Superlattices and Microstructures 93 (2016) 18–26

Contents lists available at ScienceDirect

Superlattices and Microstructures

journal homepage: www.elsevier.com/locate/superlattices

Molecular dynamics investigation into the oscillatory behavior of double-walled boron-nitride nanotubes

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ARTICLE INFO

Article history:
Received 23 January 2016
Received in revised form 27 February 2016
Accepted 29 February 2016
Available online 2 March 2016

Keywords:
Boron-nitride nanotube oscillators
Molecular dynamics simulations
Flexibility effect
Frequency of oscillation

ABSTRACT

In this paper, the oscillatory behavior of double-walled boron-nitride nanotubes is investigated based on the molecular dynamics (MD) simulations. The MD simulations are performed using the Lennard-Jones and Tersoff-like potential functions. The influences of friction between the walls of inner and outer tubes, flexibility, velocity and outer length-to-inner length ratio on the frequency of oscillations are studied. The results show that the flexibility increases the frequency during the simulation. Furthermore, it is observed that by increasing the initial velocity, the frequency decreases.

1. Introduction

Multi-walled nanotubes (MWNTs) have attracted a lot of attention in nanotechnology and related sciences. They have appropriate mechanical properties for using in nanodevices [1–3]. Using MWNTs in electro-mechanical devices such as nanoscale engines, data storage devices, surface profiling and so on, led the way to the precision engineering nowadays. After the success of Cumings and Zettl [4] in the exploration of low-friction and low-wear molecular bearings by means of multi-walled carbon nanotubes, Zheng and Jiang [5] found out the oscillatory characteristics of carbon-based nanotubes. It was believed that nanoscale oscillators can improve the science of sensors, actuator, resonators, injectors, motors, memory and switching devices. To this end, intensive studies have been carried out to investigate the various aspects of oscillation of multi-walled nanotubes. Almost all of these studies have been conducted using two main methods, namely continuum approximation approach [6,7] and molecular dynamics (MD) simulation [8,9]. In this respect, Girlfalco et al. [10] applied continuum approximation successfully to different molecular systems. Boawen and Hill [11] employed continuum approximation to determine the van der Waals (vdW) interaction force and oscillation frequency of two single-walled carbon nanotubes (SWCNTs). In addition, the mechanisms of other carbon nanotube (CNT)-based oscillators such as CNT bundles [12,13], CNT-fullerene [14] and CNT-nanotori [15] have been explored in the literature. Also, MD simulations have been employed as a powerful method by different researchers to study the vdW interaction force and oscillatory behavior of nanotube-based oscillators. For instance, Legoas and his coworkers [16] on the basis of MD simulation indicated that the frequency of CNT oscillators is in the GHz range. Those authors by examining CNT with various chiralities found that the frequency and stability of these oscillators are not dependent on the chirality. They also indicated that CNTs with interlayer spacing of 3.4 Å are dynamically stable and can generate frequencies as large as 87 GHz. The damping effect of oscillatory

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http://dx.doi.org/10.1016/j.spmi.2016.02.049
0749-6036/

motion of double-walled carbon nanotube (DWCNT) oscillators was explored by Revera and his associates [17,18] via MD-based models. Liu et al. [19,20] examined the multi-walled carbon nanotube (MWCNT) and fullerene-CNT oscillators based on the MD simulations. Zhang and Li [21] demonstrated a feasible approach to fabricate ultrafast axial nano-oscillators on the basis of carbon nanoscrolls utilizing MD simulations. The oscillatory behavior of a DWCNT with a rotating inner tube was examined by Cai et al. [22] through MD simulations. Further, Ansari et al. [14] examined the mechanisms of a C_{60} fullerene in CNT based on the continuum approximation and MD simulations. In their study, it was shown that the results obtained based on the continuum approximation are in good agreement with those from MD simulations.

In recent years, synthesizing inorganic nanotubes like boron-nitride nanotubes (BNNTs) which have similar properties to carbon ones has attracted considerable interest of researchers. So far, different studies have been performed on BNNTs in order to understand their physical and chemical characteristics [23–27].

A review of recent literature shows that the oscillatory behavior of BNNTs has been studied by a few researchers. Lee [28] utilizing classical molecular dynamics simulations, studied the gigahertz oscillatory behavior of double-walled BNNTs and compared the results with carbon and hybrid carbon @ BN nanotubes. It was found that the frequency of BNNT oscillators is higher than that of similar carbon and hybrid nanotube oscillators. That study had some essential drawbacks which were attributed to the short length of nanotubes as well as the low temperature of simulation. Kang and Hwang [29] carried out a comparative investigation on hybrid (5,5)C@(10,10)BN oscillator and (5,5)C@(10,10)C, and found out that hybrid oscillators have higher frequencies than those of carbon ones. Using a continuum approach, Thamwattana and Hill [30] examined certain fullerene-nanotube bundle oscillators. In addition, they demonstrated similar results for boron-nitride structure oscillators in their study.

In the present article, a comprehensive study on the gigahertz oscillatory behavior of double-walled BNNTs is performed via MD simulations. In order to conduct the MD simulations, the Lennard-Jones and Tersoff-like potential functions are utilized. The effects of different parameters including the friction between the walls of inner and outer tubes, flexibility, velocity and outer length-to-inner length ratio on the frequency of oscillations are investigated. Also, the rocking motion phenomenon is detected.

2. Methodology

The schematic view of a double-walled BNNT oscillator is shown in Fig. 1. The configuration of atomic structure of such oscillator is also indicated in this figure. In Refs. [31–33], Tersoff potential parameters of BN have been reported. Since the potential parameters given in Refs. [32,33] have not been tested for sp^2 structures of BN, they are not suitable to simulate the behavior of BNNTs. Albe and Möller [31] employed a Tersoff-like potential function with appropriate parameters which can accurately model BNNTs with considering the sp^2 structure for BN bonding [34–36]. Hence, the Tersoff-like potential function with parameters reported in Ref. [31] is chosen herein to simulate the BNNTs with sp^2-hybridized boron and nitrogen atoms. The vdW interaction force between the walls of the nanotubes is calculated by employing the Lennard-Jones (LJ) potential function [37] as a non-bonded energy function. Therefore, the total potential energy of system is obtained by summing the Tersoff–like and the LJ potential energies. In order to carry out the simulations, Velocity-Verlet algorithm [38] is employed to solve the Newtonian equations of motion in the basic time step of 1 fs. Nose-Hoover thermostat [39] algorithm is also applied to perform the simulation in the canonical ensemble at the 300 K which results in insignificant fluctuation during temperature stabilization. In the simulations, the nanotubes are considered to be rigid and flexible. To simulate rigid tubes, after initial relaxation of tubes, atom positions in radial direction are not allowed to update in the integration algorithm, but for the flexible ones, atoms are allowed to change their positions during the oscillation. To simulate simply supported-simply supported boundary conditions one ring of atoms in the both sides of nanotubes are held fix.

3. Results and discussion

In this section, numerical results are presented for MD simulations of BN-BN nanotube oscillators. In the simulations, the effect of rigidity and flexibility of BNNTs are examined in details. The (5,5)@(10,10) BNNTs of length 25 Å are generated in the simulations. It is worth mentioning that the chirality does not considerably affect the oscillatory behavior of nanotubes [16]. The BNNT with smaller radius is assumed to be released with no initial velocity in the simulations, unless otherwise stated. It is remarkable to note that only the stable oscillations of BN-BN nanotube oscillators are discussed in this paper. Further, in Figs. 2–9, the length ratio, i.e. the outer tube's length-to-inner tube's length ratio, is set to unity.

Plotted in Fig. 2 is the variation of vdW force in the x and y direction with respect to the simulation time. According to this figure, one can understand that the magnitude of vdW force in the x and y directions is not zero so that the core oscillation is eccentric with respect to the external BNNT. In other words, because in the flexible BNNT oscillator, the radial vdW forces are unbalanced, the eccentricity occurs which causes the inner BNNT to oscillate. It is worth mentioning that in the case of rigid BNNT oscillators, the eccentricity does not occur and the central axis of inner nanotubes coincides with the outer one.

Depicted in Fig. 3 is the eccentricity of the tube axis during the simulation. This eccentricity which is along the x and y directions is due to the existance of small vdW force in these directions. As it can be observed, the eccentricity of nanotube axis increases sharply in the beginning of the simulation in both x and y directions. However, after the peaks of diagrams, the eccentricity of tube axis in both directions remains constant, as the time of simulation gets larger.