Rotation-excited perfect oscillation of a tri-walled nanotube-based oscillator at ultralow temperature

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Received 2 December 2016, revised 17 February 2017
Accepted for publication 22 February 2017
Published 16 March 2017

Abstract
In recent years, carbon-nanotube (CNT)-based gigahertz oscillators have been widely used in numerous areas of practical engineering such as high-speed digital, analog circuits, and memory cells. One of the major challenges to practical applications of the gigahertz oscillator is generating a stable oscillation process from the gigahertz oscillators and then maintaining the stable process for a specified period of time. To address this challenge, an oscillator from a triple-walled CNT-based rotary system is proposed and analyzed numerically in this paper, using a molecular dynamics approach. In this system, the outer tube is fixed partly as a stator. The middle tube, with a constant rotation, is named Rotor 2 and runs in the stator. The inner tube acts as Rotor 1, which can rotate freely in Rotor 2. Due to the friction between the two rotors when they have relative motion, the rotational frequency of Rotor 1 increases continuously and tends to converge with that of Rotor 2. During rotation, the oscillation of Rotor 1 may be excited owing to both a strong end barrier at Rotor 2 and thermal vibration of atoms in the tubes. From the discussion on the effects of length of Rotor 1, temperature, and input rotational frequency of Rotor 2 on the dynamic response of Rotor 1, an effective way to control the oscillation of Rotor 1 is found. Being much longer than Rotor 2, Rotor 1 will have perfect oscillation, i.e., with both stable (or nearly constant) period and amplitude—especially at relatively low temperature. This discovery can be taken as a useful guidance for the design of an oscillator from CNTs.

Supplementary material for this article is available online

Keywords: Nano-oscillator, carbon nanotube, molecular dynamics, rotation

(Some figures may appear in colour only in the online journal)

1. Introduction

Since their discovery in 1991 [1], carbon nanotubes (CNTs) have attracted significant attention from researchers due to their potential applications in various engineering fields [2, 3]. Owing to the $sp^2$ carbon–carbon bonds in its shell, a defect-free CNT has a super-high modulus along its axis [4]. At the same time, a permeable large variation of bond angles leads to perfect durability [5–7], which can be adopted in the application of nanosprings [8, 9]. Besides the two favorable mechanical properties mentioned, the friction between two adjacent tubes is ultralow [2, 10], which makes CNTs particularly suitable for acting as a component in most nanodevices such as nanoscale molecular bearings [11–14], nanostrain sensors [15, 16], nanomotors [17–21], and gigahertz oscillators [22–32].

When releasing inner CNTs which had been pulled out partly from their outer fixed tubes, Cumings and Zettl [2] discovered that the inner CNTs retracted back into the outer tubes rapidly. Their experimental results illustrated the
ultralow friction between the adjacent tubes. Following this line, Zhang et al [10] presented a way of modifying intertube friction by means of the concept of superlubricity. Due to the existence of intertube friction, the oscillator itself behaves as an obvious damped oscillation [25]. However, without external force, the motion of the inner tube will behave as a damped motion, e.g., damped oscillation (relative sliding along the tube axis) or damped rotation (relative sliding along the tube tangent). From then on, it becomes an open issue to explore the mechanism of intertube friction and find a feasible way to generate and maintain a perfect oscillation of the nano-oscillator. In particular, Legoa et al [23] found that the oscillation could be kept stable when the radii difference of tubes is ~0.34 nm. Guo et al [24] built a relationship between the intertube friction force and the energy dissipation of a multi-wall CNT-based gigahertz oscillator. Neil et al [26] suggested a method to control the oscillation by exerting a periodic external force on the oscillator. Ershova et al [27] estimated the controlling efficiency of the oscillator by providing a non-uniform electric field. Kang et al [29] simulated the effect of the gap between two stators on the frequency of oscillation in such an oscillator. Cai et al [28] found that the oscillation of the free inner CNT in a fixed outer CNT can be excited when the inner tube initially has a high rotational frequency. Gao et al [33] investigated the oscillation of a curve rotor [6, 7] with high-speed rotation in two short stators from CNTs. Recently, Shi et al [34] proposed a model for exciting the oscillation of the inner tube in a thermally driven nanomotor [35–37].

Unlike the works just summarized, we focus on investigating mechanisms of generating stable or perfect oscillation and constructing the corresponding nanotube system in this work. By means of a molecular dynamics approach, we propose a nano-oscillator from triple-walled CNTs, which is different from those proposed by Motevalli and his colleagues [38, 39]. In our model, the outer tube is fixed as a stator and the middle tube is specified with a constant rotational frequency. The inner tube, which is longer than the middle tube, may have both rotating and oscillating motions if the system is placed in a canonical NVT ensemble, where N is the number of atoms, V is the volume of the simulation system, and T is the temperature. We investigate the dynamic behavior of the inner tube affected by inner tube length, temperature, and the input rotational frequency of the middle tube. The mechanism for the inner tube to generate a perfect oscillation is also discussed.

2. Model and methodology

To explore the dynamic stability of the nanodevice shown in figure 1, we place two tubes in a fixed tube (the stator). The middle tube (Rotor 2) is run with a constant rotational frequency and has no axial oscillation during rotation. Due to friction between the two rotors, Rotor 1 will be driven into rotation when Rotor 2 is rotating. It is noted from our previous study [28] that a rotary nanotube may be transformed into an oscillator. To overcome the friction between the stator and Rotor 2, we use a thermal nanomotor to drive the rotation of Rotor 2, which further drives the motion of Rotor 1 by friction. Hence, friction may act as a reaction in driving the motion of Rotor 2 or act as an action in driving the motion of Rotor 1. Therefore, dynamic responses such as rotational frequency, oscillatory amplitude, and frequency of oscillation in Rotor 1 could perform in a controllable way, which is important in most engineering applications. Considering the length of Rotor 1 is an essential factor, and we adopt the following four models in the present study. Moreover, the system works under a canonical NVT ensemble. Therefore, we study the temperature effect on the dynamic responses as well. In our analysis, four different temperature values are used: 8 K (which is considered a relatively low temperature), 150 K, 500 K, and 800 K, with the last three being used for purposes of comparison.

In our numerical study, the system is simulated using the open-code LAMMPS program [41, 42]. To draw the interaction among atoms in the C–H system, the AIREBO potential [43] is adopted. The update of the atoms’ positions in the system is determined by the numerical integral of Newton’s Second Law of Motion, with a time step of 0.001 or 0.0005 ps (only for λ = 1.2 at 800 K). There are eight steps for obtaining the dynamic response of Rotor 1 before and after simulation:

1. Build an initial model of the system featured, with the coordinates of atoms, masses, and atom types;
2. Initiate the parameters in algorithms for unit, boundary types, potential type, cutoff, time step, etc;
3. Define groups of atoms for related control, calculation, and outputs;
4. Minimize the potential energy of the system by steepest descending algorithm with tolerance of 10⁻⁴ and 10⁻⁶ units for energy and force, respectively. The maximal iterations are 100 and 1000, respectively;
5. After potential minimization, fix the carbon atoms on the two rings of each end of the outer tube (stator) with respect to their degrees of freedom. The two rotors are fixed partly, i.e., the carbon nanotubes at the second and third circular rings at each end of the stator are fixed before the end of 100 ps of relaxation under the canonical NVT ensemble with specified temperature. When discussing the effect of ω₂ on the dynamic response, the temperature is set to be 300 K. When the temperature is different from 300 K, ω₂ = 200 GHz;
6. After relaxation, release the two rotors to let them move freely; the stator is still fixed as before. The tubes are under the same canonical NVT ensemble during operation;
7. Calculate the relevant data and output them for post-processing;
8. Stop when the number of iterations reaches its maximum or when Rotor 1 escapes from the middle tube.
The output rotational frequency of Rotor 1 at $\omega_1 = 20$ GHz is shown in figure 2(a). It can be found that the mean value of the rotational frequency of Rotor 1 is around 20 GHz after a period of acceleration, driven by Rotor 2 via the inter-tube friction [11, 12, 44–47]. It can also be found that the fluctuation of the frequency of Rotor 1 with $\lambda = 1.2$ is $\sim 20$ GHz, which is the highest among the four cases in figure 2(a). From figure 1(b), the length difference between Rotor 1 and Rotor 2 with $\lambda = 1.2$ is only $\sim 0.81$ nm, which is larger than the cutoff of potential function (3 times of 0.335 nm in the present study). Hence, the adjacent ends of both rotors have strong van der Waals (vdW) interaction. As the system is under a canonical NVT ensemble with $T = 300$ K, the atoms (both carbon and hydrogen atoms) on both tubes have drastic vibration (phonon scattering). During their vibration, the spatial distance between the two tubes decreases to less than 0.335 nm, i.e., the equilibrium distance between neighboring carbon nanotubes or layers of graphene. Hence, the repulsive force increases rapidly as the spatial distance decreases. Further, the two tubes depart due to the repulsive force. The collision between the two tubes is completed from the appearance until disappearance of the repulsive force. Due to the collision (see Movie 1, available at stacks.iop.org/NANO/28/155701/mmedia), Rotor 2 exerts upon Rotor 1 a momentum which leads to the variation of configuration of Rotor 1. In a three-dimensional problem, a momentum vector has three independent components along three orthogonal directions—axial, radial, and circular—of a tube (see figure 3). Since the axial component $F_{\text{axis}}$ is not equal to zero, Rotor 1 will have a translatonal acceleration along the axial direction. With time, the position of the mass center of Rotor 1 has a deviation along the axial direction, i.e., Rotor 1 oscillates along the axis as shown in figure 2(a'). If the radial component $F_{\text{rad}}$ does not equal zero, Rotor 1 has a breath-like vibration of the cross section which will produce further collision between the two rotors. When the circular component $F_{\text{circ}}$ is nonzero, it generates a moment of momentum along the tube axis. Therefore, the circular component will drive the rotation of Rotor 1. In particular, the atoms at the ends of the tubes have stronger vibration because of the weaker local stiffness of the tube ends. Accordingly, the vdW interaction between the adjacent ends of the tubes is much stronger than that among the internal atoms [48]. At the same time, both the mass and moment of inertia of Rotor 1 become smaller as the length of Rotor 1 decreases. Hence, under the same impact-loading during collision, the shorter Rotor 1 has higher variation in both rotation and oscillation. This conclusion can be verified from the results shown in figures 2(a) and (a').

When the input rotational frequency $\omega_2$ becomes larger, say 50 GHz (figure 2(b)), 100 GHz (figure 2(c)), or 200 GHz (figure 2(d)), the fluctuation of Rotor 1’s rotation with shorter length behaves similarly to those shown in figure 2(a). If the length of Rotor 1 becomes longer, e.g., $\lambda = 2.0$ or 4.0, the output rotation of Rotor 1 becomes unstable. In particular, there are two phenomena worthy of mention; one is that, when $\lambda = 4.0$ and $\omega_2 \gg 100$ GHz, the rotational frequency of Rotor 1 increases firstly and decreases lastly. From figures 2(c) and (d), the peak value of $\omega_1$ is lower than that of $\omega_2$ but higher than that of 0.5 $\omega_2$. Especially when $\lambda = 4.0$ and $\omega_2 = 200$ GHz, $\omega_1$ tends to be stable at $\sim 25$ GHz after about 12 ns of acceleration. First, we discuss the positive acceleration of rotation, i.e., before 3.5 ns the rotational frequency of Rotor 1 increases continuously. From figure 2(d’), we find that the oscillation of Rotor 1 has moved asymmetrically, i.e., Z1 does not vary near zero. From Movie 2, it can be found that Rotor 1 has slight eccentric rotation. Hence, before approaching 3.5 ns, the oscillation amplitude of Rotor 1 is obvious. After 4.5 ns, the oscillation amplitude of Rotor 1 becomes neglected and the value of Z1 is close to $-6$ nm, which implies that the right ends of both rotors have been absorbed into each other. Due to the rotational frequency of Rotor 1 decreasing continuously from 3.5 ns, the axial pulling force caused by the eccentric rotation of Rotor 1 is reduced synchronously. Hence, after 12 ns of acceleration, Rotor 1 reaches a dynamic equilibrium state (see Movie 3), i.e., both
Figure 2. Rotation and oscillation of Rotor 1 when driven by Rotor 2 with rotational frequencies $\omega_2 = 20, 50, 100,$ and $200 \text{ GHz}$. The temperature of the environment is 300 K.
rotational frequency and position of mass center of Rotor 1 remain unchanged.

One more phenomenon is found by which, when \( \lambda = 2.0 \) and \( \omega_2 = 200 \text{GHz} \) (figure 2(d')), the rotational frequency of Rotor 1 increases at first and decreases after about 6 ns of acceleration. Especially when the simulation time passes 14.2 ns, the rotational frequency of Rotor 1 has a periodic fluctuation with the given amplitude at the frequency of 85 GHz. Checking the mass center of Rotor 1, shown in figure 2(d'), we see that it is out of the left end of Rotor 2 (see the gray dashed line of \(-0.203 \text{ nm}\)). This means that the right end of Rotor 1 has entered Rotor 2, overcoming the potential barrier \([48, 49]\) at the right end. Owing to super-lubricity of the CNT shell, the axial resistance acting upon Rotor 1 by Rotor 2 can be neglected. At the same time, Rotor 1 is in an eccentric rotation state (see the second inserted snapshot at 13 448 ps in figure 2(d')). Rotor 1 escapes from Rotor 2 quickly under the action of the centrifugal force due to eccentric rotation (see the second inserted snapshot at 14 245 ps in figure 2(d'), \( Z_1 < -6.09 \text{ nm} \)); this process can be found in Movie 4. After leaving Rotor 2, Rotor 1 is free of external force, which leads to the velocity of the mass center, and the magnitude of rotational velocity of Rotor 1 is unchanged. We calculate the rotational frequency of Rotor 1 according to the projection of the rotational velocity onto the tube axis of Rotor 2. From the movie, we can also observe that Rotor 1 is rolling along a certain axis, which is different from the tube axis of Rotor 2. Hence, \( \omega_1 \), i.e., the magnitude of the projection of rotational velocity on the angular, varies periodically. Now we can answer the question as to why Rotor 1 with \( \lambda = 2.0 \) escapes from Rotor 2 during rotation while Rotor 1 with \( \lambda = 4.0 \) does not: the only reason is that the rotational frequency of Rotor 1 with \( \lambda = 4.0 \) is only \( \sim 25 \text{GHz} \), which provides weaker pulling force on Rotor 1 during eccentric rotation.

When \( \lambda = 4.0 \) and \( \omega_2 = 20 \text{GHz} \), the rotation of Rotor 1 becomes relatively stable after about 7 ns of acceleration. Having observed the configuration of Rotor 1, we found that the mass center of Rotor 1 has the highest amplitude of axial oscillation among the four cases with respect to \( \lambda \). When \( Z_1 \) is more than \( 2.03 \text{ nm} \) or less than \(-2.03 \text{ nm} \), the mass center of Rotor 1 is out of the middle CNT. When \( Z_1 \) is between \(-6.09 \text{ nm} \) and \( 6.09 \text{ nm} \), the right or left end of Rotor 1 is still out of Rotor 2. Constrained by the potential barrier at the ends of Rotor 2, Rotor 1 does not escape from Rotor 2 during rotation because the eccentric rotation of Rotor 1 is small (see the two inserted snapshots in figure 1(a'')) and has no influence on its axial oscillation. Hence, a conclusion can be made that Rotor 1 does not escape from Rotor 2, as the input rotational frequency is relatively small.

### 3.2. Temperature effect on dynamic outputs

Temperature can significantly affect the dynamic response of a nanosystem in a canonical NVT ensemble. It is known that the atoms in a system with high temperature have drastic thermal vibration. From the state equation \( E_{\text{Kinetic}} = \frac{3}{2} k_B T / 2 \), we can see that temperature \( T \) is proportional to \( E_{\text{Kinetic}} \) (the sum of average kinetic energy of all the atoms in the system). In the equation, \( k_B \) is the Boltzmann constant \((1.3806505 \times 10^{-23} \text{J/K})\). In this study, the value of \( E_{\text{Kinetic}} \) is obtained by subtracting the kinetic energy of rigid body motion of the tubes from the total kinetic energy of the tubes. Hence, the interaction between the two rotors is sensitive to the temperature of the system. Here, we investigate the temperature effect on the dynamic response of Rotor 1, which is driven by Rotor 2 with 200 GHz input rotational frequency, by following four cases. From figure 4, one can find that the rotational frequency of Rotor 1 at 8 K increases more slowly but is more stable than any other cases. When \( T = 800 \text{K} \), the rotational frequency of Rotor 1 has the highest fluctuation, nearly 200 GHz; this is due to the strong vdW interaction between the two rotors. When Rotor 1 is relatively short, say \( \lambda = 1.2 \) or 1.5, Rotor 1 does not escape from Rotor 2 at any temperature, which can be verified from figures 4(a), (a''), (b), and (b''). From figures 4(a'') and (b''), it can also be found that Rotor 1 has no oscillation at 8 K after a period of running. At higher temperature, Rotor 1 has pseudo-periodic oscillation with the highest possible amplitude, e.g., the amplitude is about the length difference between the two rotors. This implies that one can generate or confine the oscillation of Rotor 1 by changing the temperature, and is an interesting and valid approach to a practical design for NEMS or nanomotors.

When the length of Rotor 1 becomes longer, say 2.0 or 4.0 of \( L_2 \), the dynamic outputs of Rotor 1 are significantly different from those of a shorter Rotor 1. In figures 4(c) and (d), the rotational frequency of Rotor 1 increases first and decreases later. Even in some cases, e.g., \( \lambda = 2.0 \) at \( T \geq 150 \text{K} \) or \( \lambda = 4.0 \) at \( T = 800 \text{K} \), Rotor 1 escapes from Rotor 2. This can be verified from the periodic variation of rotational frequency of Rotor 1 (figures 4(c) or (d)) and the sharp drop of \( Z_1 \) (mass center of Rotor 1) (figures 4(c'') or (d'')). Hence, the system with a longer Rotor 1 is unstable at higher temperature. If, for example, we need both rotation and oscillation of a longer Rotor 1, we have to place the system at relatively low temperature, e.g., 8 K from figure 4(d'').

Figures 4(d) and (d'') show that the oscillation of Rotor 1 increases directly proportional to the time and is perfectly stable, i.e., with a stable period, and the amplitude is without decay as time passes. From figure 4(d''), there are \( \sim 64.2 \) periods during 30 ns of oscillation, i.e., frequency of oscillation is \( \sim 2.14 \text{GHz} \) (Movie 5). The major reason for this is that Rotor 1 has slight eccentric rotation due to negligible thermal vibration of atoms on tubes. Simultaneously, the inter-tube

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**Figure 3.** Schematic of action forces on the inner tube exerted by its adjacent tube during collision.
Figure 4. Dynamic response of Rotor 1 driven by Rotor 2 with $\omega_1 = 200$ GHz at NVT ensemble for different temperature. When $\lambda = 1.2$ at 800 K, time step is 0.0005 ps.
friction between the two rotors is very small at relatively low temperature. Finally, the rotating CNT becomes an oscillator due to strong interaction between adjacent ends of both rotors when they move together too closely [28]. Considering the amplitude of oscillation as \( \sim 14.2 \text{ nm} \) \((2.03 \times 2 \times 4 - 2.03 = 14.21 \text{ nm})\) (figure 5), the oscillator is suitable for various engineering applications.

4. Conclusions

We suggest a new model for building a CNT-based nano-oscillator, with stable oscillation, in which the outer tube is fixed (stator) and the middle tube, acting as Rotor 2, is with a constant rotational frequency. The inner tube, which is longest among the three tubes and acts as Rotor 1, will be driven to rotation firstly by the interaction forces between the two rotors. According to the rotation-oscillation transmission law [28], closely followed with rotation, the oscillation of Rotor 1 will be excited. By investigating effects of the length of Rotor 1, temperature, and input rotational frequency of Rotor 2 on dynamic behavior of the oscillator, some conclusions can be made which are useful for potential applications of the proposed model to practical design:

1. During collision between the two rotors, Rotor 2 exerted a reaction force upon Rotor 1. The axial component of reaction force controls the oscillation of Rotor 1; the circular component determines the rotational acceleration of Rotor 1; and the radial component, which depends on thermal vibration, influences the friction force between the two rotors.

2. At 300 K, when the input rotational frequency of Rotor 2 is relatively low, Rotor 1 can be excited to have a pseudo-periodic oscillation. If the input rotational frequency is high, Rotor 1 can easily have an eccentric rotation which may result in Rotor 1 escaping from Rotor 2. Avoiding the eccentric rotation is essential to generating the oscillation of Rotor 1.

3. When Rotor 1 is short, the pseudo-periodic oscillation of Rotor 1 can be easily actuated when temperature is not too low. For a longer Rotor 1, a perfect oscillation can be generated and kept when the system is under a canonical NVT ensemble with relatively low temperature. The amplitude of oscillation approximately equals the difference between the length of Rotor 1 and half-length of Rotor 2.

References


Figure 5. Sequential snapshots of system with 200 GHz Rotor 2 and Rotor 1 with \( \lambda = 4.0 \) at 8 K during a period from 20 756–21 177 ps.
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