Research Article

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Ultrasensitive analysis of SW-BNNT with an extra attached mass

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Abstract: In this article, the ultrasensitive analysis of single-walled boron nitride nanotubes (SW-BNNTs) with an extra attached mass is studied by employing atomistic analysis technique. Numerical examples are carried out for vibration characteristic of SW-BNNT with an extra attached mass. Our results show that the vibration frequencies and magnitudes of SW-BNNT are very sensitive to the extra attached mass. In addition, the influence of length and chirality of SW-BNNT on the vibration frequencies and magnitudes of SW-BNNT with an extra attached mass are also examined in detail. This investigation indicates that SW-BNNTs have a great potential in the field of sensor technology.

Keywords: ultrasensitive analysis, vibration, atomistic simulation, SW-BNNT

1 Introduction

Pure boron nitride nanotubes (BNNTs) were first synthesized in 1994 by Chopra et al. [1]. In recent years, many investigations related to BNNTs have already been carried out [2–12]. The atomic structure of BNNTs is similar to that of the carbon nanotubes (CNTs), and can be regarded as replacements of carbon atoms in CNT by boron and nitrogen atoms. The elastic material properties of multiwalled BNNTs were determined experimentally by Chen et al. [13] in 2004. They also presented that due to the effect of nitrogen and boron atoms, the oxidation resistance of BNNTs is stronger than that of CNTs.

Furthermore, boron nitride structures have high chemical and thermal stability. Therefore, the material superiorities of BNNT make it a potential candidate for many applications.

In the past years, much attention has been paid to the BNNTs' mechanical properties. It is reported that the axial Young's modulus of an individual multiwalled BNNT was about 1.22 ± 0.24 [14]. Li et al. [15] examined the mechanical properties of both single-walled (SW)-BNNTs and CNTs. Serhan et al. [9] presented the impact of electronic properties of defected boron nitride nanotubes with different chiralities. They also found that near the Stone-Wales defect area, the bond angles and lengths of all BNNTs vary significantly. Salavati et al. [16] predicted the piezoelectric coefficients and elastic modulus of BNNTs. Vaccarini et al. [17] investigated axial stiffness, bending, and torsion dynamic behaviors of both BNNTs and CNTs. Ansari et al. [18] studied the buckling properties of SW-BNNTs with different boundary conditions and geometries by using a 3-D FEM model. Jiang and Guo [19] studied the elastic material properties of SW-BNNTs by using a small-scale molecular model. Patra and Batra [20] studied the axial stress wave propagation in BNNTs with different lengths and chiralities under adiabatic conditions. Song et al. [21] examined the stress-strain curves, Young's modulus, and nonlinear bifurcation in BNNTs. They discovered that the diameter and length of the BNNTs have little effect on the mechanical behavior of the BNNTs, but the mechanical behavior of BNNTs is strongly dependent on the helicity. Rezanian and Aghaiimanesh [22] studied the influence of a transverse magnetic field on the electronic properties of both boron nitride monolayer and zigzag nanotubes with Hubbard model at the antiferromagnetic sector.

One potential application of BNNT is serving as highly sensitive nanomechanical resonators and sensors. When there is additional mass attached onto the surface of BNNT, the resonance frequency or surface stress changes of BNNT can be used for defining the sensitivity of BNNT [23,24]. Yan et al. [4] studied the free vibration behaviors of SW-BNNTs using a multiscale simulation approach. They indicated that there is a critical radius for the

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vibration fundamental frequency of BNNTs. Based on non-local piezoelectricity cylindrical shell theory, Ghorbanpour Arani et al. [25] investigated the nonlinear vibration and instability of the embedded double-walled BNNTs conveying viscous fluid. Aydin [26] calculated IR, non-resonance Raman spectra, and vertical electronic transitions of the zigzag single-walled and double-walled BNNTs. Using continuum plate model and molecular dynamics simulation, Yi et al. [27] studied the vibrational behaviors of the single-layered hexagonal boron nitride. Fakrach et al. [28] calculated the Raman spectra of SW-BNNTs based on the force constants model. They discovered that the change in the diameter of the SW-BNNTs will significantly change the modes in the low-frequency region.

It is noteworthy that the generalized continuum mechanics such as nonlocal elasticity theory are suggested to replace the classical continuum mechanics when studying the nanomaterials since scale effect has to be considered. Nevertheless, how to exactly determine the scale parameter is still quite difficult and many literatures are focused on the study of the variation of scale parameter on the mechanical behaviors of nanomaterials [29]. Based on the above literature review, there is little investigation for the ultrasensitive analysis of SW-BNNTs with an extra attached mass. In this work, an atomistic simulation is employed for studying the vibration frequency shifts of cantilevered SW-BNNT with an extra mass attached on the surface at different positions. Different numerical cases are provided to investigate the influence of length and chirality on the vibration frequencies and magnitudes of SW-BNNT.

2 Atomistic simulation for BNNTs

In this investigation, we employ an atomistic simulation for analysis of vibration frequency changes of SW-BNNT with an extra mass attached to the surface at different positions. For the atomic finite element method (AFEM), a system that contains a number of NN boron and nitrogen atoms is considered. In BNNT, there is only covalent bond between B and N atoms, and the energy stored in the B–N bonds is a function of all atoms' positions, which can be expressed as:

$$U_{nb} = U_{nb}(\mathbf{q}_1, \mathbf{q}_2, \dots, \mathbf{q}_N) = \sum_{I < J}^{NA} V_{IJ}(\mathbf{q}_I - \mathbf{q}_J), \quad (1)$$

where $V_{IJ}(\mathbf{q}_I - \mathbf{q}_J)$ and $\mathbf{q}_I$ are the empirical potential and atom positions, respectively. To describe the atomic interaction, here we use the Tersoff-Brenner multi-body interatomic

potential, where the atomic bond energy $V_{IJ}(\mathbf{q}_I - \mathbf{q}_J)$ is related to the atoms outside the bond.

The atomic system potential energy is given as:

$$E_{tot}(\mathbf{q}) = U_{nb}(\mathbf{q}) - \sum_{I=1}^{NA} \bar{\mathbf{F}}_I \cdot \mathbf{q}_I, \quad (2)$$

where $\bar{\mathbf{F}}_I$ denotes the external force on the atom I . The state of the equilibrium configuration is presented as:

$$\frac{\partial E_{tot}(\mathbf{q})}{\partial \mathbf{q}} = 0. \quad (3)$$

By taking the Taylor expansion of $E_{tot}(\mathbf{q})$ around an initial guess of $\mathbf{q}^0 = (\mathbf{q}_1^0, \mathbf{q}_2^0, \dots, \mathbf{q}_{NA}^0)^T$ for the equilibrium state, we can obtain the following equation:

$$E_{tot}(\mathbf{q}) \approx E_{tot}(\mathbf{q}^0) + \left. \frac{\partial E_{tot}(\mathbf{q})}{\partial \mathbf{q}} \right|_{\mathbf{q}=\mathbf{q}^0} \cdot (\mathbf{q} - \mathbf{q}^0) + \frac{1}{2} (\mathbf{q} - \mathbf{q}^0)^T \cdot \left. \frac{\partial^2 E_{tot}(\mathbf{q})}{\partial \mathbf{q} \partial \mathbf{q}} \right|_{\mathbf{q}=\mathbf{q}^0} \cdot (\mathbf{q} - \mathbf{q}^0). \quad (4)$$

Substituting equation (4) in equation (3), we can obtain the following equation for $\Delta \mathbf{q} = (\mathbf{q} - \mathbf{q}^0)$ as:

$$\mathbf{K}_A \Delta \mathbf{q} = \mathbf{P}, \quad (5)$$

where

$$\mathbf{K}_A = \frac{\partial^2 E_{tot}}{\partial \mathbf{q} \partial \mathbf{q}} = \frac{\partial^2 U_{nb}}{\partial \mathbf{q} \partial \mathbf{q}}, \quad (6)$$

$$\mathbf{P} = - \frac{\partial E_{tot}}{\partial \mathbf{q}} = \bar{\mathbf{F}} - \frac{\partial U_{nb}}{\partial \mathbf{q}}, \quad (7)$$

where the external force vector is described by $\bar{\mathbf{F}} = (\bar{\mathbf{F}}_1, \bar{\mathbf{F}}_2, \dots, \bar{\mathbf{F}}_{NA})^T$. By iteratively solving equation (5) using Newton–Raphson method until the nonequilibrium force vector $\mathbf{P}$ reaches zero and the hexagonal boron nitride (h-BN) sheet equilibrium configurations under external loading are achieved. In this model, the atomic-scale finite elements are dependent not only on the atomic structure but also on the atomic interactions.

Here the nonequilibrium force vector and the element stiffness matrix are given by the following equations:

$$\mathbf{P}^{\text{element}} = \begin{bmatrix} \left(\bar{\mathbf{F}}_1 - \frac{\partial U_{tot}}{\partial \mathbf{x}_1} \right)_{3 \times 1} \\ (\mathbf{0})_{27 \times 1} \end{bmatrix}, \quad (8)$$

$$\mathbf{K}^{\text{element}} = \begin{bmatrix} \left(\frac{\partial^2 U_{tot}}{\partial \mathbf{x}_1 \partial \mathbf{x}_1} \right)_{3 \times 3} & \left(\frac{1}{2} \frac{\partial^2 U_{tot}}{\partial \mathbf{x}_1 \partial \mathbf{x}_i} \right)_{3 \times 27} \\ \left(\frac{1}{2} \frac{\partial^2 U_{tot}}{\partial \mathbf{x}_i \partial \mathbf{x}_1} \right)_{27 \times 3} & (\mathbf{0})_{27 \times 27} \end{bmatrix}, \quad (9)$$

where the external force imposed on the central atom is denoted by $\bar{\mathbf{F}}_1$, and i ranges from 2 to 10 in $\frac{\partial^2 U_{tot}}{\partial \mathbf{x}_i \partial \mathbf{x}_1}$ and $\frac{\partial^2 U_{tot}}{\partial \mathbf{x}_1 \partial \mathbf{x}_i}$.

The stored atomic bond energy is a combination of attractive and repulsive pairs, which is described by the widely used Tersoff-Brenner multi-body potential [30]

$$V_B(r_{IJ}) = V_R(r_{IJ}) - B_{IJ}V_A(r_{IJ}), \quad (10)$$

$$V_R(r_{IJ}) = \frac{D^{(e)}}{S-1} e^{-\sqrt{2S}\beta(r_{IJ}-R^{(e)})} f_c(r_{IJ}), \quad (11)$$

$$V_A(r_{IJ}) = \frac{D^{(e)}S}{S-1} e^{-\sqrt{2/S}\beta(r_{IJ}-R^{(e)})} f_c(r_{IJ}), \quad (12)$$

$$B_{IJ} = \left[1 + \sum_{K \neq I, J} G(\theta_{IJK}) f_c(r_{IK}) \right]^{-\delta}, \quad (13)$$

where r_{IJ} is the bond length between atoms I and J and V_R and V_A denote the repulsive and attractive potentials, respectively. Due to atoms I and J located in different environments, Brenner suggested an average value to replace B_{IJ} (a coupling multi-body parameter):

$$\bar{B}_{IJ} = \frac{1}{2}(B_{IJ} + B_{JI}). \quad (14)$$

The angle function $G(\theta_{IJK})$ is given as:

$$G(\theta_{IJK}) = a_0 \left[1 + \frac{c_0^2}{d_0^2} - \frac{c_0^2}{d_0^2 + (1 + \cos(\theta_{IJK}))^2} \right], \quad (15)$$

where θ_{IJK} denotes the angle between bonds $I-K$ and $I-J$.

The cutoff function f_c is presented as:

$$f_c(r) = \begin{cases} 1, & r \leq R^{(1)} \\ \frac{1}{2} \left\{ 1 + \cos \left[\frac{\pi(r - R^{(1)})}{R^{(2)} - R^{(1)}} \right] \right\}, & R^{(1)} \leq r \leq R^{(2)} \\ 0, & r \geq R^{(2)}, \end{cases} \quad (16)$$

in which the valid ranges of the cutoff function are $R^{(1)}$ and $R^{(2)}$. In the present study, the revised values of parameters related to h-BN nanosheets for the Tersoff-Brenner potential are selected from the literature [31].

Based on the AFEM, the governing equation of vibration of SW-BNNT with an extra mass attached on the surface at different positions is given as:

$$\sum_{i=1}^{NN} (m_i \ddot{\mathbf{q}}_i + \mathbf{K}_A \mathbf{q}) = \mathbf{0}, \quad (17)$$

in which m_i is the mass per atom.

Considering the field function $\mathbf{q}(t) = \mathbf{A} \exp(i\omega t)$, the dynamic equation is given as:

$$\sum_{i=1}^{NN} (\mathbf{K}_A \mathbf{x}_0 - \omega^2 m_i \mathbf{q}) = \mathbf{0}. \quad (18)$$

The vibration frequency of SW-BNNTs can be obtained from the solution of equation (18).

Table 1: The average potential per atom for the three kinds of BNNTs with different lengths

BNNT (nm)	Potential per atom (eV)		
	(3,3)	(6,6)	(9,9)
4.05	-6.02086	-6.33045	-6.38814
6.09	-6.03835	-6.35017	-6.40842
8.13	-6.04722	-6.36018	-6.41871

3 Numerical results and discussion

An atomistic simulation is presented to investigate the resonant frequency of cantilevered SW-BNNT with an extra mass attached on the surface at different positions. The AFEM has been used to study the free vibration behaviors of BNNTs by Yan et al. [4]. They also developed a novel multiscale atomistic-continuum approach under the same empirical potential of the present AFEM to fast predict the vibrational behaviors with high consistency, which can be observed from the results shown in Table 1. As the tubular length and radius increasing, the edge dangling bonds and the curvature effect of the BNNTs become smaller and smaller, and the average potential per atom becomes close to that of the semi-analytical result, -6.4979 eV [31,32].

In this investigation, (3,3), (6,6), and (9,9) SW-BNNTs with lengths of 4.05, 6.09, and 8.13 are considered. Figure 1 shows the geometric figure of cantilevered SW-BNNT with an extra mass attached on the surface at the free end. The BNNT atomic structure can be regarded as replacing the carbon atoms by boron and nitrogen atoms, as shown in Figure 2.

Figure 3 depicts the frequency-attached mass curves for cantilevered (3,3), (6,6), and (9,9) SW-BNNTs with the extra mass attached on the surface at the free end. The length of SW-BNNT is 4.05 nm. It can be seen that when the extra mass attached on the surface at the free end is larger than 10^{-21} g, an obvious variation of resonant frequency is observed, which implies that the mass sensitivity for SW-BNNT is at the level of 10^{-21} g. Figure 4 shows the variation of frequency shifts for cantilevered

Figure 1: The geometric diagram of cantilevered SW-BNNT with an extra mass attached on the surface at the free end.

Figure 2: The atomic structure of BNNTs by replacing carbon atoms of CNT by boron and nitrogen atoms.

(3,3), (6,6), and (9,9) SW-BNNTs with the extra mass attached on the surface at the free end. The frequency shift for a cantilevered (3,3) SW-BNNT with the extra mass of 10^{-21} g attached on the surface at the free end is 71.0684 GHz, and those for the (6,6) and (9,9) SW-BNNTs are 157.9924 and 230.7156 GHz, respectively. Since it is easier to detect large frequency change, (9,9) SW-BNNT is more sensitive than (3,3) and (6,6) SW-BNNT. When we change the extra mass attached on the surface at the free end from 10^{-20} to 10^{-21} g, the frequency changes for the (3,3), (6,6), and (9,9) SW-BNNT are 125.1134, 81.5113,

Figure 3: Resonant frequencies for (3,3), (6,6), and (9,9) cantilevered SW-BNNT with length 4.05 nm for different attached masses.

Figure 4: Frequency shifts for (3,3), (6,6), and (9,9) cantilevered SW-BNNT with length 4.05 nm for different attached masses.

and 40.6197 GHz, respectively. Furthermore, when we change the extra mass attached on the surface at the free end from 10^{-21} to 10^{-22} g, the frequency changes for the (3,3), (6,6), and (9,9) SW-BNNT are 36.6987, 30.2546, and 23.711 GHz, respectively. Therefore, it can be concluded that the mass sensitivity for the (9,9) cantilevered SW-BNNT is at the level of 10^{-22} g.

Figures 5 and 6 present the resonant frequencies and frequency changes for (3,3), (6,6), and (9,9) cantilevered SW-BNNT with the extra mass attached on the surface at the free end for length 6.09. It can be seen that the chirality of SW-BNNT has a significant effect on the resonant frequencies. From Figure 6, it can be seen that when the extra mass attached on the surface at the free end is larger than 10^{-20} g, the three frequency change curves are almost parallel. It means that the mass sensitivities of (3,3), (6,6), and (9,9) cantilevered SW-BNNT are the same in this case. Also, it can be found that an increase in the size of the SW-BNNT leads to a slight reduction in the accuracy.

Figures 7 and 8 present the resonant frequencies and frequency changes for (3,3), (6,6), and (9,9) cantilevered SW-BNNT with the extra mass attached on the surface at the free end for length 8.13 nm. Compared with the results of Figures 1–4, similar conclusions can be obtained. For this case, we further studied the high performance of (3,3), (6,6), and (9,9) SW-BNNT in mass detection with

Figure 5: Resonant frequencies for (3,3), (6,6), and (9,9) cantilevered SW-BNNT with length 6.09 nm for different attached masses.

Figure 7: Resonant frequencies for (3,3), (6,6), and (9,9) cantilevered SW-BNNT with length 8.13 nm for different attached masses.

the extra mass attached at arbitrary places on the surface. Here we use symbol a to denote the distance between the attached point and the free end in axial direction, and an

additional geometrical parameter $\xi = \frac{a}{L}$ is introduced, where L is the total length of SW-BNNT. Figures 9 and 10 present the resonant frequencies for (3,3), (6,6), and

Figure 6: Frequency shifts for (3,3), (6,6), and (9,9) cantilevered SW-BNNT with length 6.09 nm for different attached masses.

Figure 8: Frequency shifts for (3,3), (6,6), and (9,9) cantilevered SW-BNNT with length 8.13 nm for different attached masses.

Figure 9: Resonant frequencies for (3,3), (6,6), and (9,9) cantilevered SW-BNNT with length 8.13 nm with mass of 10^{-20} g attached at different locations.

Figure 11: The variations of resonant frequency shift for (3,3), (6,6), and (9,9) cantilevered SW-BNNT with length 8.13 nm with an extra mass of 10^{-20} g versus different attached positions on the surface.

Figure 10: Resonant frequencies for (3,3), (6,6), and (9,9) cantilevered SW-BNNT with length 8.13 nm with mass of 10^{-21} g attached at different locations.

Figure 12: The variations of resonant frequency shift for (3,3), (6,6), and (9,9) cantilevered SW-BNNT with length 8.13 nm with an extra mass of 10^{-21} g versus different attached positions on the surface.

(9,9) cantilevered SW-BNNT with length 8.13 nm with the extra masses of 10^{-20} and 10^{-21} g attached at different locations. Figures 11 and 12 show the frequency changes for (3,3), (6,6), and (9,9) cantilevered SW-BNNT with length 8.13 nm with the extra masses of 10^{-20} and 10^{-21} g attached at different locations. From Figures 11 and 12, it can be seen that the frequency shifts for cantilevered (3,3), (6,6), and (9,9) SW-BNNT-based mass resonators decrease significantly as the value of ξ increases, which reveals that the mass detection sensitivity significantly depend on the location of the extra attached masses. From the frequency change curves for (3,3), (6,6), and (9,9) cantilevered SW-BNNT, we can also conclude that the most sensitive location is the free end of SW-BNNT. Finally, it can also be seen that when the value of additional geometrical parameter $\xi = \frac{a}{L}$ is more than 0.6, the differences of frequency shift for (3,3), (6,6), and (9,9) SW-BNNT become smaller and smaller.

4 Conclusion

In this article, the potential application of cantilevered SW-BNNT for mass detection was studied based on an atomistic simulation. Results show that the frequencies of SW-BNNT with the extra mass attached on the surface are at extremely high level, and when the lengths of SW-BNNT increase, the frequencies decrease quickly. We also found that the effect of length, of SW-BNNT with the extra mass attached on the surface, on the frequency changes proves that the mass sensitivity of SW-BNNT depends on the tube length. The effect of the attached mass position on the frequency shift is also investigated. Our investigation indicates that the most sensitive location is the free end of SW-BNNT.

Conflict of interest: Author states no conflict of interest.

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