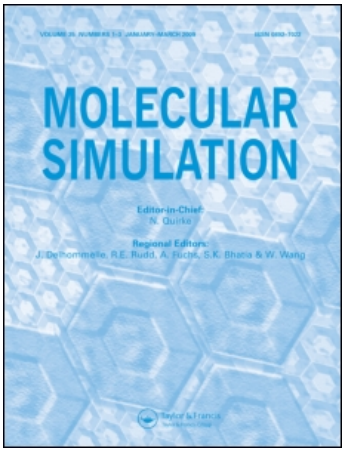

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Neon atoms oscillating inside carbon and boron nitride nanotubes: a fully atomistic molecular dynamics investigation

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Neon atoms oscillating inside carbon and boron nitride nanotubes: a fully atomistic molecular dynamics investigation

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In the present work, based on extensive fully atomistic molecular dynamics simulations, we discuss the dynamics of neon atoms oscillating inside (5,5) single-walled carbon nanotubes (CNTs) and boron nitride nanotubes (BNNTs). Our results show that sustained high-frequency oscillatory regimes are possible for a large range of temperatures. Our results also show that the general features of the oscillations are quite similar to those observed in CNT and BNNT, in contrast with some speculations in previous works in the literature about the importance of broken symmetry and chirality exhibited by BNNTs.

Keywords: nanotubes; nano-oscillator; molecular dynamics

1. Introduction

Since the pioneering work of Cumings and Zettl [1], carbon nanotube (CNT)-based oscillators have become the object of many theoretical works. Cumings and Zettl demonstrated the controlled and reversible telescopic extension of multiwalled CNTs, thus realising ultra low-friction nanoscale linear bearing. Zheng and collaborators [2,3] proposed that this phenomenon could be exploited to build nano-oscillators in the frequency range of gigahertz. Legoas et al. [4,5] carried out molecular dynamics (MD) simulations and concluded that sustained oscillations are possible when the radii difference between inner and outer oscillator moving parts is about $\simeq 3.4$ Å. Frequencies as high as 40 GHz are possible and even clear chaotic signatures were observed [6]. Rivera et al. [7] studied the behaviour of oscillator damping via MD, and they showed that the damping depends on the inverse of the CNT length, which is in good agreement with the predictions of analytical models [2,3]. They also showed [8] that the frequencies (GHz) decrease as the length of the tubes increases. Zhao et al. [9] studied the oscillator energy dissipation energy mechanism, also using MD simulations. They demonstrated the importance of the overlap length of double CNTs and the mechanical deformation of the outmost CNT to this mechanism. In spite of the intense investigation of CNT-based oscillators, some aspects remain not well understood, especially in relation to friction mechanisms [10–12]. In this sense, it is important to study other related systems, such as oscillators made of different materials and also atoms and molecules oscillating inside the tubes. Only very few studies have been reported along these lines: oscillators composed of boron nitride nanotubes (BNNTs) [13], BNNTs in association with CNT ones [14], C_{60} molecules [15,16] and rare-gas atoms [17–20] inside CNTs. The choice for using rare-gas atoms is associated with their inert nature which prevents chemical reactions (bond formation with the tubes). It has been demonstrated [17,18] that sustained oscillations are possible for a large range of energy variations and also, in some circumstances, the tube chirality is important to determine the oscillatory patterns. However, there are conflicting data for the behaviour of the oscillator frequency decaying with the tube diameter. Further studies are thus necessary to better understand these aspects. Recently, Zhao and Cummings [21] have shown that, for constant energy and low temperatures, a double-walled CNT could have a sustained oscillation, which is consistent with our results for Ne atom oscillations obtained here. In the present work, we report extensive fully atomistic MD simulations for the study of Ne atoms oscillating inside (5,5)CNTs and (5,5)BNNTs. To our knowledge, this is the first study of rare-gas atoms oscillating inside BNNTs.

2. Methodology

We have carried out MD simulations using the universal force field [22,23], as implemented in the *Cerius2* package (*Cerius2* is a suite of simulation programs available from Accelrys, http://www.accelrys.com). This force field includes van der Waals, bond stretch, bond angle bend, inversion, torsion and rotation terms. It has been used with success in the study of dynamical properties of carbon-based nanostructures [4,5,24–26]. Initially, we perform a

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Table 1. Calculated frequencies (GHz) for a Ne atom inside a (5,5) CNT.

	Temperature (K)						
CNT (Å)	5	10	20	40	80	160	240
25	136.71	136.71	136.71	136.71	136.71	136.71	117.18
50	78.12	78.12	78.12	78.12	78.12	58.59	58.59

molecular mechanics energy minimisation to optimise the geometry of each isolated nanotube. Then, a Ne atom is placed about 1 Å from the nanotube ends and the dynamical simulations are carried out.

For all the simulations, we have used a microcanonical ensemble (NVE). We have considered different energy values, defined through different initial kinetic energy values (corresponding to temperatures of 5, 10, 20, 40, 80, 160, 240 and 300 K). We have used an integration step of 1 fs. In order to avoid spurious results as a consequence of fluctuations, initial runs of 200 ps were carried out, followed by runs of 50 ps, where the magnitudes to be investigated were averaged. From the trajectory data, we perform a fast Fourier transform analysis to obtain the oscillatory frequencies. In order to investigate the frequency dependence on the tube lengths, we have considered tubes of 25 and 50 Å. The (5,5) nanotubes were chosen because they present the minimum diameter that allows the Ne atom encapsulation. Also, this particular chirality implies fewer atoms in the unit cells, which substantially reduces the computational cost of the simulations.

3. Results and discussion

In Table 1, we present the calculated oscillatory frequencies for a Ne atom inside a CNT, for temperatures from 5 up to 240 K. For 300 K, we observed that the Ne atom is not encapsulated. In our simulations, all the atoms of the nanotube are free to vibrate and, with the increase in temperature, the amplitude of vibrations of the atoms at the ends of the tube increases. These large amplitude movements create a dynamical barrier that, due to the van der Waals interactions, prevents the Ne atom encapsulation. As can be seen from Table 1, stable frequencies are possible for a large range of temperatures. For the 25 Å CNT, from 5 up to 240 K, the frequencies are 136.71 GHz and then they drop to 117.18 GHz. For the longer tube (50 Å), as expected, this occurs at lower temperature (160 K), the frequencies drop from 78.12 to 58.59 GHz. This sustained oscillatory regime is better visualised in Figures 1 and 2. These results are consistent with the ones obtained by Zeng et al. [18] in spite of their different protocol simulations. They used an impulse dynamics that can be mapped into our NVE simulations varying the

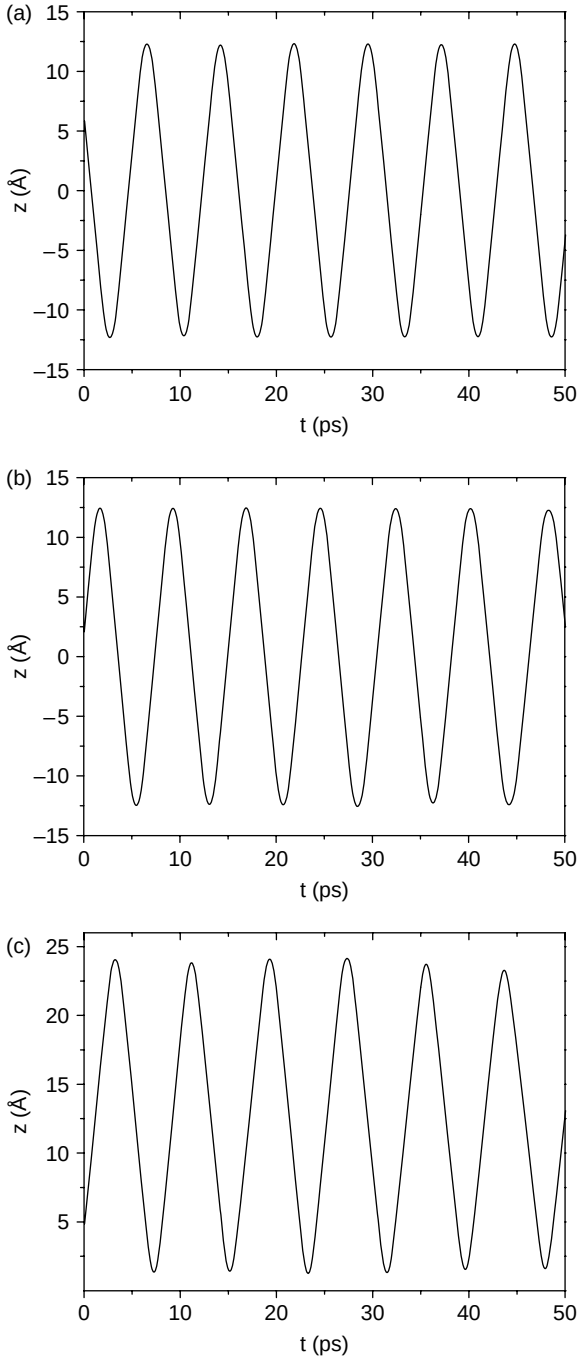

Figure 1. MD simulation results for Ne atom oscillations inside a CNT of 25 Å length for the following temperatures: (a) 80 K, (b) 160 K and (c) 240 K.

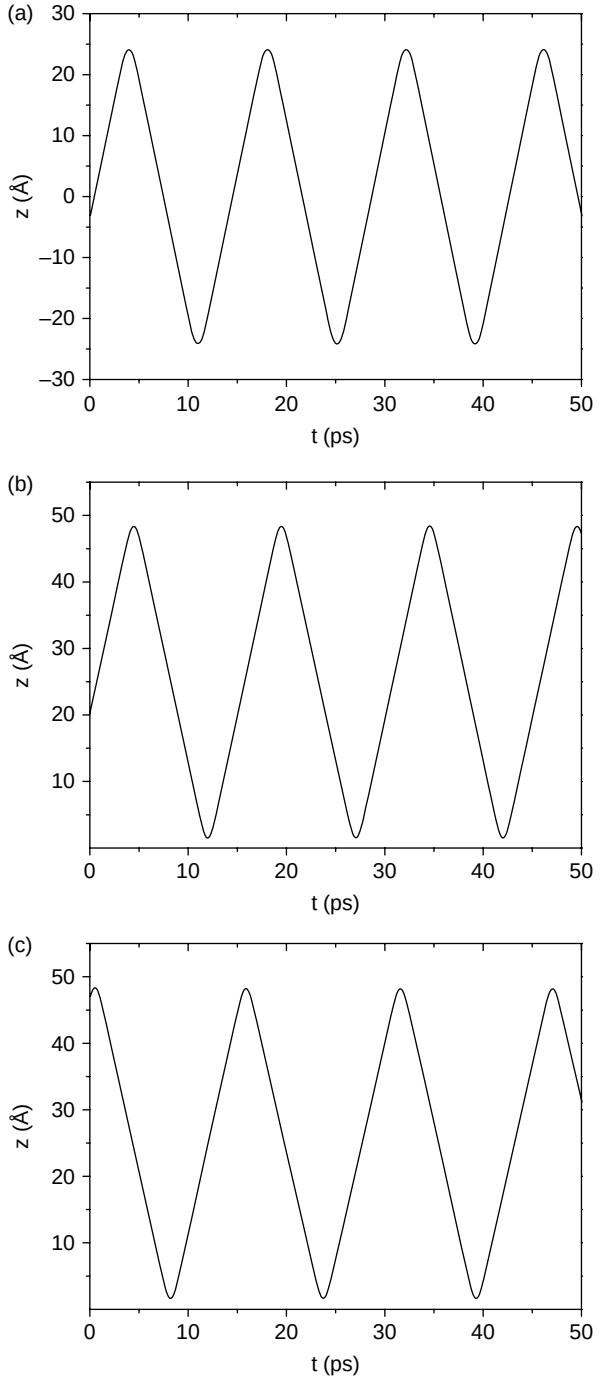

Figure 2. MD simulation results for Ne atom oscillations inside a CNT of 50 Å length for the following temperatures: (a) 80 K, (b) 160 K and (c) 240 K.

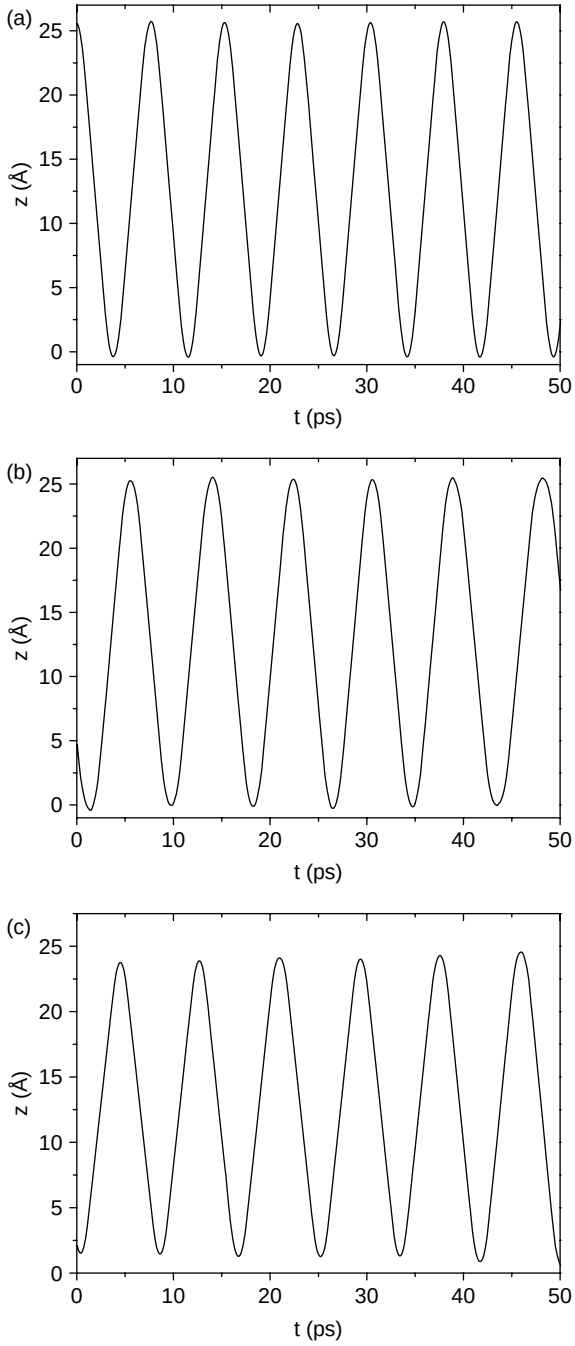

Figure 3. MD simulation results for Ne atom oscillations inside a BNNT of 25 Å length for the following temperatures: (a) 80 K, (b) 160 K and (c) 240 K.

initial conditions with respect to the temperature of simulations.

In Table 2, we present the equivalent results for the case of a Ne atom inside a (5,5)BNNT. Again, for the cases investigated, the temperatures at which the Ne atom is not encapsulated was 300 K for the tube of 25 Å, and 240 and 300 K for the tube of 50 Å. We believe that this occurs for the same reasons (large end atom tube movements creating a dynamic barrier) as in the case of the CNT. The lower temperature in the BNNT case can be attributed in part to different symmetries (i.e. B and N atoms are located in a slightly different diameter position) and also due to the small diameter differences between the CNT (6.8 Å) and

Table 2. Calculated frequencies (GHz) for a Ne atom inside a (5,5) single-walled BNNT.

	Temperature (K)						
BNNT (Å)	5	10	20	40	80	160	240
25	136.71	136.71	136.71	136.71	136.71	117.18	117.18
50	78.12	78.12	78.12	78.12	78.12	78.12	–

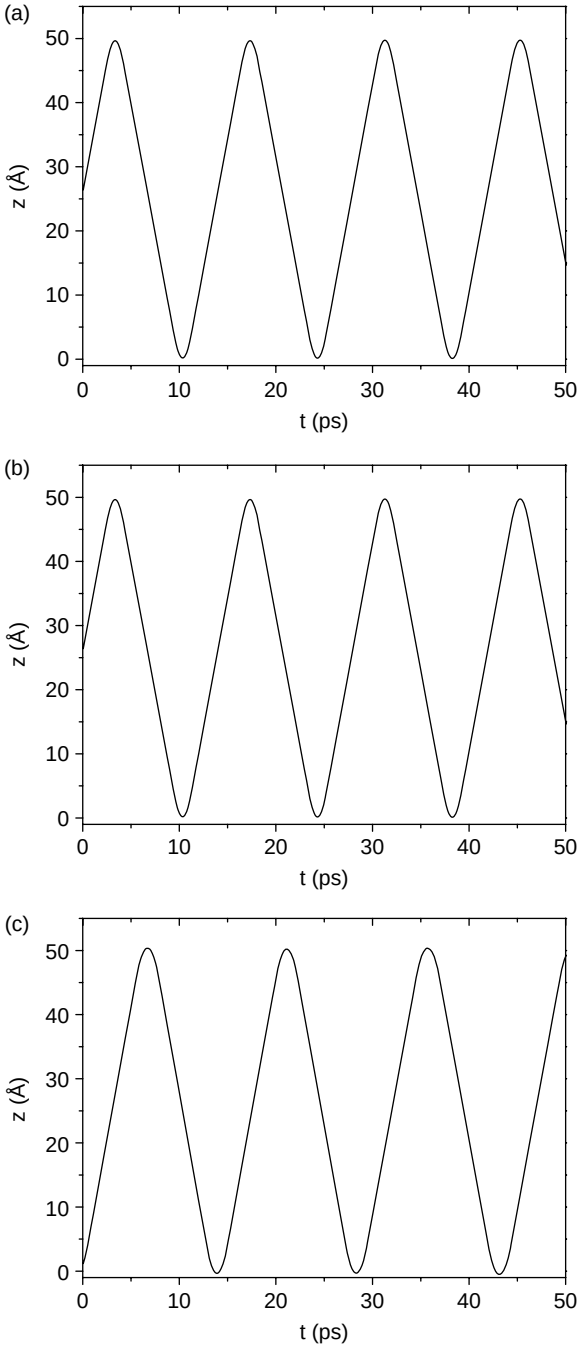

Figure 4. MD simulation results for Ne atom oscillations inside a BNNT of 50 Å length for the following temperatures: (a) 40 K, (b) 80 K and (c) 160 K.

the BNNT (6.9 Å). We expect larger fluctuations for tubes of larger lengths due to mass differences.

Again, as observed for the CNT case, sustained oscillatory regimes are possible for a large range of temperatures, and almost at the same frequency values. The only major differences occurring are the temperature at which we observe dropping frequency values and the absence of encapsulation at 240 K for the BNNT of 50 Å. However, the major point is that, in contrast to some previous speculations [17] for the systems investigated here, the symmetry breaking and chirality of the BNNT do not seem to play important roles in determining the oscillatory regimes. The general oscillatory behaviour (Figures 3 and 4), frequency values and axial displacement movements (Figure 5) are quite similar to those observed in the CNT. Similarly to the case of double-walled CNT oscillators [21], we observed that the frequency can be temperature independent (Table 1). However, if the temperature is increased above a certain limit, the thermally activated 'breathing mode' of the nanotube can create a 'scattering' potential that reduces the net atom velocities and, consequently, its oscillatory frequency.

In summary, we have carried out a detailed analysis of extensive fully atomistic MD simulations for Ne atoms oscillating inside (5,5)CNTs and (5,5)BNNTs of different lengths (25 and 50 Å) and at different temperatures. Our results show that well-defined sustained oscillatory regimes are possible for a large range of temperatures (from 5 up to 240 K). There are several stable frequencies for the nano-oscillator configuration studied here, ranging from 58 to 137 GHz. Another interesting aspect of these

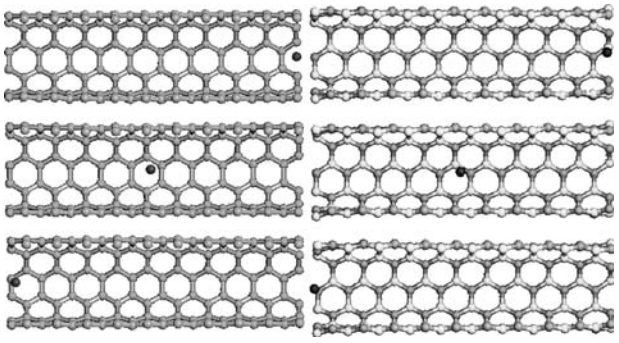

Figure 5. Snapshots from the MD simulations. Left: Ne atom oscillating inside a CNT of 25 Å length for the temperature of 160 K. Right: Ne atom oscillating inside a BNNT of the same length and at the same temperature.

nanostructures is that we can tune the frequency by a suitable modification of the nanotube length and/or type. Our results showed that the results for the BNNT are quite similar to the CNT ones in terms of general oscillatory behaviour, frequency values and axial displacement movements. In this sense, our results are closer to those obtained by Zeng et al. [18] and in disagreement with the ones obtained by Lin and Su [17].

Acknowledgements

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