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MOLECULAR DYNAMICS SIMULATIONS OF CARBON NANOTUBE-BASED OSCILLATORS HAVING TOPOLOGICAL DEFECTS

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Effect of vacancy and Stone–Wales defects on the oscillatory behavior of (5,5)/(10,10) carbon nanotube-based oscillator are studied using NVE molecular dynamics simulations. Results show that defects reduce stability of the oscillators. Effect of single vacancy defect on stability is very small, whereas Stone–Wales defect considerably reduces the stability thereby damping the oscillations quickly. Further increase in density of vacancy defects causes a monotonic decrease of stability of oscillator. In all cases the initial temperature (1 and 300 K) had almost no effect on the oscillation stability.

Keywords: Carbon nanotube; oscillator; molecular dynamics; defect.

1. Introduction

There is a growing interest in the development of carbon nanotube (CNT)-based mechanical systems. Recently, fabrication of CNT-based oscillators has been realized by John Cumings and Zettl[1] who observed extremely low-friction oscillations between the walls of multiwalled CNT. CNT oscillators have been proposed in various applications viz. actuators,[2] surface profiling devices,[3] nonvolatile memory devices,[4] and inertial measurement systems.[5] Legoas *et al.*[6] were the first to simulate CNT-based oscillator using molecular dynamics (MD). They observed the oscillator frequencies to be as large as 38 GHz and predicted that the difference between outer and inner wall radii in order to have sustained oscillations should be around 0.34 nm. The energy dissipation in double-walled CNT oscillators was studied by Guo *et al.*[7] using NVE MD simulations.

Any nonhexagonal ring structures present in the CNT hexagonal structure can be regarded as a defect. Stone–Wales (SW) defects and vacancies are common topological defects present on the nanotube.[8,9] The manufacturing process itself may introduce the defects; defects may also occur while manipulating the tubes with the tips of positioning instruments. Creating and healing/annealing of defects at selective locations is possible using the electron irradiation.[10] Presence of a defect on the CNT surface can change the local energy profile thereby altering various properties. There are few studies of CNT oscillators having topological defects. The effect of single SW defect (grooving) on the oscillatory behavior of double-walled CNT oscillators was studied by Wang *et al.*[11] using MD simulations. They showed a significant reduction in oscillation energy leakage with the presence of a defect on the outer tube which in turn reduces the

frictional effects between the sliding nanotubes. They also showed that the effect of grooving reduces as the initial temperature increases. Liu *et al.*[12] studied the oscillation characteristics and instability of double- and triple-walled CNT-based oscillators containing a vacancy or a SW defect using MD simulation. Their study shows that defect-free oscillators exhibit least energy dissipation, thus stable oscillations than that of oscillators with defects which is in contrast with the result of Wang *et al.*[11] They showed a vacancy defect creates more instability than a SW defect. The change in potential energy profile due to the defect creates a complicated force pattern on the oscillating core causing large fluctuations of lateral force and instability in the oscillations. Song *et al.*[13] investigated the effect of radius and vacancy defect on the oscillatory behavior of C60-nanotube oscillators using MD simulations. Their results showed that the energy dissipation is sensitive to the radius and vacancy defect. They found the energy dissipation is mainly through the self-rotation motion and lateral oscillation of C60. They studied various diameters of CNTs, but among all they studied, surprisingly C60-(17,0) nanotube oscillator with vacancy defect is found more stable than that without defect. It is clear that there is ambiguity in the results on the effect of defects on oscillation stability in CNT-based oscillators. Furthermore, there have been no attempts to study the effect of multiple defects.

In this paper, we conducted MD simulations to study the oscillatory characteristics of (5,5)/(10,10) CNT-based oscillator containing single and multiple defects. Results show that single SW defect greatly affected the oscillation stability than single vacancy defect. Further multiple vacancy defects can monotonically decrease the oscillation stability with increased defect density.

2. Method

Interactions among carbon atoms belonging to the same CNT are modeled here by the modified Morse potential,[14] which have been successfully used to study the mechanical properties of CNTs.[15,16] The parameters for the modified Morse potential are given in Ref. 14. The interactions between walls of different CNTs are described by the Lennard−Jones potential using the parameters $\sigma = 3.37\,\text{Å}$, $\varepsilon = 4.2083\,\text{meV}$, and a cut-off radius $r_c = 15\,\text{Å}$ is used. In the present simulation, a double-walled CNT consisting of (5,5) and (10,10) CNTs is used. The capped (5,5) inner SWNT is 3 nm long and is composed of 260 atoms, while the open (10,10) outer SWNT composed of 800 atoms is 4.7 nm long. Initially the whole system is relaxed for 30 ps at constant temperature using Berendsen thermostat.[17] Velocity Verlet integration scheme is used to solve the equations of motion and a time step of 1 fs is used for all the simulations. Vacancy and SW defects are modeled by removing an atom from the CNT's hexagonal network and by rotating a C−C bond by 90 degrees, respectively. To study the effect of size of vacancy defect, we modeled double and triple atom vacancy defects. Effect of multiple vacancy defects with various densities on the outer (10,10) tube is also studied. To model the multiple vacancies, vacancy defects were modeled on the CNT by randomly removing some carbon atoms. A range of inter-defect distances, i.e., 2.9−75.5 nm were reported experimentally[18] for the study of tuning of conductance of CNTs by ion irradiation, and observed that irradiation time is the key parameter which defines the average inter-defect distance. Here we have maintained 7 Å as the minimum radial distance between any two randomly created vacancies. Starting from 0.5%, up to 2% of total atoms were removed in steps of 0.5% to create the vacancy defects. Half of the inner core is telescoped out and released at zero velocity to kick off oscillations. Atoms of two rings at both ends of the outer SWNT are constrained throughout the oscillation period.

3. Results and Discussion

Single vacancy defect, single SW defect, and multiple vacancy defects on the outer CNT atoms are modeled and studied on how they affect the behavior of CNT-based oscillator. Figure 1 illustrates the atomic structure of double-walled CNT-based oscillator considered in our study which is at the start of oscillation. Single vacancy defect is modeled by removing an atom, and the surrounding bonds are

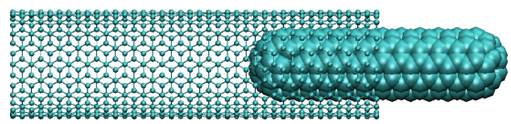
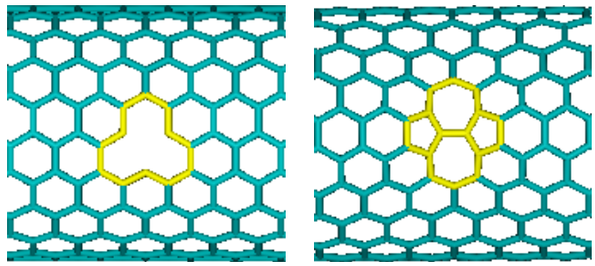


Fig. 1. Double walled CNT oscillator composed of a (5,5) movable inner tube with both ends capped and a (10,10) outer tube is constrained at both end rings.



(a) (b)

Fig. 2. Single defect in outer (10,10) CNT. (a) Vacancy defect (b) SW defect.

illustrated in Fig. 2(a). The configuration of SW defect is produced by rotating a C−C bond by 90° which gives two pairs of pentagons and heptagons as shown in Fig. 2(b).

3.1. *Effect of single defects*

Simulations are conducted to study the oscillation behavior of (5,5)/(10,10) CNT-based oscillator. We first study the oscillator without any defects and the location of the CNT center of mass of the inner CNT is recorded with time. Frequency is found in the range of 40 GHz which is in agreement with earlier studies.[6,7] After this, simulations are conducted for oscillators having single vacancy defect (single atom, double atom and triple atom vacancy). It can be seen that from Fig. 3 the effect of vacancy defect on oscillation is very small and the oscillations last up to the end of simulation period. SW defect considerably affects the oscillations and the oscillator with SW defect failed at around 1 ns of

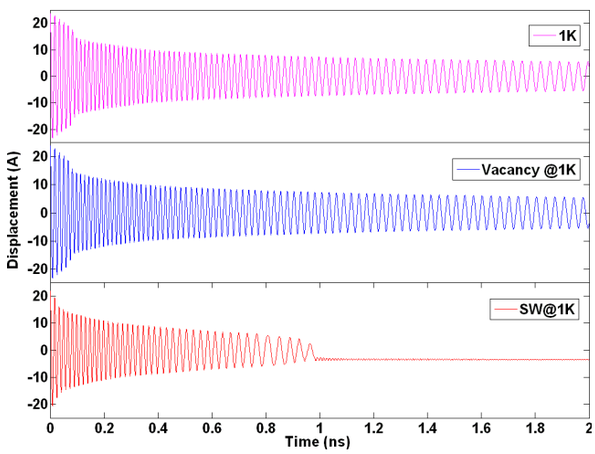


Fig. 3. Comparison of oscillation profiles at 1 K.

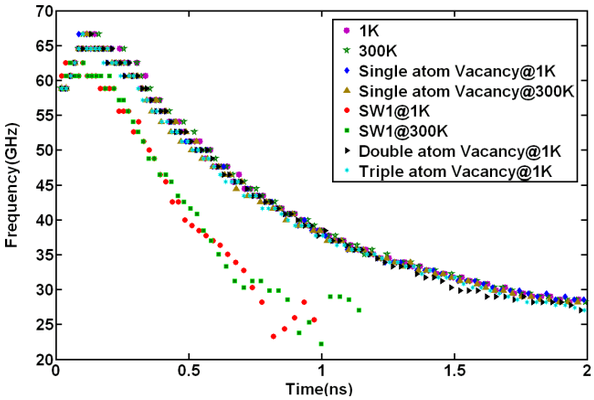


Fig. 4. Frequencies of damped oscillations of all cases with and without single defects.

simulation time. The SW defect causes more damping owing to larger variations in the force field in the axial direction compared to vacancy defect. CNTs with double and triple atom vacancy defects also almost affect in a similar manner to single atom vacancy, which can be seen from Fig. 4.

Another set of simulations is conducted at an initial temperature of 300 K. The effect is the same as that at 1 K except for SW defect case where the oscillations lasts up to 1.2 ns of simulation time. The added thermal effects due to raised initial temperature (300 K) provide a small enhancement in the duration of oscillation.

Frequency of oscillation for each cycle is calculated for all cases and plotted as a function of time as shown in Fig. 4. In all cases average frequencies are found in the range of 40 GHz. Initially frequency in all cases started from around 55 GHz and

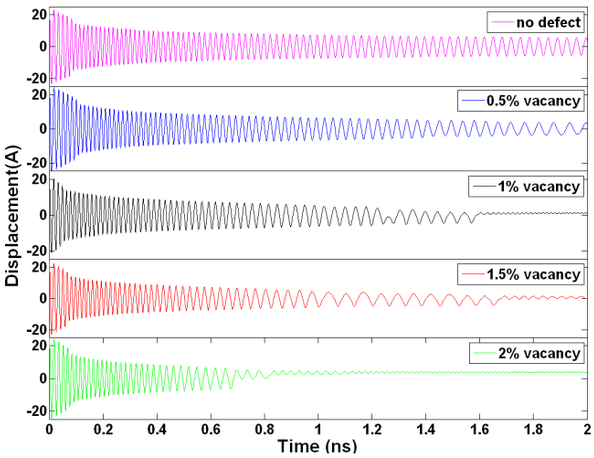


Fig. 5. Comparison of oscillation profiles at 1 K.

Table 1. Values of the damping ratio.

Temp.	No defect	V	SW	0.5%	1%	2%
1K	0.0046	0.00475	0.00761	0.00559	0.00639	0.00861
300K	0.0045	0.00473	0.00779	0.00547	0.00674	0.0084

increased linearly up to 65 GHz in 0.2 ns of simulation time. Afterward the frequencies of oscillator having SW defect decreased more rapidly compared to the oscillator having vacancy defect. As a result of constrained ends of outer CNT where almost all dangling bonds have been constrained, effect of initial temperature on damping of oscillations due to the presence of defects is found insignificant.

3.2. *Effect of multiple vacancy defects*

To study the effect of defect densities on the oscillation stability, we used four cases by creating multiple vacancy defects of densities ranging from 0.5%−2% of carbon atoms on the outer CNT of the oscillator. The oscillation profiles for all the cases are given in Fig. 5 along with the case without any defect for comparison. All these cases are conducted at initial temperature of 1 K and 300 K. From Fig. 5 we can see that the oscillator fails quickly as the density of defects increases. It is also observed that the drop in oscillation frequency becomes sharper as the defect density increases. It seems that more defects on the outer CNT surface cause more friction to the oscillator.

By considering a simplified system of oscillator and using the logarithmic decrement δ of the oscillation amplitude, average damping ratio ζ of the oscillations can be written as

$$\zeta = \frac{1}{\sqrt{1 + \left(\frac{2\pi}{\delta}\right)^2}}\,, \tag{1}$$

where logarithmic decrement

$$\delta = \frac{1}{n}(\ln x_0/x_n)\,. \tag{2}$$

For quantitative comparison of the effect of various defect cases on stability of CNT-based oscillator, Eq. (1) is used to analyze the envelopes of oscillation amplitudes in Figs. 3 and 5. The estimated average values of damping ratio over the period of oscillation for all the cases are shown in Table 1. We can see that at initial temperature of 1 K, the damping ratios, ζ, of the oscillator with single vacancy and single SW defect are around 3% and 65% higher, respectively, than that of oscillator without any defect. Also, at the initial temperature of 300 K, damping ratios are approximately 4% and 71% higher, respectively.

Similarly, oscillators with multiple vacancy defects having up to 2% defect density at initial temperatures of 1 and 300 K have a maximum of 87% and 84% higher damping ratios, respectively, than the oscillators without any defect.

4. Conclusions

In this paper, the role of single vacancy, SW defect, and multiple vacancy defects of various densities in the oscillatory behavior of (5,5)/(10,10) CNT-based oscillator was explored by MD simulation using modified-Morse potential. It was found that the SW defect significantly reduces the stability of the oscillator when compared to the vacancy defect. In case of multiple vacancy defects, as the defect density increases the stability of oscillator decreases monotonically. We found no major distinction at the initial temperatures of 1 and 300 K for all the cases studied.

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