Transverse vibration analyses of cantilevered boron nitride nanocones

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The free transverse vibration characteristics of cantilevered boron nitride nanocones (BNNCs) have been systematically investigated by utilising classic molecular dynamics simulations. The natural frequencies of the transverse vibrations of cantilevered BNNCs with different apex angles, cone heights and top radii are achieved by using fast Fourier transformation. The influences of the geometric parameters of the BNNCs on the natural frequencies are extensively investigated based on the established methodology.

1. Introduction: Low dimensional nanostructures have many advantages relating to the mechanical, physical and electronic aspects, and thus they possess great potential for science and engineering applications. Recent research efforts have been directed towards single-layer graphenic nanomaterials [1–3]. The formation and characterisation techniques for carbon-based nanostructures have been extensively explored by using theoretical and experimental methodologies [4–7]. The achieved advanced knowledge paves the way for practical applications of such kinds of graphenic nanostructures.

As one of the isomorphs of the graphenic nanostructures, boron nitride (BN) nanostructures exist in a crystalline form similar to carbon. Thus, a number of single-layer BN nanostructures including white graphenes, BN nanotubes (BNNTs) and BN nanocones (BNNCs) have also been theoretically predicted and/or experimentally synthesised and observed [8–10]. It is found that the BNNTs have a wide bandgap, which does not rely on tube morphology and chirality, and the measured elastic modulus up to 850 GPa, as well as excellent thermal and chemical stability. Therefore extensive research efforts have been directed towards such kinds of BN nanostructures relating to the aspects of mechanical, physical and electronic properties.

The single-layer cone-shaped nanostructures including carbon nanocones (CNCs) and BNNCs are considered as potential candidates for electron field emitters, resonators/mass detectors and high-speed AFM probe tips [11–14]. The BNNCs with different apex angles have been experimentally synthesised and observed using transmission electron microscopy and the electron diffraction technique [15–17]. The electric structures have been investigated using first principles calculations. It is noted that the electronic structures are strongly affected by the non-B–N bonds with the BNNCs. Recently, the formation energy and geometric vacancies of BNNCs with disclination angles of 60° and 120° have been investigated using *ab* initio calculations [18]. The tensile and compressive behaviours of BNNCs have been investigated using molecular dynamics (MD) simulation [19]. The buckling and post-buckling behaviour have been systematically explored. The deformation patterns are extensively investigated to further understand the mechanical properties of such kinds of BNNCs. The effects of the apex angle and the cone height on the buckling pattern, critical buckling load and failure strain are also analysed. These experimental investigations and theoretical studies have established advanced knowledge of such kinds of BNNCs. However, there is no research on the natural frequencies of BNNCs, which is one of the crucial issues to be solved for the potential applications of BNNCs. Thus, it is necessary to conduct investigations on the free vibration behaviour of BNNCs under initial lateral displacement excitation at the top section.

This Letter investigates the free transverse vibration characteristics of BNNCs utilising classic MD simulations. The natural frequencies of the transverse vibrations of the cantilever BNNCs with different apex angles, cone heights and top radii are achieved by using fast Fourier transformation. The influences of the geometric parameters of the BNNCs on the natural frequencies are extensively investigated based on the established methodology.

2. Computational model and methodology: The BNNCs can be formed by rolling up the circular white graphene with certain disclination angles. To form a pristine cone shape without non-B–N bonds, the BNNCs should have a disclination angle of $120°\cdot n$ ($n = 1, 2$), indicating that the corresponding apex angles are 83.6° and 38.9°, respectively. These kinds of BNNCS have already been observed in the experimental synthesis. However, BNNCs with disclination angles of 60° and 300° were also discovered in previous investigations. These BNNCs are generally considered as defective nanocones induced by the non-B–N bonds. In our computational analyses, the BNNCs with apex angles of 19.2°, 38.9° and 60° have been investigated with both closed and open tips.

Fig. 1 shows the schematic diagram of the BNNC with an apex angle of 60°. The B–N bond length is set to 1.45 Å based on the previous work done by Moon and Hwang [20]. To conduct the computational calculations, the entire nanocone has been divided into several layers. The top layer at the upper section is used to apply initial lateral displacement loads, whereas the fixed layer at the bottom section is used to constrain the BNNC by setting the velocity and the force on the atoms to zero. The middle section is the free layer, where the positions and the velocities of the atoms obey Newton's second law. The measuring layer is defined among the free layers to collect the free vibration of the BNNC. The atoms of the fixed layer are not subject to internal forces. However, they provide internal forces to the atoms in the free layer.

In this Letter, the classic MD method is utilised to explore the free transverse vibration characteristics of the BNNCs. The Tersoff-like potential is adopted to model the interactions between the atoms, which is in the form of an interactive empirical bond order potential

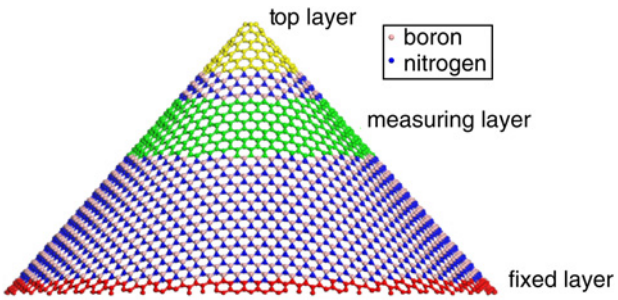

Figure 1 *Schematic diagram of the BNNC with an apex angle of 60°*

[21]. The potential function can be expressed as

$$E = \frac{1}{2}\sum_{i\neq j} V_{ij} = \frac{1}{2}\sum_{i\neq j} f_{\mathrm{C}}\left(r_{ij}\right)\left[f_{\mathrm{R}}\left(r_{ij}\right) + b_{ij} f_{\mathrm{A}}\left(r_{ij}\right)\right] \quad (1)$$

where $f_{\mathrm{C}}, f_{\mathrm{R}}$ and f_{A} are the cutoff function, repulsive pair potential and attractive pair potential, respectively. r_{ij} is the distance between the atoms i and j. b_{ij} is the bond order function. These parameters can be obtained by

$$f_{\mathrm{C}}\left(r_{ij}\right) = \begin{cases} 1 & r_{ij} < R_{ij} - D_{ij} \\ \frac{1}{2} - \frac{1}{2}\sin\left(\frac{\pi}{2}\frac{r_{ij} - R_{ij}}{D_{ij}}\right) & R_{ij} - D_{ij} < r_{ij} < R_{ij} + D_{ij} \\ 0 & r_{ij} > R_{ij} + D_{ij} \end{cases},$$

$$f_{\mathrm{R}}\left(r_{ij}\right) = A\exp\left(-\lambda_1 r_{ij}\right)$$

$$f_{\mathrm{A}}\left(r_{ij}\right) = -B\exp\left(-\lambda_2 r_{ij}\right), \quad b_{ij} = \left(1 + \beta^n \zeta_{ij}^n\right)^{-(1/2n)},$$

$$\zeta_{ij} = \sum_{k\neq i,j} f_{\mathrm{C}}(r_{ik}) g\left(\theta_{ijk}\right) \exp\left[\lambda_3^3\left(r_{ij} - r_{ik}\right)^3\right]$$

$$g\left(\theta_{ijk}\right) = 1 + \frac{c^2}{d^2} - \frac{c^2}{d^2 + (h - \cos\theta)^2}$$

where θ_{ijk} is the bond angle between the bonds ij and ik. These Tersoff-like potential parameters can be achieved by fitting the first principles and the experimental data.

Recently, several Tersoff-like potential parameters have been obtained for BN materials by first principle calculations or the force matching method [9, 22, 23]. These potential parameters can be classified into two categories: one treats the BN as a one component system and develops the uniform potential parameters for both B and N; the other considers the BN as a two component system and calculates the different parameters for B and N. The developed Tersoff-like potentials are used to investigate the mechanical, physical and electrical properties of the single layer BN nanostructures.

In this MD simulation, the parameters for the Tersoff-like potential developed by Liao *et al.* [23] have been used to conduct the computational analyses, and the values of the parameters are listed in Table 1. An microcanonical ensemble (NVE) ensemble is used in the MD simulations of the free vibration of the BNNCs. The NVE ensemble means that the number of molecules, the volume and the energy of the system are kept constant. The system temperature is set at 1 K with the aid of the Nose-Hoover thermostat algorithm to reduce the temperature-induced fluctuation of the atoms. The velocity Verlet algorithm with a time step of 1 fs is utilised to integrate the Hamiltonian equations of motion determined by Newton's second law. Before the lateral displacement load on the top layer is applied, the BNNC is completely relaxed for a certain period under the canonical ensemble (NVT) ensemble to minimise the internal energy and reach an equilibrium state. The NVT ensemble indicates that the number of molecules, the volume and the temperature of the system are kept constant. Then, the

Table 1 Tersoff-like interatomic potential parameters for the BNNCs

A, eV	4570.8	c	1093.28
B, eV	3732.28	$\beta(\times 10^{-7})$	1.1134
λ_1, Å^{-1}	2.99038	d	14.82145
λ_2, Å^{-1}	2.77618	h	−0.6815
λ_3, Å^{-1}	0	R, Å	2.0
n	0.351653	D, Å	0.1

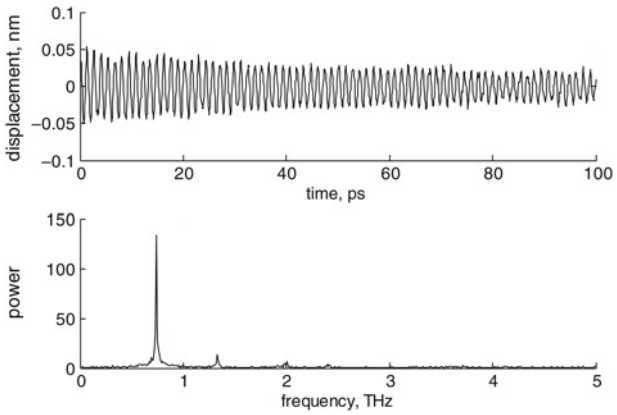

Figure 2 *Free vibration of the BNNC with disclination angle 240° in the time and the frequency domains*

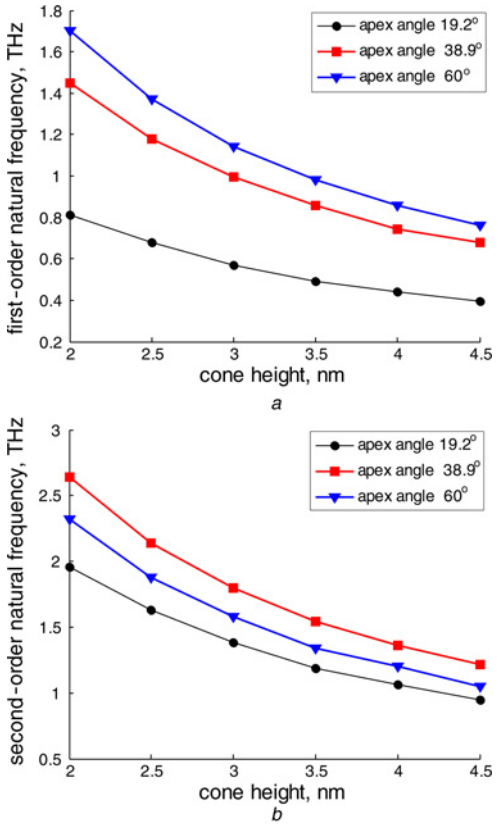

Figure 3 *First two order natural frequencies of the BNNCs with closed tips*
a First-order natural frequencies
b Second-order natural frequencies

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ensemble switches to NVE, and the atoms at the top layer of the BNNC are laterally moved away 0.1 nm from the equilibrium position, and meanwhile the atoms at the fixed layer remain constant. After several times relaxation, the top layer atoms are released and thus the BNNC will undergo free vibration. The moving trajectory of the measuring layer can be recorded during the MD simulations. Based on the obtained vibration signals, the natural frequencies of the BNNC can be obtained using the fast Fourier transform (FFT) technique. In this Letter, only the first two natural frequencies are obtained and analysed.

3. Results and discussion: Based on the developed computational methodology, the MD simulations can be conducted to study the free transverse vibration properties of the BNNCs with different apex angles, cone heights and top radii. Fig. 2 shows the time history of the free vibration of the BNNC and the power spectrum using FFT. It can be seen that the BNNC will oscillate around its equilibrium position with decreased amplitude. The time of the trajectory through the equilibrium position with the same velocity direction is the damping vibration period of the BNNC. However, it is noted that the damping ratio of the BNNC is negligibly small, and thus the damping natural frequency can be considered as the natural frequency of the BNNC. The power spectrum shows the first two natural frequencies, corresponding to the two peaks of the curves. It is demonstrated that the first-order and the second-order natural frequencies of the BNNC are 0.74 and 1.33 THz, respectively.

Fig. 3 shows the first two order natural frequencies of the BNNCs with a closed tip and apex angles of 19.2°, 38.9° and 60°, respectively. It is noted that the first two order natural frequencies of the BNNCs decrease with the increasing of the cone height. This phenomenon is similar with that of the CNCs provided by Hu *et al.* [13], and Firouz-Abadi *et al.* [14]. The apex angle has also significant influence on the first-order natural frequencies of the BNNCs, and the increasing apex angle will increase the first-order natural frequencies, which is in agreement with the result obtained by Hu *et al.* [13]. However, the BNNCs with an apex angle of 38.9° have larger second-order natural frequencies than those with an apex angle of 60° under the same cone height condition. This indicates that the apex change does not affect the mode shapes and the corresponding frequencies linearly and uniformly. It must be pointed out that with the increasing of the cone height, the difference between the natural frequencies becomes smaller.

Fig. 4 shows the computational results of the BNNCS with top radii of 0.77 nm and apex angles of 19.2°, 38.9° and 60°, respectively. It can be seen that the influences of the cone height on the natural frequencies of the open tip BNNCs are similar with those of the closed tip BNNCs. The natural frequencies decrease in the form of the power function with the increasing cone height. The increasing apex angles of the BNNCs will increase the first-order natural frequency of the BNNCs with the same cone height. However, the second-order natural frequencies will decrease with the increasing apex angles. This is different from the phenomenon of the closed tip nanocone. The reason is mainly because of the open tip changing the topography of the nanocone, and this makes the second-order natural frequency decrease with the increasing apex angle.

Fig. 5 shows the natural frequencies of the BNNCs with an apex angle of 19.2° and different top radii. It is noted that the increasing top radii will increase the first-order natural frequencies of the BNNCs with same cone heights. This is because the entire radius of the nanocone with the same height is increased with the increasing top radius, which will increase the lateral bending stiffness. With the increasing of the cone heights, the influence of the top radii on the first-order natural frequencies becomes smaller.

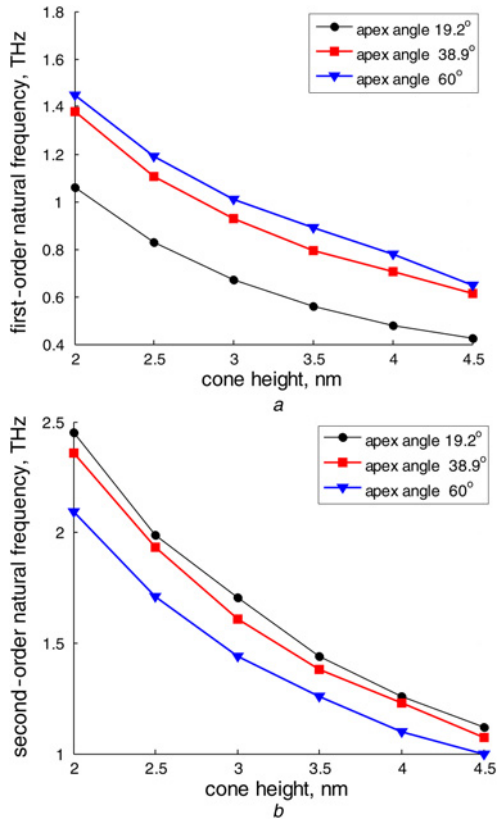

Figure 4 *First two order natural frequencies of the BNNCs with a top radius of 0.77 nm*
a First-order natural frequencies
b Second-order natural frequencies

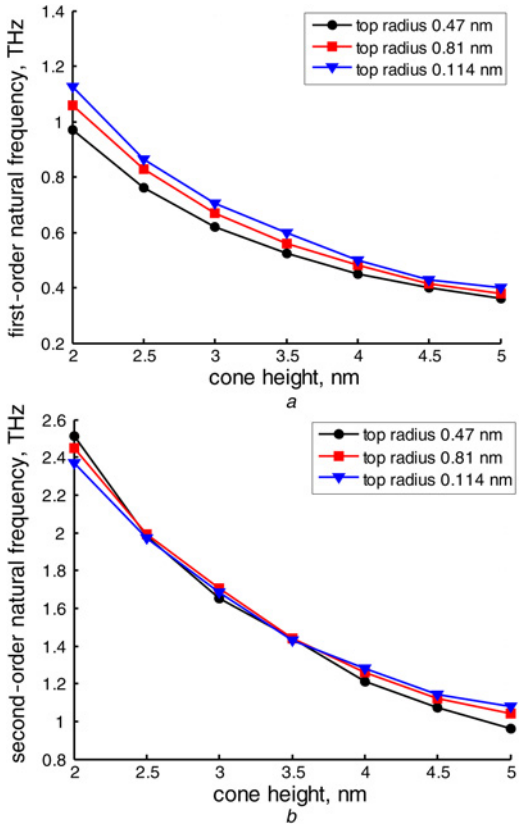

Figure 5 *First two order natural frequencies of the BNNCs with an apex angle of 19.2°*
a First-order
b Second-order

However, the influences of the top radii on the second-order natural frequencies are negligible small.

4. Conclusions: The free transverse vibrations of the BNNCs have been investigated by using MD simulations. The first two order natural frequencies have been obtained based on the time history of the vibrations of the BNNCs and the FFT technique. It is observed that the increasing cone height will exponentially decrease the natural frequencies of the BNNCs with both the open and the closed tips. The first-order natural frequencies of the BNNCs with the same cone heights increase with the increasing apex angles, and the increment becomes smaller with the increasing cone height. However, the influences of the apex angles and the top radii on the second-order natural frequencies are different from those of the first-order natural frequencies.

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