin walled tubes, using the finite element method. In a similar effort [16], they have performed dynamic analysis of SWBNNT as resonant nanomechanical sensor, by developing a molecular structural mechanics finite element model based on the use of three dimensional elastic beams and point masses. In a more detailed manner, Panchal and Upadhyay [17] have investigated the vibrational behavior of SWCNTs using finite element based atomistic models for both armchair and zigzag chiralities and different aspect ratios. Chandra et al. [18]. have addressed the length and the temperature-dependent sensitivity of precompressed armchair BNNTs towards their use as sensors by utilizing MD. In a recent attempt, Asari and Ajori [19] have computed the natural frequency of pure single and double walled BNNTs together with carbon and boron nitride double walled hybrid nanotubes and have investigated the effects of geometrical parameters and boundary conditions. In their excellent work, Chowdhury et al. [20]. have captured the unique features of axial, torsional, transverse and radial breathing vibrations for armchair and zigzag SWBNNTs based on MM simulations and CM mechanics theories.

In the present study, the static elastic as well as the free vibration behavior of single walled boron nitride nanotubes (SWBNNTs) is investigated by using an atomistic, structural mechanics, finite element method which utilizes appropriate three dimensional spring-like, line elements and point mass elements to simulate, according to the molecular theory and atomistic structure of the nanotubes, the interatomic force field as well as inertia effects. To the authors' best knowledge, it is the first time that the calculation of static stiffness and the modal analysis of SWBNNTs are numerically conducted by using a spring based structural mechanics approach. The influence of the size, aspect ratio and chirality of the nanotubes on their effective elastic modulus, the natural frequencies and corresponding mode shapes is thoroughly investigated. The impact of the boundary conditions on the free vibration of SWBNNTs is also discussed. The proposed numerical technique is found to be simple, effective and time saving compared with other standard numerical techniques such as molecular dynamics (MD).

2. Analysis method

2.1. Molecular mechanics equations

The potential energy function within a BNNT, by neglecting Van der Waals interactions, may be expressed as follows:

$$U = \sum U_r + \sum U_\theta + \sum U_\tau \tag{1}$$

where U_r represents the energy due to bond stretching, U_θ the energy due to bond angle bending and U_τ the energy due to both dihedral angle and out-of-plane torsion. The simplest harmonic forms of the aforementioned potential energies are:

$$U_r = \frac{1}{2}k_r(\Delta r)^2;\ U_\theta = \frac{1}{2}k_\theta(\Delta\theta)^2;\ U_\tau = \frac{1}{2}k_\tau(\Delta\varphi)^2 \tag{2}$$

Where k_r, k_θ and k_τ are the bond stretching, bond angle bending and bond angle torsion resistance force constants which, at the room temperature, are respectively equal to 486.5 nN nm^{-1}, 0.6952 nN nm rad^{-2} and 0.6255 n N nm rad^{-2} [21]. Similarly, the parameters Δr, $\Delta\theta$ and $\Delta\varphi$ represent the bond length, bond angle bending and bond angle torsion change, respectively.

2.2. Transformed total potential energy

Let us assume the *ijn* nanostructure of Fig. 1, in an equilibrium state. The nanostructure contains three atoms, i.e., two B atoms bonded with one N atom or two N atoms bonded with one B. The centers of these atoms are denoted by *i*, *j* and *n*. The BN bond equilibrium length is taken equal to $r_0 = 0.145$ nm [22]. As shown in Fig. 1, two different local coordinate systems are adopted, i.e., the $(\widehat{x},\ \widehat{y},\ \widehat{z})$ for the analysis of bond stretching interaction and the $(\widehat{x},\ \widehat{y},\ \widehat{z})$ for the analysis of both bond angle bending and bond angle torsion interaction. Notice that $\overline{x}$-axis coincides with *ij* line, $\widehat{x}$-axis coincides with *in* line while $\widehat{y}$-axis lies on *ijn* plane. With respect to these local coordinate systems and by assuming small deformations, the following geometric expressions arise:

$$\Delta r = \Delta\overline{x};\ \Delta\theta = \frac{\sqrt{\left(\Delta\widehat{x}\right)^2 + \left(\Delta\widehat{y}\right)^2}}{r_0};\ \Delta\varphi = \frac{\Delta\widehat{z}}{r_0} \tag{3}$$