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Stress wave propagation in Boron-Nitride nanotubes

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ABSTRACT

The propagation of axial stress waves in Boron-Nitride nanotubes of different chirality and length under adiabatic conditions has been studied using molecular dynamics (MD) simulations. The velocities of the axial stress waves are found using three methods - (i) direct MD simulations, (ii) harmonic approximation of the nanotubes, and (iii) one-dimensional (1-D) wave equation. The MD simulation results indicate a small dependence of the wave velocities on the nanotube chirality and the excitation frequency – in armchair and zigzag nanotubes waves travel faster than that in chiral nanotubes, and wave velocities decrease with an increase in the frequency of excitation. The wave speed obtained from the harmonic approximations is ≈ 20—25% higher than that found from the MD simulations. Likewise, the frequencies of vibrations from the two approaches differ by 15–20% for most of the cases. The computation of the wave speed from 1-D equation requires a prior knowledge of the elastic modulus and the nanotube wall thickness. The values of these parameters are found from MD simulation results – axial tensile tests provide an estimate of the wall thickness scaled elastic modulus and the transverse vibration data relates the standard deviation of the tip displacement with material properties of the nanotube. The wave speed predicted from the 1-D wave equation agrees with that obtained from the MD simulations at low excitation frequencies. The contribution of the anharmonicity to the dynamics during wave propagation is found by matching the response of the anharmonic Fermi-Pasta-Ulam chain with the MD simulation results.

1. Introduction

The discovery of nanotubes, both Boron-Nitride (BNNT) and Carbon (CNT), has been one of the most promising findings in nanotechnology. These nanotubes possess exceptional specific mechanical strength [1,2], chemical properties [3], thermal stability [4] and electronic properties [5]. Experimental investigations with electric field induced resonance [6], X-ray scattering measurements [7] and bending tests using high-resolution transmission electron microscope [8] have revealed that Young's modulus of a BNNT is ≈722 GPa to 1.22 TPa, orders of magnitude higher than that of steel when the mass density is considered.

By using different analytical and simulation tools – classical molecular dynamics (MD) [9–13], ab initio [14] and tight-binding [15] MD, and first principles based study [16], it has been found that the elastic and the shear moduli of BNNTs depend upon their chirality and aspect ratio [17]. The chirality also significantly influences the torsional response of the nanotubes. The MD studies indicate that BNNTs are thermally stable up to ≈3700 K [9]. Thus BNNTs have been used in several interesting applications such as protective shields for nanomaterials [18], adsorption of gases [19], hydrogen storage [20], water purification [21] and nanomechanical sensors [22].

While the aforementioned computational methods are powerful, they require large computational resources. Researchers have, therefore, used structural mechanics and combined finite-element modeling to develop the atomic scale finite-element models (AFEM) [23,24]. Utilizing AFEM, Tao et al. [25] studied elastic properties of BNNTs, and evaluated buckling characteristics and Young's modulus by assuming the wall thickness of 0.34 nm. The stiffness matrix was formed by numerically displacing the atoms from their equilibrium positions. Similarly, Giannopoulos et al. [26,27] investigated the free vibration response of BNNTs and the tensile fracture behavior of Boron-Nitride nanoribbons along with the boundary conditions, the length and the diameter dependence of elastic properties, assuming the wall thickness to be 0.333 nm. Chowdhury et al. [28] used molecular mechanics (MM) simulations for finding optimized structures of BNNTs and their vibrational behaviors. Using the Euler-Bernoulli beam theory and MM, Chowdhury and Adhikari [29] modeled BNNT resonators. Jiang and Guo [30] developed an analytical model using MM to evaluate the size dependent elastic properties of BNNTs. The development of these models has enabled the bridging of scales through

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equivalent continuum structures (ECSs) [31]. However, the understanding of the BNNTs deformations significantly depends on the assumed material properties like the wall thickness and Poisson's ratio [28,32,33]. For example, the wall thickness of the nanotubes has been assumed to vary from 0.065 nm [33] to 0.34 nm [23]. Likewise, the Poisson's ratio varies from being negative [34] to positive [35]. It must be noted that MM and other related techniques do not account for thermal fluctuations present in the nanotube.

Bridging the nano- and the continuum scales in an ECS requires an in-depth analysis of differences in behaviors of the nano- and the continuum models. Here we focus on studying the propagation of axial stress waves in BNNTs. While the propagation of thermal waves has been extensively studied [36,37], only a few studies exist regarding the propagation of stress waves in BNNTs. Stress waves have been found to fracture nanotubes under excessive tensile loadings upon the release of the accumulated elastic energy [38]. In this work, the stress wave propagation results from MD simulations are compared with those obtained from the harmonic approximations (HAs). The method of obtaining the HA equivalent structure is similar to that of the AFEM from the MM. Specifically, the speed of the axial stress waves and the frequencies of vibration are compared to assess the suitability of the HAs in solving nanoscale problems. While the wave speeds through MD simulations show frequency dependence, they are frequency-independent from the HAs. Additionally, the wave speeds and frequencies are found to vary by 15–25%. The contribution of the anharmonicity to the dynamics is ≈20%, obtained by matching the response of an anharmonic Fermi-Pasta-Ulam chain with that from the MD simulations. Results of transverse vibrations and axial tensile tests are utilized to find the wall thickness and the elastic modulus of the BNNTs by handshaking MD results with the vibration properties of a beam. Using these thickness and elastic modulus values, the wave speed obtained from the continuum 1-D wave equation is found to agree well with that from the MD simulations at low excitation frequencies.

2. Simulations and analysis

2.1. Modeling the system

A BNNT may be imagined to be obtained by rolling a hexagonal Boron-Nitride sheet comprised of hexagonal rings in which every Boron atom is covalently bonded to three other Nitrogen atoms (and vice versa), with the nearest BN bond length, $a = 1.4457$ Å [39]. A typical BNNT is characterized by three parameters - the length (l), and the chiral indices (n, m) that determine the rolling direction of the hexagonal sheet. The diameter, D, and the chiral angle, θ, of a nanotube in terms of the chiral indices are given by:

$$D = \frac{a}{\pi} \times \sqrt{3(m^2 + mn + n^2)} \tag{1}$$

$$\theta = \tan^{-1}\left(\frac{\sqrt{3}m}{2n + m}\right) \tag{2}$$

Depending upon values of m and n, one gets three different types of nanotubes: (i) $m = n$ gives an armchair nanotube, (ii) $m = 0, n > 0$ gives a zigzag nanotube, and (iii) $0 < m < n$ gives a chiral nanotube. It is evident that the chiral angle θ is in the range $[0, 30^\circ]$. Nanotubes of 4 different chiralities: $(10,10), (12,8), (15,4)$ and $(17,0)$, and three different lengths, $l = 70$ nm,140 nm and 210 nm, have been investigated in this study. The nanotubes have been chosen such that each has $D \approx 1.38$ nm. The three different lengths help us identify essential features of the stress wave propagation, and the interaction between the incident and the reflected waves. The atoms of an BNNT interact with each other through the three-body Tersoff type potential [40]. Details of the potential function are given in Ref. [41]. Several different Tersoff parameters have been proposed for the Boron-Nitride interactions. Here, values of parameters given by Sevik et al. [41] that have been shown to provide good agreement between experimental and computational results are used.

All MD simulations have been performed by using the open-source software, LAMMPS [42]. The simulation begins with a conjugate gradient energy minimization. The simulation domain is then divided into three regions along the axial (z) direction - the 1 nm long leftmost region, the 1 nm long rightmost region, and the middle region comprised of the rest of the nanotube. Only the rightmost region is kept fixed for the remainder of the simulations. Subsequently, the MD simulations are conducted at the constant temperature of 0.01 K using the Langevin thermostat for 40,000 time steps with an integration time-step of 1.0 fs.

2.2. Computing wave speeds from MD simulations

A stress wave is imposed on the nanotube by axially displacing atoms of the leftmost region in a sinusoidal manner:

$$z(t) = z(0) + 0.5 \sin\left(\omega_f t\right), \tag{3}$$

and the frequency ω_f is varied systematically from 0.5 THz to 5 THz in 10 simulation runs. The boundary conditions imposed at the two end faces of the BNNT are shown in Fig. 1. While atoms on the rightmost boundary are kept fixed, those on the leftmost boundary are allowed to move only in the axial direction. As mentioned above, atoms in the middle region are un-constrained. Furthermore, the Langevin thermostat is removed and simulations are performed at a constant energy ensemble.

The displacement is imposed for 600,000 time steps where each integration time step equals 0.1 fs. In order to compute the wave speeds, we find the distance through which the first peak of the wave propagates since the beginning of the simulation by closely studying snapshots of the wave at 10 different times. If the distance travelled by the wave in time t_k is d_k, then the average wave speed is computed as:

$$\langle c \rangle = \frac{\sum_{k=2}^{10} \frac{d(t_k) - d(t_1)}{t_k - t_1}}{9}. \tag{4}$$

The entire procedure is shown in Fig. 2. Alternatively, the speed may be obtained from the time at which the wave crosses a fixed location of the nanotube [43].

2.3. Wave speed using the harmonic approximations

At very low temperatures, the dynamics of the nanotubes is harmonic [44]. We thus numerically compute the Hessian matrix. As schematically shown in Fig. 3, for the post minimization and equilibration runs, each ring of a nanotube is treated as a single particle with its z-coordinate equal to the axial location of the ring. The boundary conditions considered are the same as those shown in Fig. 1. The distance between two adjacent particles is ≈ 0.125 nm. Thus, for a 70 nm long nanotube there are 560 particles. A particle is first displaced by $\Delta = 0.001$ nm in the positive z direction, and forces on all particles are computed. Similarly, the particle is displaced by $-\Delta$ along the z direction and the resulting forces are obtained. Stiffness terms are then computed using the relation:

$$K_{ij} = -\frac{F_{ij}(\Delta) - F_{ij}(-\Delta)}{2\Delta}, \tag{5}$$

where F_{ij} denotes the force on the equivalent particle j when the particle i is displaced. To ensure real eigenvalues, the matrix $[K]$ is