Deformation of Carbon Nanotube Oscillators Encapsulating Cu Nanowires

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ABSTRACT

Pure carbon nanotube (CNT) oscillators are compared to CNT oscillator encapsulating copper nanowire (M@CNT) by molecular dynamics simulations. The excess forces of the Cu@CNT oscillator are slightly higher than that of the CNT oscillator and the excess van der Waals forces induced by the inter-wall interactions are 17 times higher than the excess forces induced by the Cu nanowire-CNT interactions. Since the masses of copper atoms are higher than those of carbon atoms, the carbon atoms are easier accelerated than the copper atoms and the collisions between the inner nanotube and then the encapsulated copper nanowire make a repelling force to decrease the total excess force. Structural deformations of CNT induced by the encapsulated copper nanowire are more important factor than the mass of the copper nanowire for its oscillation frequency.

Keywords: molecular dynamics, carbon nanotube, oscillator

1 INTRODUCTION

After Cumings and Zettl [1] reported an ideal low-friction and low-wear bearing carved out of a multi-walled carbon nanotube (CNT) with a diameter of a few tens of nanometers, gigahertz CNT-based oscillators were proposed by Zheng and Jiang [2]. Nanoelectromechanical devices based on CNTs have been considered for various applications such as precision engineering, electronic devices, medicines, etc. Gigahertz nanotube oscillators may be applied to nanoscale sensors, actuators, resonators, injectors, motors, engines, filters, memory and switching devices. Molecular dynamics (MD) has often been used to study and to predict the performance of nanoscale machine components, and has been applied to investigating multi-walled CNT oscillators [3]. The oscillatory behavior of the multi-walled CNT oscillators can be initialized by precision mechanical controllers [1], and remotely with electromagnetic fields, lasers and electrostatic forces.

The CNTs encapsulating metal nanowires or clusters (M@CNT) have been synthesized and investigated [4]. M@CNT can be also applied to a gigahertz CNT oscillator. CNT encapsulating potassium ions was applied to a gigahertz CNT oscillator initialized by the external electric field [5]. Therefore, in this paper, M@CNT oscillator is investigated using classical MD simulations. The oscillatory behaviors of double-walled CNT oscillators encapsulating copper nanowire are considered, and the mass-dependent frequency change can not be estimated using classical oscillation theory when the encapsulated nanowire deforms the encapsulating CNT.

2 METHODS

To perform MD simulations for double-walled CNT oscillator encapsulating copper nanowire, we used two empirical potential functions. For carbon–carbon interactions, we used the Tersoff–Brenner potential function [6-8] that has been widely applied in carbon systems. The long range interactions of carbon were characterized with the Lennard-Jones 12–6 (LJ12–6) potential with the parameters obtained from Mao *et al.* [9]. The potential parameters were determined from the known experimental values of cohesive energy and lattice constant at room temperature [10]. Agrawal *et al.* [31] showed that using this Lennard-Jones potential, the activation energies and pre-exponential factors of the self-diffusions of Cu were in a good agreement with other experimental and theoretical data. For carbon–copper, the LJ12-6 potential function with the cutoff distance of 10 Å has been used classical molecular dynamics simulations to study carbon–copper interface [11]. The LJ12-6 potential function for carbon-copper is unsuitable to make quantitative discussions on physical phenomena because both CNT and Cu nanowires with metallic .properties are expected to take place the substantial charge transfer. However, since this work uses the LJ12-6 potential function, the Coulomb interactions between polarized electrons can not be included, and thus effect should be considered in future works.

Two double-walled CNTs of (10,10)(5,5) and (15,15)(10,10) were considered. The open outer (15,15) and (10,10) CNTs were composed of 500 and 750 atoms with the length of 3 nm and the capped inner (5,5) and (10,10) CNTs were composed of 270 and 640 atoms with the length of 3.3 nm. Figure 1 shows the atomic structure of the double-walled CNTs encapsulating copper nanowires. The copper nanowires consisted of 46 and 330 atoms obtained from our previous work investigating the optimized copper nanowires encapsulated in armchair CNTs [12]. The initial structures were relaxed by simulated annealing simulations; then, Cu@(10,10)(5,5) CNT was optimized without

deforming whereas Cu@(15,15)(10,10) CNT was optimized with surface deformation because the Cu nanowire structure was not perfect cylindrical shape.

CNT oscillators can be realized when the outer CNT is fixed or in contact with other materials to obtain the oscillatory behaviors. Therefore, for the outer CNT of all the MD simulations, its center-of-mass was constantly maintained using the position rescaling method by every MD steps. The core CNTs were initially displaced from the relaxed structures, and then, the oscillation frequencies (f) were analyzed by the fast Fourier transform (FFT) using data obtained 300-ps MD simulations.

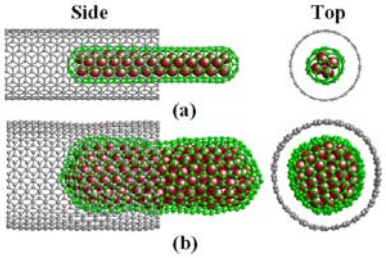

Figure 1. Atomic structure of the double-walled CNTs encapsulating copper nanowires. (a) Cu_{46}@(10,10)(5,5) CNT and (b) Cu_{330}@(15,15)(10,10) CNT oscillators. The open outer (15,15) and (10,10) CNTs were composed of 500 and 750 atoms with the length of 3 nm and the capped inner (5,5) and (10,10) CNTs were composed of 270 and 640 atoms with the length of 3.3 nm.

3 RESULTS AND DISCUSSION

MD simulation results of double-walled CNT oscillators were compared to double-walled CNT oscillators encapsulating Cu nanowires with the initial displacements. Figures 2 and 3 show the MD results for the Cu@(10,10)(5,5) CNT with the initial displacements of 13 Å and for the Cu@(15,15)(10,10) CNT with the initial displacement 10 Å, respectively. In Fig. 2, (a)-(d) show the displacements of the (5,5) CNT center-of-mass, the total excess force (F_x) induced on the inner (5,5) CNT or Cu@(5,5)CNT, the binding energy ($U_{C\text{-}Cu}$) between Cu nanowire and (5,5)(10,10) CNT, the total inter-wall vdW energies (U_{vdW}) as functions of the MD time. In Fig. 3, (a)-(d) show the displacements of the (10,10) CNT center-of-mass, the total excess force (F_x) induced on the outer (10,10) CNT or Cu@(10,10) CNT, the binding energy ($U_{C\text{-}Cu}$) between Cu nanoiwre and (10,10)(15,15) CNT, the total inter-wall vdW energies (U_{vdW}) as functions of the MD time. In the static calculation, the excess forces of the Cu@CNT oscillator were slightly higher than that of the CNT oscillator. The F_x of the CNT oscillators are composed of the only excess C-C vdW forces (F_{vdW}) whereas the F_x of the Cu@CNT oscillators are composed of the metal-carbon interaction force ($F_{C\text{-}Cu}$) as well as the F_{vdW}. For Cu@(10,10)(5,5), the $U_{C\text{-}Cu}$ and the $F_{C\text{-}Cu}$ were around 1 % of the U_{vdW} and the F_{vdW}, respectively, and for Cu(15,15)(10,10), the $U_{C\text{-}Cu}$ and the $F_{C\text{-}Cu}$ were around 3 % of the U_{vdW} and the F_{vdW}, respectively. From our calculations, the excess vdW force induced by the inter-wall interactions is 17 times higher than the excess force induced by the Cu nanowire-CNT interactions. This implies that the $F_{C\text{-}Cu}$ effects are much lower than the F_{vdW} effect for the Cu@CNT oscillator. If you assume that the $F_{C\text{-}Cu}$ be zero, since the mass of the Cu@(10,10)(5,5)CNT oscillator is 1.895 times higher than that of the (10,10)(5,5)CNT oscillator, the operation frequency (f) of the Cu@(10,10)(5,5) CNT oscillator is 0.726 times lower than that of the (10,10)(5,5) CNT oscillator in the classical oscillation theory as expressed by $2\pi f = \sqrt{k/m}$, where m is the mass of the oscillator. If we assume that the CNT oscillator approximate a classical oscillator with a spring constant, the relation between the F_x and the operating frequency ($f_{M@CNT}$) of M@CNT oscillator could be expressed as

$$f_{M@CNT} \propto \sqrt{\frac{F_x}{m}} . \qquad (1)$$

Figures 5(a)-(b) show the frequencies of both the (10,10)(5,5) CNT and the Cu@(10,10)(5,5) CNT oscillators for the initial displacements. As the initial displacements were increased, the frequencies decreased. The frequencies of the CNT oscillators were 76 and 57 GHz for the initial displacements of 13 and 23 Å, respectively. This result is in good agreement with the previous works [2,3] that have shown that the operation frequency of the CNT oscillator was inversely proportional to the square root of its initial displacement, which was predicted by an explicit formula [2,3] and was verified by Rivera *et al* [19]. The frequencies of the Cu@(10,10)(5,5) CNT oscillator were 53 and 42 GHz for the initial displacements of 13 and 23 Å, respectively. For a simple linear spring-mass system, the frequency is proportional to the square-root of the ratio of the spring constant over the mass, according to the classical theory. Using Eq. (1) and the frequencies of the (10,10)(5,5) CNT oscillators Ref. 39, the corresponding frequencies of the Cu@(10,10)(5,5) CNT oscillators are 55 and 41 GHz for the initial displacements of 13 and 23 Å, respectively. The systems of these oscillators are, of course, highly nonlinear as discussed above but nevertheless, the classical theory provides a fairly good estimate.

Figure 5(c) shows the frequencies of both the (15,15)(10,10) CNT and the Cu@(15,15)(10,10) CNT oscillators for the initial displacement of 10 Å. The frequencies of the (15,15)(10,10) CNT and the Cu@(15,15)(10,10) CNT oscillators were 76 and 23 GHz, respectively. For the same initial displacement, as the diameter of the double-walled CNT oscillator increases, its operating frequency decreases as expressed by $95\exp(-2.3d) + f_\infty$, where d is the diameter of the outer CNT in the nanometer scale and f_∞ = 11.8 GHz is the frequency of double-walled CNT oscillator with very large diameter. For the (15,15)(10,10) CNT oscillator with the initial displacement of 10 Å, this relation provides a good estimate of 77 GHz. For Cu@(15,15)(10,10) CNT oscillator, the

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frequency, 39 GHz, estimated from Eq. (1) is very different from the frequency, 23 GHz, obtained from the MD simulation. While the frequencies of Cu@(10,10)(5,5) CNT oscillator were reasonably estimated by Eq. (1) showing the mass-frequency dependence, the frequency of the Cu@(15,15)(10,10) CNT oscillator was not. These results, at least, can be explained by two reasons. The first is the mass-dependence of encapsulated Cu nanowire. For the Cu@(10,10)(5,5) CNT oscillator, the mass of the Cu nanowire is less than that of the (5,5) CNT whereas for the Cu@(15,15)(10,10) CNT, the mass of the Cu nanowire is 2.7 times higher than that of the (10,10) CNT. As the portion of the Cu nanowire mass increases, the Cu@CNT oscillator motion is influenced on the Cu nanowire mass rather than the CNT mass. Ripples shown in Figs. 2(b)-(c) and 3(b)-(c) induce the velocity decrease of the Cu@CNT oscillator. When the Cu@CNT oscillator is moving, the Cu nanowire slightly collides with the encapsulating CNT as discussed above; then, Cu nanowire motion with large mass is more important than the CNT motion with small mass in the aspects of momentum and energy transfers. Therefore, as the nanowire size increases, the nanowire motion is important more and more. However, the frequency of the Cu@(15,15)(10,10) CNT oscillator was much less than that obtained from Eq. (1) showing the mass-frequency dependence. Therefore, the frequency of the Cu@(15,15)(10,10) CNT oscillator was influenced on other effects as well as the mass increase effect. The second is the interwall friction-dependence. As shown in Fig. 1(a), for Cu@(10,10)(5,5) CNT oscillator, the (5,5) CNT was not deformed, and it oscillated with very low surface friction and energy dissipation. However, for Cu@(15,15)(10,10) CNT oscillator, the (10,10) CNT was deformed as shown in Fig. 1(b). Therefore, the deformed Cu@(10,10) CNT oscillated with a high surface friction during the translational motion, and this induced high energy dissipation. The high surface friction made a rotational motions of the Cu@(10,10) CNT. Since the MD simulations in this work did not include the thermal effects, we could not provide information on the frequency variations and the noise effects due to the thermal motions of the double-walled CNT oscillator encapsulating the copper nanowire. Therefore, since thermal energy dissipations, interwall energy exchanges, and interwall frictions can affect the operations frequencies and the oscillation damping of the multi-walled CNT oscillators, further work should be performed by using the MD simulations for different conditions of the temperatures. A multi-walled CNT encapsulating a magnetic material has a potential for a CNT oscillator initiated by the external magnetic fields, and this can be applied to nano-magnetic source and nano-magnetic memory. Therefore, multi-walled CNT oscillators encapsulating magnetic nanowires should be investigated by further work. The Coulomb interactions induced by the charge transfer between the CNT and Cu nanowire should be also investigated by further work.

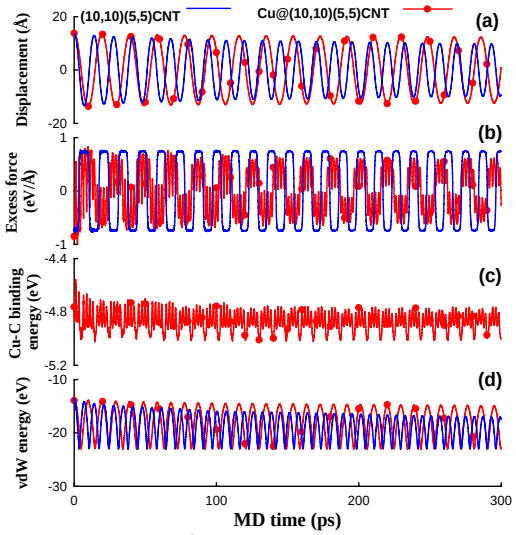

Figure 2. MD results for the Cu@(10,10)(5,5) CNT with the initial displacements of 13 Å. (a) Displacements of the (5,5) CNT center-of-mass, (b) total excess force (F_x) for (5,5) CNT and Cu@(5,5)CNT, (c) Cu-C binding energy ($U_{C\text{-}Cu}$), and (d) C-C vdW energies (U_{vdW}) as functions of the MD time.

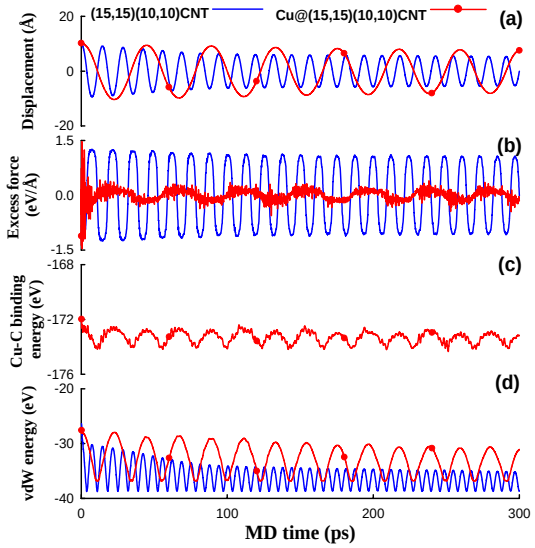

Figure 3. MD results for the Cu@(15,15)(10,10) CNT with the initial displacement 10 Å. (a) Displacements of the (10,10) CNT center-of-mass, (b) total excess force (F_x) for (10,10) CNT and Cu@(10,10) CNT, (c) Cu-C binding energy ($U_{C\text{-}Cu}$), and (d) the C-C vdW energies (U_{vdW}) as functions of the MD time.

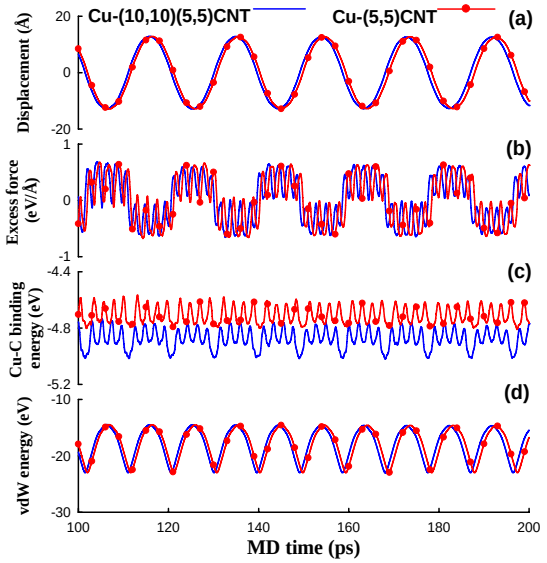

Figure 4. The MD simulation results when the copper atoms interacted with the (5,5) CNT were compared to those when the copper atoms interacted with both the (5,5) and the (10,10) CNTs. (a) Displacements of the inner CNT center-of-mass, (b) excess forces, (c) Cu-C binding energy, and (d) C-C vdW energies as functions of the MD time for the different copper-carbon interaction ranges from 100th and 200th ps.

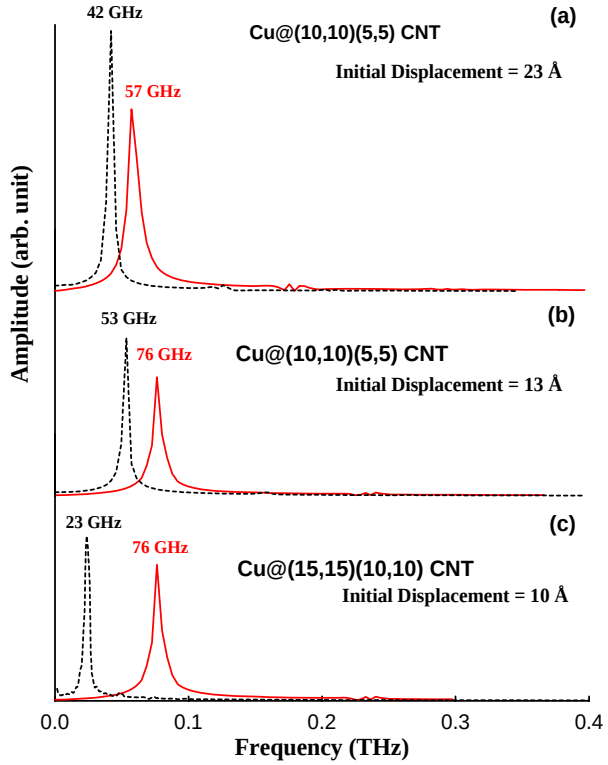

Figure 5. Frequencies of (a) the (10,10)(5,5) CNT, (b) the Cu@(10,10)(5,5) CNT, and (c) Cu@(15,15)(10,10) CNT oscillators for the initial displacements.

4 SUMMARY

Double-walled CNT oscillators encapsulating Cu nanowire were investigated by MD simulations. The excess forces of the Cu@CNT oscillator are slightly higher than that of the CNT oscillator and the excess vdW forces induced by the inter-wall interactions are 17 times higher than the excess forces induced by the Cu nanowire-CNT interactions. Since the masses of copper atoms are higher than those of carbon atoms, the carbon atoms were easier accelerated than the copper atoms; then, this induced the collision between the inner CNT and the encapsulated copper nanowire; finally, this repelling force due to this collision made a decrease of the total excess force. The systems of the CNT oscillators were highly nonlinear but nevertheless, the classical oscillation theory provided a fairly good estimate of the operating frequency when the CNT surface was not deformed by the Cu nanowire. However, when the encapsulating CNT was deformed due to the encapsulated Cu nanowire, the frequency could not be estimated by the mass-frequency dependence.

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REFERENCES

[1] J. Cumings and A. Zettl: Science 289 (2000) 602.
[2] Q. Zheng and Q. Jiang: Phys. Rev. Lett. 88 (2002) 045503.
[3] Q. Zheng, J. S. Liu, and Q. Jiang: Phys. Rev. B 65 (2002) 245409.
[4] M. Monthioux: Carbon 40 (2002) 1809.
[5] J. W. Kang and H. J. Hwang: J. Appl. Phys. 96 (2004) 3900.
[6] J. Tersoff: Phys. Rev. B 38 (1988) 9902.
[7] J. Tersoff: Phys. Rev. B 39 (1989) 5566.
[8] D. W. Brenner: Phys. Rev. B 42 (1990) 9458.
[9] Z. Mao, A. Garg, and S. B. Sinnott: Nanotechnology 10 (1999) 273.
[10] P. M. Agrawal, B. M. Rice, and D. L. Thompson: Surf. Sci. 515 (2002) 21.
[11] S. Dorfman, K. C. Mundim, D. Fuks, A. Berner, D. E. Ellis, and J. Van Humbeeck: Mater. Sci. Eng. C 15 (2001) 191.