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Ultra-fast oscillation of cobalt clusters encapsulated inside carbon nanotubes

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Abstract

Using molecular dynamics (MD) simulations, the authors have studied the oscillatory characteristics of the 2Co@CNT oscillator systems. Each of these oscillator systems consists of a hosting carbon nanotube (CNT) and two encapsulated cobalt (Co) clusters, and oscillations are initiated by prescribing an initial kinetic energy to each of the two cobalt clusters. The non-symmetric oscillation mode, in which the two cobalt clusters always move towards the same direction, was found to be stable over a wide range of initial energy. However, the symmetric oscillation mode, in which the two cobalt clusters move towards or away from each other, bouncing off each other in each oscillation, is stable only when the initial kinetic energies are lower than a threshold value. Above this threshold, the oscillation becomes increasingly unstable with the increasing initial kinetic energy. The instability is found to take place through transferring energy from the translational motion to the rotational motion of the cobalt clusters, due to the fact that the impact of the cluster–cluster collisions can be slightly off-center, causing the clusters to roll and rock. The rocking motion of the cobalt clusters serves as the channel for the energy transfer. The rocking motion can be retarded and may even be eliminated by reducing the hosting CNT diameter. But a smaller hosting CNT does not always lead to more stable translational oscillation. There apparently exists an optimal CNT for a given size of clusters for stabilizing the translational oscillation. A hosting CNT that is too much smaller than optimum causes severe cobalt–carbon atomic interactions, which lead to losses of energy from the ordered translational motion of clusters to disordered thermal motions of the atoms.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

Investigations on carbon nanotubes (CNTs) have been inspired primarily by their extreme physical properties, such as the axial Young's modulus and mechanical strength, and/or their versatile electronic properties (semi-conducting versus metallic behavior, for example). This has led to the promise of a variety of novel application concepts [1]. The application concept that is most relevant to the present study is the proposal that the inter-wall translational oscillation of multi-walled CNTs may be utilized to design mechanical oscillators of frequencies in the gigahertz (GHz) range [2, 3]. There have been much interest and many investigations [4–45] of the CNT oscillators. Much of this interest is because nano-electro-mechanical-systems (NEMSs) of ultra-high frequencies have long been sought for a range of envisioned novel applications, including mechanical devices for high-frequency signal processing, sensitive mechanical

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charge detectors, and quantum measurements [46–48]. One of the critical issues is how to initiate and subsequently drive the oscillatory motion for such a system in a controlled manner. The oscillatory behavior of the CNT oscillators can be manipulated by precision mechanical controllers [6, 17], and may possibly be controlled remotely with electromagnetic fields [5, 18, 19], lasers [31] and electrostatic forces [41]. Legoas *et al* [5, 18] discussed the possibility of initiating the oscillatory motions of these systems using internal metallic (or filled with metallic materials) or an external semi-conducting nanotube and by applying an external electric field, through charge injection, or by applying a variable magnetic field. Kang *et al* studied the feasibility of initiating oscillatory motions of the CNT oscillators using an electric field [19] or a thermo-mechanical mechanism [31].

Filling CNTs with nanoparticles has led to the discovery of a more intriguing class of hybrid materials [49–51]. The fillings could be oxides, e.g. PbO [52], Bi_2O_3 [53], V_2O_5, or MoO_3 [54], or carbides of various elements such as transition metals (Cr, Mn, Fe, Co, Ni) and rare earths (Sm, Gd, Dy, Yb, La) [55–57], as well as pure metals, including Mn [58], Cu [59], Ge [60, 61] or Ga [62]. Some nanoparticles, including fullerenes, endo-fullerenes, and nanoclusters of nickel and cobalt, have been found to form ordered arrays nested along the axes of the hosting CNTs. Such a supra-molecular structure is often referred to as a 'peapod' structure, due to its resemblance to peas in a pod. The configuration of a peapod assembly is understood to be the result of the delicate balance of the interactions among the nanoparticles and the hosting CNT, which include both short-range and long-range interactions for electrically charged or magnetized nanoparticles [49, 63, 64]. This new class of material points to a very promising opportunity for synthesizing supra-molecule nanostructured materials of extreme or versatile properties and/or special functionality. Studies on the NT-based GHz oscillators have largely focused on double-walled and multi-walled CNTs [2, 3, 5, 7, 8, 18–20, 30–36, 38, 43], and boron nitride nanotubes (BNNTs) [9, 21–24, 37]. In several recent studies [23, 33, 42, 45], systems consisting of a hosting CNT and one or more encapsulated fullerenes have been investigated as oscillators, which can generate much higher frequencies than their double-walled or multi-walled CNT counterparts. In this report, we present our study of a Co@CNT oscillator system, which is composed of a hosting CNT and two encapsulated cobalt (Co) clusters. Using MD simulations, we have studied the oscillatory characteristics of such an oscillator system. The simulation results show that for an initial cluster velocity ranging from 0.5 to 1.2 Å ps^{-1} (or equivalently for the initial cluster kinetic energy ranging from 0.94 to 5.43 eV), such a system oscillates with frequencies of several tens of GHz in its two basic oscillation modes: the symmetric mode, in which the two cobalt clusters move towards or away from each other, and the non-symmetric mode, in which the two cobalt clusters always move towards the same direction. The non-symmetric oscillations of this system are found to be stable, i.e., the oscillation amplitude experiences no significant change with the MD simulation time. The symmetric oscillations, however, are stable only when the initial kinetic energies are lower than a threshold value, and above this threshold, the oscillation becomes increasingly unstable with the increasing initial kinetic energy. The instability is found to take place through transferring energy from the translational motion to the rotational motion of the cobalt clusters, due to the fact that the impact of the cluster–cluster collisions can be slightly off-center, causing the clusters to roll and rock. The rocking motion of the cobalt clusters serves as the channel for the energy transfer. The rocking motion can be retarded and may even be eliminated by reducing the hosting CNT diameter. But a smaller hosting CNT does not always lead to more stable translational oscillation. There apparently exists an optimal CNT for a given size of clusters for stabilizing the translational oscillation. A hosting CNT that is too much smaller than optimum causes severe cobalt–carbon atom interactions, leading to losses of energy from the ordered translational motion of clusters to disordered thermal motions of the atoms.

2. Method and modeling

Molecular dynamics (MD) has been broadly used to study the properties of nanodevices. Legoas *et al* [5, 18] have performed MD simulations on a number of CNT oscillator systems and have shown that these nano-oscillators are dynamically stable when the radii difference between the inner and the outer tubes is ∼3.4 Å. Guo *et al* [10] have thermally equilibrated double-walled CNT oscillators with a bath to reach an initial temperature, and then switched to a microcanonical ensemble for simulations. A similar approach is used by Zhao *et al* [7] on nano-oscillator setups to study their energy dissipation mechanisms. In a previous study [45] on a $2C_{60}$/CNT oscillator system, we thermally heated the system, after initial optimization, up to a desired temperature and assigned the two fullerenes initial translational kinetic energies, superimposed on their equilibrium status to start the subsequent dynamics—a microcanonical ensemble run.

Our model system consists of a hosting CNT with two encapsulated cobalt nanoclusters, as illustrated in figure 1(a). The cobalt clusters are assumed to have a face-centered cubic (FCC) close-packed structure and a diameter of 3 nm, approximately, as reported according to both theoretical construction using molecular dynamics (MD) simulations [65, 66] and experimental observation using high-resolution transmission electron microscopy (HRTEM) [66]. We note that the cobalt clusters may exhibit faceting properties due to the complex features in various environments [66], which are not taken into account in this analysis. To perform simulations, we use the MM3(2000) force field of Allinger *et al* [67] to characterize the short-range C–C and Co–Co interactions, while the C–Co interaction is calculated using the mixed rule, i.e., interpolating between the C–C interaction and the Co–Co interaction as an approximation. To account for the magnetic interaction between two cobalt clusters, we have included the following dipole potential in the manner employed by Gennes and Pincus [68] and by Morimoto and Maekawa [69]:

$$u_m = -m_i \cdot H_{ij} = \frac{1}{4\pi\mu_0}\left[\frac{m_i \cdot m_j}{r_{ij}^3} - \frac{3}{r_{ij}^5}(m_i \cdot r_{ij})(m_j \cdot r_{ij})\right], \quad (1)$$

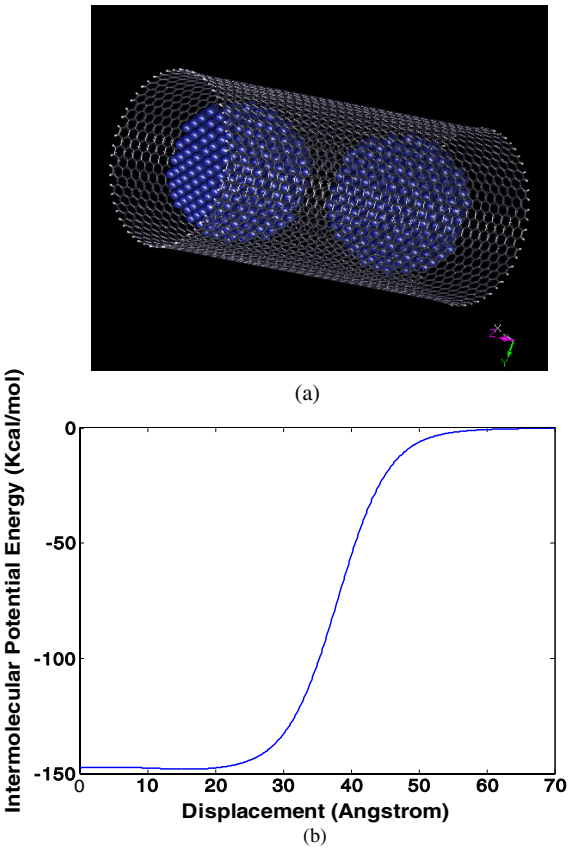

Figure 1. (a) An illustration of the 2Co@(28, 28) CNT oscillator system in the optimized configuration, in which the two cobalt clusters are well aligned symmetrically along the axis of the hosting CNT axis; (b) variations of the potential energy of a single cobalt cluster versus its displacement along the axis of the hosting (28, 28) CNT.

where μ_0 and m_i are, respectively, the free space permeability and the magnetic moment of cluster i. H_{ij} stands for the magnetic field at the position of cluster i produced by cluster j, and r_{ij} presents the distance between the two clusters. As reported by Xie and Blackman [70], the magnetic moment of a cobalt cluster initially decreases rapidly with an increasing number of constituent cobalt atoms and approaches a constant value of about $1.8\mu_0\mu_B$ when the number of atoms is larger than 500. We first performed minimization, leading to an optimized system configuration, in which the two cobalt clusters are well aligned symmetrically along the axis of the hosting CNT, with an inter-cluster spacing of 45.36 Å, approximately, for a (26, 26) CNT. The system is then heated to a pre-assigned temperature by performing a canonical run with the Berendsen thermostat. This is the initial temperature of the microcanonical ensemble. The initial temperature is set to be 3 K for all the simulations, except those shown in figures 7(a) and (b) for illustrating the thermal effect. For the subsequent MD simulations, we have used essentially the same approach as in our previous study [45]. The dynamics simulations are carried out utilizing the open source code TINKER [71] with our customized features. A time step of 1 fs is used for all simulations. However, much smaller time steps, such as 0.1 fs, have been tested to ensure that qualitative features from the simulations are robust.

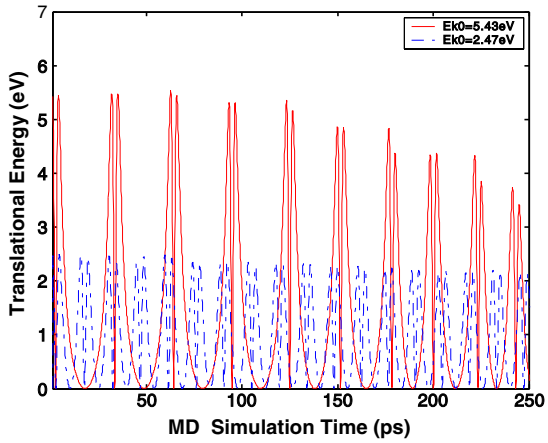

Figure 2. Variations of the kinetic energy per cluster in the translation motion for the 2Co@(28, 28) CNT system in the symmetric oscillation initiated with prescribed kinetic energies, respectively, $E_{k0} = 2.47$ eV/cluster and $E_{k0} = 5.43$ eV/cluster.

3. Results and discussion

We began MD simulations with the 2Co@(28, 28) CNT system. The CNT length in the simulations is set to be 86.1 Å, which is equal to 35 times of the periodicity length of the armchair CNTs. This length has been tested to be long enough to minimize the edge effect on the optimized configuration, while it is not too long to challenge our computation capacity. For illustration, we have plotted in figure 1(b) variations of the potential energy of a single cobalt cluster versus its displacement along the axis of the hosting CNT. The system has two basic oscillation modes: the symmetric mode, in which the two cobalt clusters move towards and then away from each other, and the non-symmetric mode, in which the two cobalt clusters always move in the same direction. We generated the oscillations in the symmetric and non-symmetric modes by assigning the two cobalt clusters initial velocities (or initial energies, equivalently) of the same magnitude and, respectively, with opposite and the same directions. We studied the oscillations in these two basic modes by prescribing the initial cluster velocity (v_0) in the range 0.5–1.2 Å ps^{-1}, or equivalently the initial kinetic energy per cluster (E_{k0}) in the range 0.94–5.43 eV. The simulation results confirm the expected trend for such a nonlinear oscillation system that the oscillation magnitude increases and the oscillation frequency decreases with increasing initial kinetic energy. Within this range of initial kinetic energy, the oscillation frequency ranges from 33 to 80 GHz for the symmetric mode and from 26 to 60 GHz for the non-symmetric mode, respectively. What has caught our particular interest is the observation that the non-symmetric mode is stable, with no reduction in the oscillation amplitude with time, for the entire range of initial kinetic energy (E_{k0}), while the symmetric mode becomes increasingly unstable with increasing initial kinetic energy. As shown in figure 2, the amplitude of oscillation energy for the symmetric mode experiences little reduction with time when the initial kinetic energy (E_{k0}) is prescribed at 2.47 eV per cluster (or $v_0 = 0.8$ Å ps^{-1}, equivalently). But the reduction is substantial within the first 250 ps, for $E_{k0} = 5.43$ eV. The energy

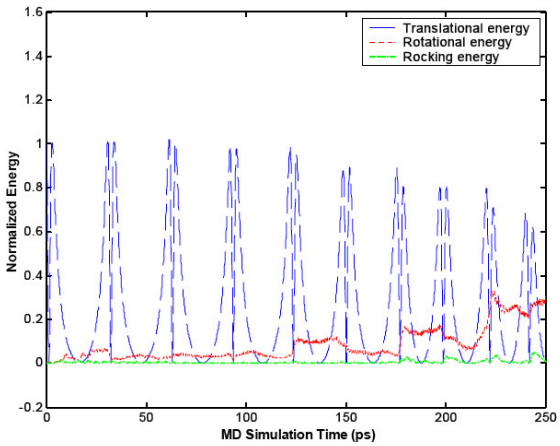

Figure 3. The normalized energy components of the 2Co@(28, 28) CNT oscillator system with the initial kinetic energy $E_{k0} = 5.43$ eV/cluster: the dashed (blue) line is the normalized translational energy; the dotted (red) line is the normalized rotational energy; and the dashed–dotted (green) line is the normalized rocking energy.

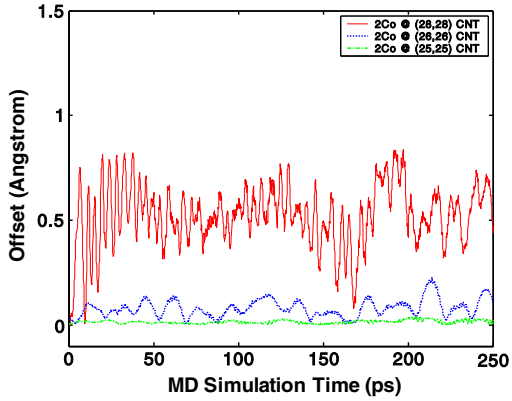

Figure 4. Variations of the cluster offset distance from the CNT axis, in oscillation initiated with prescribed kinetic energy $E_{k0} = 5.43$ eV/cluster: the solid (red) line is for the 2Co@(28, 28) CNT oscillator system; the dashed (blue) line is for the 2Co@(26, 26) CNT oscillator system; and the dashed–dotted (green) line is for the 2Co@(25, 25) CNT oscillator system.

plot of the higher energy case reveals that the energy in the translational motion experienced little reduction during the first 125 ps. Most of the reduction occurred in the subsequent time interval from 125 to 250 ps. Within this later time interval, the translational motion lost about 35% of its energy. Our detailed examination of the components of the total kinetic energy for each cobalt cluster indicates that the energy in the rotational mode of a cluster became significant and increasingly large after the 125th ps. To study the mechanisms for the energy transfer in this process, we have plotted the normalized energies in the translational mode, the rotational mode and the rocking mode (with a velocity perpendicular to the CNT axis) all together in figure 3. The energy components were normalized using the initial kinetic energy per cluster. We note that sharp increases in the rotational energy occurred at approximately three time instants, $t = 125$, 180, and 225 ps. At each of these three time instants, the two cobalt clusters collided against each other. This suggests that the energy transfer from the translational mode into the rotational mode primarily took place during the collisions. The inter-colliding of two clusters subjects the clusters to large repelling forces. These repelling forces are not necessarily aligned perfectly along the CNT axis, nor precisely pointing towards the mass centers of the clusters. The misalignment causes the clusters to rock around the CNT's axis, while the offset from the mass center cause a cluster to rotate. The rocking motion, being severely confined by the hosting CNT, does not gain much energy itself, but instead, channels energy from the translational motion to the rotational motion.

Hoping to retard the channel that transfers the energy to the rotational motion, we have run the MD simulations for systems with smaller CNTs, by keeping all the other parameters, i.e., the CNT length, the initial energy and the initial temperature, the same as those for the case shown in figure 3. To illustrate the confinement effect of a hosting CNT on the rocking motion of the clusters, we have plotted, in figure 4, the variations in the offset of a cluster (the distance to the cluster mass center from the CNT axis) versus the

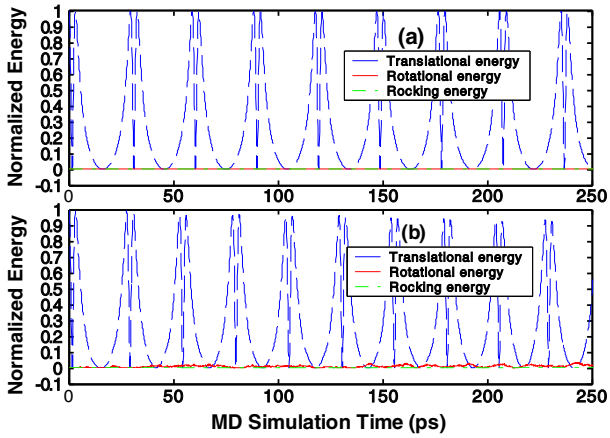

Figure 5. The normalized energy components for (a) the 2Co@(26, 26) CNT oscillator system and (b) the 2Co@(25, 25) CNT oscillator system, in oscillation initiated with prescribed kinetic energy $E_{k0} = 5.43$ eV/cluster: the dashed (blue) line is the normalized translational energy; the dotted (red) line is the normalized rotational energy; and the dashed–dotted (green) line is the normalized rocking energy.

MD simulation time, for three systems, namely the 2Co@(28, 28) CNT system, the 2Co@(26, 26) CNT system and the 2Co@(25, 25) CNT system. The offset for the 2Co@(26, 26) CNT system is substantially smaller than that for the 2Co@(28, 28) CNT system, and the offset for the 2Co@(25, 25) CNT system is negligibly small compared to those for the other two systems. The energies for the translational motion, rotational motion and the rocking motion are plotted, respectively, in figure 5(a) for the 2Co@(26, 26) CNT system and in figure 5(b) for the 2Co@(25, 25) CNT system. The confinement appears to be very effective in retarding the rocking motion and hence starving the rotational motion, as seen in figure 5. What surprised us are the observations from figure 5 that the 2Co@(26, 26) CNT system experienced no loss in the translation energy during the entire MD simulation and that the 2Co@(25, 25) CNT system, with a smaller CNT and thus a

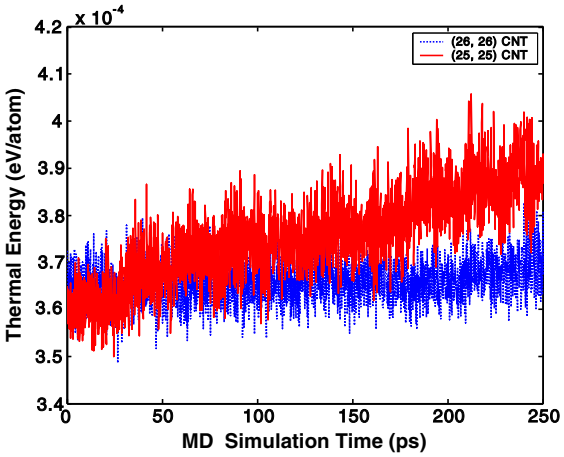

Figure 6. The thermal energies of the hosting CNTs for oscillation initiated with prescribed kinetic energy $E_{k0} = 5.43$ eV/cluster: the solid (red) line is for the 2Co@(25, 25) CNT oscillator system; and the dotted (blue) line is for the 2Co@(26, 26) CNT oscillator system.

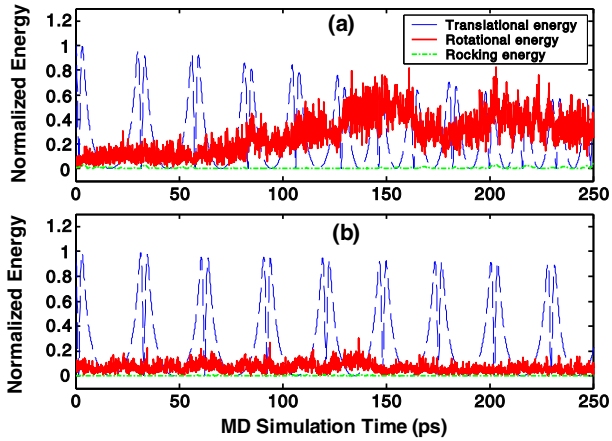

Figure 7. The normalized energy components for oscillation initiated with prescribed kinetic energy $E_{k0} = 5.43$ eV/cluster and with the initial temperature of 300 K, for (a) the 2Co@(28, 28) CNT oscillator system and (b) the 2Co@(26, 26) CNT oscillator system: the dashed (blue) line is the normalized translational energy; the dotted (red) line is the normalized rotational energy; and the dashed–dotted (green) line is the normalized rocking energy.

stronger confinement, had lost some energy in the translational motion, although the loss is merely 5%, approximately, of the initial kinetic energy. Our detailed examination reveals that the cluster was 'shaking' about its mass center (rotating with a tiny magnitude and with a violently changing axis of rotation), and this 'shaking' is responsible for the rotation energy barely seen in figure 5(b), which had increased to about 2% of the initial kinetic energy over the 250 ps MD simulation time. We note that this increase in the rotation energy is not enough to account for the loss in the translational energy—about 5%. Naturally, one would wonder where the energy had gone and what had caused this loss. We find no energy accumulations in other ordered motion modes, for both the clusters and the CNT. We therefore looked into the disordered motion of atoms and calculated the corresponding thermal energies. We have plotted the thermal energies versus the MD time in figure 6 for both the 2Co@(25, 25) CNT system and the 2Co@(26, 26) CNT system, with the results from the same simulations as shown in figure 5. Initially, the thermal energies of the two systems, measured per atom, were approximately the same. The thermal energy of the 2Co@(25, 25) CNT system increased significantly with the increasing MD simulation time, while the thermal energy of the 2Co@(26, 26) CNT system exhibited no trend of accumulating energies. In particular, the total thermal energy for the 2Co@(25, 25) CNT system had increased nearly 0.3 eV, which is just about 3% of the initial kinetic energy for the two clusters. We note that the diameters for the (26, 26) CNT and the (25, 25) CNT are 35.2 and 34.0 Å, respectively, and the diameter reduction from 35.2 to 34.0 Å corresponds to the reduction from 2.6 to 2.0 Å in the minimum distance between a cobalt atom in a cluster and a carbon atom on the CNT. As expected, such a reduction in the atom–atom distance leads to substantially stronger interactions between the cobalt atoms and the carbon atoms, and this is the mechanism for the increasingly larger thermal energy and the energy of the 'shaking' motion of the clusters for the 2Co@(25, 25) CNT system.

Comparing the 2Co@CNT system with the $2C_{60}$@CNT system investigated in a previous study [45], we note that the oscillation frequencies of the 2Co@CNT system are about one tenth of the frequencies of the $2C_{60}$@CNT system, for the same initiation velocities. The fact that the mass of a cobalt cluster is approximately 100 times of the mass of a C_{60} reminds us the classic relation for a linear spring–mass system, i.e., the frequency is inversely proportional to the square root of the mass. This is an interesting observation because the inter-particle interaction forces are highly nonlinear in both these systems. A more interesting observation is that the energy exchange between the translation mode and the rotation mode is far greater in the $2C_{60}$@CNT system than in the 2Co@CNT system. With the initiation velocities in the same order, the energy transferred from the translation motion to the rotation motion reaches as high as 80% of the initial total kinetic energy for the $2C_{60}$@CNT system within the first 50 ps of the simulation run, while it remains less than 30% for the 2Co@CNT system even after 250 ps. In fact, the cobalt cluster does not rotate in the convention manner, but instead it shakes violently about its mass center while it translates along the axis of the hosting CNT axis. We note that the 2Co@CNT system has a size 12 times larger than the $2C_{60}$@CNT system and that the mass of a cobalt cluster is more than 100 times larger than that of a C_{60}. These characteristic differences between the two systems are primarily responsible for the differences in their oscillatory behaviors, while the effect of the magnetic dipole–dipole interaction appears to be minor. We have made our best attempt to quantify the effect of the magnetic dipole–dipole interaction, but we have found, however, that we are unable to obtain conclusive understanding with the present approach, because the effect on translation motion is insignificant while on rotation motion it is tiny compared with the effect of inter-cluster collisions.

4. Concluding remarks

The non-symmetric oscillations of a 2Co@CNT oscillator system are found to be stable. That is, the oscillation amplitude experiences no significant change over the MD simulation time. The symmetric oscillations, however, are stable only when the initial kinetic energies are lower than a threshold value. Above this threshold, the oscillation becomes increasingly unstable with increasing initial kinetic energy. The instability takes place through the energy transfer from the translational motion to the rotational motion of the clusters. The rocking motion of the clusters serves as the channel for the energy transfer. The rocking motion can be retarded and may even be eliminated by reducing the hosting CNT diameter. However, a smaller hosting CNT does not always lead to more stable translational oscillation. There apparently exists an optimal CNT for a given size of clusters for stabilizing the translational oscillation. A hosting CNT that is too much smaller than optimum causes severe cobalt–carbon atomic interactions, leading to severe losses of energy from the ordered translational motion of clusters to disordered thermal motions of the atoms. Our results from MD simulations for these systems at selected temperatures indicate that the above conclusions remain valid as the temperature increases to room temperature. To illustrate the thermal effects, we have plotted the energy components in figure 7(a) for the 2Co@(28, 28) CNT system and in figure 7(b) for the 2Co@(26, 26) CNT system, respectively. The conditions for these simulations are the same as for those shown in figures 3 and 5(a), except that the initial temperature was set at 300 K, instead of 3 K.

Acknowledgments

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