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Beat vibration of hybrid boron nitride-carbon nanotubes – A new avenue to atomic-scale mass sensing

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ABSTRACT

In this paper a beat phenomenon is reported in molecular dynamics simulations for vibrating boron nitride-carbon nanotubes (BN-CNTs) and then analysed based on a continuum mechanics theory. It was shown that the distinctive dynamic behaviour is a result of the superposition of two orthogonal transverse vibrations whose frequencies are slightly different due to the oval cross-section of the hybrid nanotubes. In particular, the interaction between the two vibrations in BN-CNTs will facilitate to resolve the fundamental issue in developing mass nanosensors for atomic-scale mass measuring. To reach this goal, efforts should be made to maintain high quality factor of the BN-CNT oscillating system by minimising the damping effect of its surrounding environment. This issue turns out to be essential for the beat mode-based nanosensors as large damping will reduce the hybrid nanotubes to conventional resonators with only one transverse vibration same as that reported for homogeneous nanotubes.

1. Introduction

In the past decades, superior mechanical and other physical properties of quasi-one-dimensional nanomaterials such as carbon nanotubes (CNTs) and boron nitride nanotubes (BNNTs) have triggered a great deal of interest due to a broad range of their potential engineering applications [1,2]. Among the most promising applications are the nanoresonators with ultra-high frequency and the nanosensors for measuring atomic-scale mass [3–8], which exploit the extreme stiffness [9–12], super high strength [13,14] and relatively low mass density [3] of CNTs and BNNTs, and the sensitivity of their nature frequency to the mass absorbed on the nanotubes [7,8]. Nevertheless, a long-standing issue remains in measuring the mass of a single atom as the frequency shift varies with not only the mass of the atom but also its position on the nanotube [15,16]. To locate the position of the attached atom, one has to resort to additional experimental equipment, such as a scanning electron microscope [17,18] and optical microscope [19]. This will make the measurement much more complicated and time-consuming [18]. Under this circumstance, efforts are required to resolve the issue on the nanotube-based mass sensor by achieving a novel design that enables one to correlate the mass of adsorbate directly to the shift of the frequency. Recently, Gil-Santos et al. [15] confirmed that such a mass sensor can be achieved via a resonator exhibiting two orthogonal vibrations with different frequencies. This indeed provides a new avenue towards the design of a nanotube-based mass sensor.

Obviously, homogenous nanotubes, e.g., CNTs or BNNTs, only vibrate in one transverse direction due to their axisymmetric cross-sections [20–22]. Thus, newly fabricated hybrid nanotubes are expected to provide a solution to the long-standing issue in achieving the nanosensors for measuring atomic-scale mass. Inspired by this idea, the present work is focused on the vibration of boron nitride-carbon nanotubes (BN-CNTs), which are fabricated by doping a BN segment into the CNTs. These novel nanotubes have attracted increasing attention due to their unique physical properties and thus, great potential for the next-generation nanodevices [23–25]. The first-principles calculations and molecular dynamics (MD) simulations were employed to measure the geometric and elastic properties for BN-CNTs [26–29]. The results show that the structural stability of BN-CNTs is similar to their CNT and BNNT counterparts [26] and their Young's modulus is comparable to CNTs and BNNTs [27,28]. Such similarities between BN-CNTs and CNTs/BNNTs suggest that BN-CNTs are also promising for the design of nanoresonators. The vibrations of pristine CNTs and BNNTs have been studied extensively in the past two decades [20–22,30–34]. Different vibration frequencies were obtained for CNTs and BNNTs even with similar geometric size [22]. This observation infers that the frequency of hybrid BN-

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CNTs should change with the vibration (or bending) direction due to the fact that the bending stiffness of the hybrid nanotubes varies with the bending axis. These may lead to two orthogonal vibrations of the hybrid nanotubes with different frequencies as described in Ref. [15]. It is thus of great interest to explore the unique vibrational responses of BN-CNTs.

In this paper, the vibrational behaviours of BN-CNTs were investigated based on MD simulations. A beat phenomenon was observed, which is unique for the vibration of BN-CNTs but is absent from vibrating CNTs and BNNTs. Effort was then invested to reveal the physical mechanisms of the beat phenomena by using the continuum mechanics theory. It is found that such two-dimensional vibration characteristics make BN-CNTs an ideal candidate for the nanosensors for atomic-scale mass sensing. In addition, case studies were carried out to exam the influence of key parameters on the performance of BN-CNTs-based nanoresonators.

2. Simulation method

In the present study, we considered (10, 0) zigzag BN-CNTs with two linear C-B (N) junctions along the tube axis as shown in Fig. 1a. The composition of BN-CNTs is represented by the molar fraction of BN atoms c, which was taken as the ratio of the number of BN atoms to the total number of atoms in the system. Here c was taken as 0.55 and the length L of the nanotubes was assumed to be 100 Å. To conduct the computational calculations, the nanotube was divided into two sections, i.e., (1) the fixed layers at the two ends, where the velocities of and the forces on the atoms were set to be zero, and (2) the free layers at the middle section, where the positions and velocities of atoms obey Newton's second law. Free vibration of such BN-CNTs can be achieved by applying an initial lateral displacement on the free layers. In this study, the classical MD simulations were employed to investigate the transverse vibration characteristics of BN-CNTs. The Tersoff-like potential was adopted to model the interactions between atoms, which is in the form of an interactive empirical bond order potential [35]. The values of the parameters in Tersoff potentials were taken from Refs. [36,37]. Such interatomic interactions in the C-B-N system have been successfully employed to evaluate the mechanical and thermal transport properties of hybrid BN-C nanosheets [38,39] and study the mechanical behaviours of BN-CNTs under static loading [27,28]. These studies showed clear evidence that Tersoff potentials are reliable in measuring the mechanical properties of BN-CNT structures.

In each simulation, a BN-CNT was initially created using the lattice constant of CNTs, and then relaxed to a minimum energy state using the conjugate gradient algorithm. Subsequently, MD simulations were performed on the energy-minimized configuration of the BN-CNT in the following procedure. First, the BN-CNT was relaxed for a certain period (20 ps in this work) to minimize the internal energy and reach an equilibrium state. In doing this, with the aid of the Nosé-Hoover thermostat algorithm [40] the NPT ensemble (constant number of particles, pressure and temperature) was employed to maintain a constant temperature under a pressure of 1 atm. In addition, the velocity Verlet algorithm with the time step of 0.5 fs was utilized to integrate the Hamiltonian equations of motion determined by Newton's second law. The system temperature was set at 1 K to reduce the temperature-induced fluctuation of the atoms. Then the two ends of the nanotube were fixed and a lateral displacement load was applied at the midpoint to deflect the nanotube in transverse direction. In this step, to avoid the crystalline defects normally produced due to a high loading rate a relatively low loading rate of 0.01 Å/ps was used in the simulations. In addition, in this step the nanotube was loaded for 150 ps. As a result, the displacement was less than 2% of the nanotube length and thus the influence of the geometric nonlinearity can be neglected. Finally, upon the removal of this lateral displacement load the vibration of the nanotube started under a constant energy (NVE) ensemble. In the present study, all MD simulations were conducted using a large-scale atomic/molecular massively parallel simulator (LAMMPS) [41] with a periodic boundary condition along the axial direction.

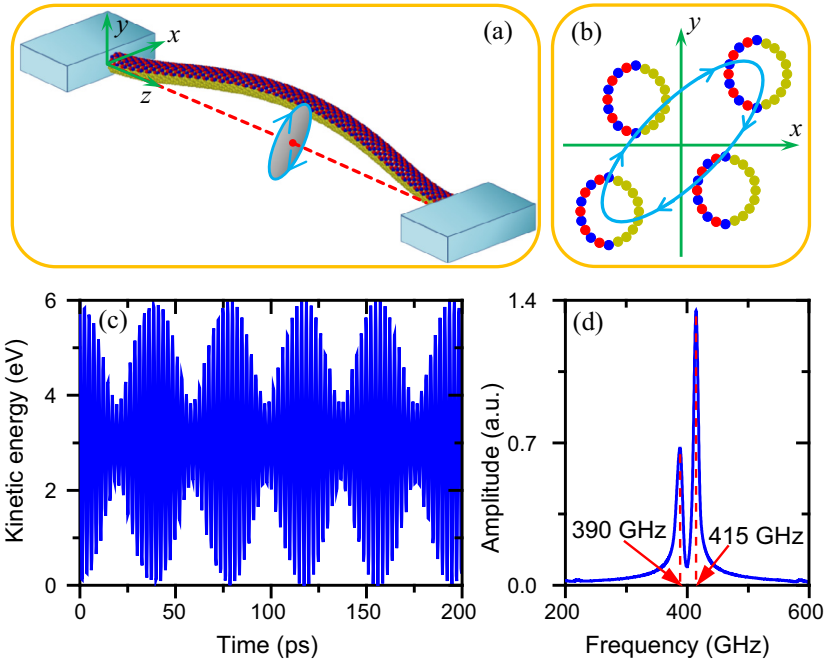

Fig. 1. (a) A schematic showing a vibrating BN-CNT modelling in the present study. Here the carbon atoms are denoted as yellow balls, while the boron and nitrogen atoms are represented by red and blue balls. (b) A typical displacement pattern of the cross-section during the vibration. (c) Kinetic energy time history of the vibrating BN-CNT. (d) Fast Fourier transform of the kinetic energy time history. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

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