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Controlled Stable Oscillation of Nanomechanical Systems Based on Carbon Nanotubes

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Abstract Numerical simulations are used to study the conditions controlling the stable oscillation of nanomechanical systems based on carbon nanotubes under periodic harmonic driving force. It is shown that the conditions to sustain the stable oscillation are not only dependent on the driving frequency, but also dependent on the amplitude and the initial phase of the driving force. Once the oscillatory frequency is given, the driving frequency must be equal to the integral multiple of the oscillatory frequency in order to sustain the stable oscillation. We determine the conditions by a combination of equations containing the parameters of the oscillator and the driving force, and solve it numerically. Sustained stable oscillation for the systems with a nonlinear dependence of the friction force on the relative velocity of the tubes can be obtained by properly choosing the amplitude and the initial phase of the periodic harmonic driving force. Both regular and irregular oscillatory modes are observed.

Keywords Carbon nanotube · Nanooscillator · Driving frequency · Stable oscillation

1 Introduction

There has been great effort in recent years to create nanomechanical devices working in the gigahertz range and beyond. Carbon nanotubes (CNTs) have attracted remarkable attention due to their great potential applications as the basis for mechanically based motion control [1–4]. In particular, extremely low friction and low wear were reported to exist between core and shell of a double-walled carbon nanotube (DWCNT), leading to much research work in exploring its possibility in making nanooscillators [5, 6], nanobearings [7], nanogears [8], nanomotors [9, 10], etc. Cumings and Zettl have managed to open one end of CNTs and telescope a core tube out of an outer-housing shell [11]. The interlayer telescoping friction force was estimated to be less than 1.5×10^{-14} N per atom. They found that when the core was partially pulled out of the outer tube and then released, the inner tube can spontaneously retract into the shell due to the intertube van der Waals (vdW). Zheng et al. proposed the first CNT-based mechanical oscillator with a natural map of molecular manufacturing [5]. Since then, a great number of experimental and theoretical studies on gigahertz oscillators and related physical and mechanical problems have been carried out. Fennimore et al. built a rotational actuator using a carbon nanotube as the motion-enabling element which is controllable by electrical field [12]. Jensen et al. reported the successful synthesis of tunable nanoactuators based on telescoping carbon nanotubes [13]. While the experimental investigation of such nanomechanical systems is limited by the available techniques, the theoretical study on the multiwalled carbon nanotube (MWCNT) oscillators is relatively straightforward. The interaction between the tubes is dominated by physical vdW force, which makes the MWCNT oscillators being studied by molecular dynamic simulations [14] and numerical calculations [15–17].

It was found that although a relatively smooth and low-frictional oscillator can be achieved by choosing an appropriate radius difference between inner and outer nanotubes, friction-induced energy dissipation is still inevitable, resulting in damping oscillation. The simulation results have shown that the axial oscillation decays quickly within a few nanoseconds. The short lifetime greatly limits its practical application because it brings difficulties for the energy supplement and signal detection. Thus, how to sustain the CNT oscillatory motion in a precise control down to the molecular level over long periods of time remains a critical problem. Reducing

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energy dissipation and applying an external field are two possible approaches. Correspondingly, different effective strategies have been proposed to study the relative motion of CNTs, e.g., by applying external electrical fields in the case where ions are located inside the movable wall [18], by using uniform magnetic fields with a conducting movable wall [19], by accelerating encapsulated charged elements located inside the inner tube [20], by periodically applying thermal gradients that are imposed on the outer tube using external agents such as electrical currents [21], and by thermal expansion of encapsulated gases which are enclosed between the walls of the nanotube [22], although it has been recognized that there are many technological challenges [23] that currently hinder the realization and implementation of the proposed CNT oscillators.

For a harmonic oscillator, the natural frequency has nothing to do with the initial displacement. However, the natural frequency of anharmonic oscillator is strongly dependent on the initial displacement. In this work, we introduce a numerical computation method for maintaining and controlling the stable motion of DWCNTs with a nonlinear dependence of the friction force on the relative velocity of the tubes. Periodic harmonic driving force is applied to the anharmonic nanooscillator in which the inner and outer nanotubes are of different length. We determined the controllable operating conditions for the stable oscillation by the parameters of the oscillators and the driving force, and investigated the relation of the stable oscillation with the amplitude and the initial phase of the periodical driving force. Our aim is to demonstrate the feasibility of the proposed method for controlling the stable motion of the oscillation system.

The paper is organized in the following way: The oscillator configurations and the model for the calculations are described in Section 2. In Section 3, we give the results from the numerical calculations and demonstrate the possibility of controlling the stable oscillation of DWCNT systems with the proposed method. Section 4 is left for conclusions.

2 Model Setting

In order to demonstrate the possibility of realizing the stable oscillation, we perform numerical simulations of the controlled operation of the double-walled carbon nanotube (10,10)@(15,15) with different lengths (20 and 30 nm) for the outer tubes and same length (10 nm) for the inner tube as shown in Fig. 1. Both ends of the inner and outer tubes are opened. The intertube distance is ~3.4 Å, which coincides that between adjacent sheets of graphite. Since covalent bonds are much stiffer than vdW interaction, the DWCNT can be modeled as a system of two rigid tubes moving coaxially. For all our computations, at the beginning of simulation (t=0), the inner tube has been pulled out of the outer nanotube so that the overlap between them is 7 nm.

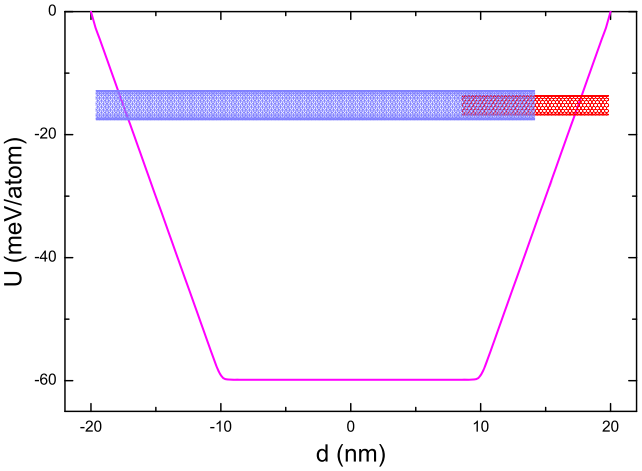

Fig. 1 The atomic configuration of the double-walled carbon nanotube (10,10)@(15,15)-based mechanical oscillator and the potential profile along the axial displacement with length of 30 nm for the outer tube and length of 10 nm for the inner tube

VdW interactions are not only prominent in driving the oscillation of nanotubes but also central to the oscillatory stability and the energy dissipation during oscillation. Several registry-independent and registry-dependent vdW potentials have been proposed for carbon fullerene structures. We perform the analysis of the controlled properties of DWCNT oscillators employing empirical Lennard-Jones (LJ) pair potential

$$U_{ij} = 4\varepsilon\left[\left(\sigma/r_{ij}\right)^{12} - \left(\sigma/r_{ij}\right)^{6}\right] \tag{1}$$

and plot in Fig. 1. In the expression, r_{ij} represents the interatomic distance, and the parameters ε=4.2038 meV and σ= 3.37 Å have been used [24]. The LJ approach has been successfully used for molecular dynamic simulations of carbon structures taking into condition its relative simplicity and satisfactory results when compared with experimental findings [25]. It is indicated that the LJ potential is suitable for nanotubes sliding on graphite surface [26], parallel single-walled CNT [27], multiwall CNTs [28], and fullerenes inside single-walled CNTs [29]. Furthermore, the LJ model has been proved to be very effective in calculating the oscillatory frequency and describing the characteristic behavior of various CNT oscillator systems [30–32].

As seen from the energy profile in Fig. 1, when there is no crossover of the ends of the outer and inner tube, the vdW potential is approximately constant, while the potential is increasing steeply at regions where crossover occurs, which provides the retraction force for the oscillation. Such a scenario also results in oscillatory frequencies dependent on displacement amplitudes. When the displacement dies down to a level at which crossover distances are very low, the frequency can drop sharply, as illustrated by MD simulations of the architecture.

3 Results and Discussion

Before we go on to the oscillatory details of nanotube, it is instructive to analyze the difference of harmonic and anharmonic oscillator. Figure 2 shows the harmonic potential as a function of translational displacement. It is known that the natural frequency of harmonic oscillator has nothing to do with the initial displacement. To illustrate the characteristic of the anharmonic potential, we consider the oscillation of two rectangular graphite blocks. When the upper and low blocks have same sizes, the potential can be obtained as shown in Fig. 2. For the initial displacements 0.7 and 1.7 corresponding to points A and B of Fig. 2, the natural frequencies are 1.326963 and 0.851821, respectively. In addition, Fig. 3 illustrates the concrete relations between the natural frequency and the initial displacement for different sizes of the upper graphite block. These results indicate that the natural frequency is strongly dependent on the initial displacement $x(0)$, and so the dynamics of an anharmonic oscillator is quite different from that of a harmonic oscillator. Under the conditions of no dissipation, in order to ensure the complete restoration of the anharmonic oscillator and the external force in a period, the displacement, velocity, and energy have strict periodicity. Once the external force is given, its period cannot change. Thus, the oscillator must adjust its parameters, such as displacement and phase, to make the oscillatory frequency and the driving frequency match.

In order to study the dynamics of the device, we consider nonlinearly damped oscillators by using numerical computations. The dissipation of the oscillation energy results in the decrease of the oscillation amplitude with time. Consequently, to sustain the stable oscillation of the commensurate DWCNT oscillators, it is necessary to supply the energy to the oscillator. We assume the dissipated energy is compensated by an external applied periodical harmonic force. If the Langevin stochastic force and vibrations in the telescopic nanotube are neglected, the oscillator dynamics may be roughly described by one-dimensional equations of relative motion

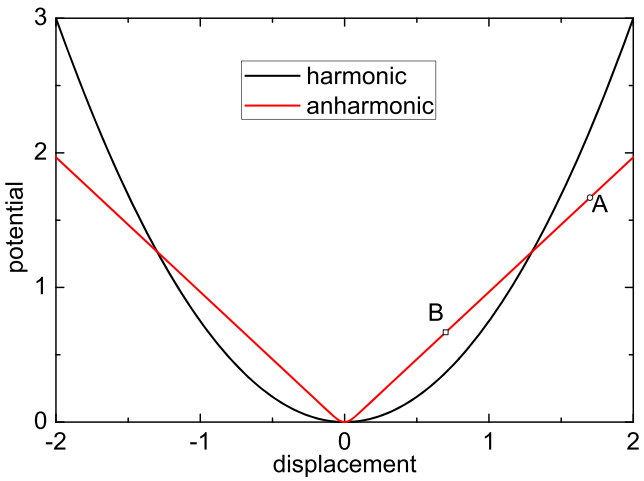

Fig. 2 Harmonic and anharmonic potential as a function of translational displacement

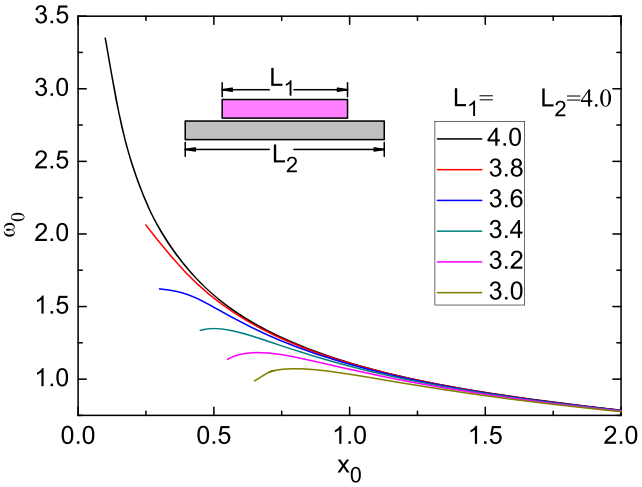

Fig. 3 Calculated natural frequency as a function of initial displacement for different size L_1 of two rectangular graphite blocks

$$\dot{x} = v \tag{2}$$

$$\mu\dot{v} = -\frac{\partial U(x)}{\partial x} - \gamma \mathrm{sgn}(v)|v|^2 + F_m \sin(\omega t + \varphi) \tag{3}$$

where μ is the mass of the movable core, x is the displacement of the core with respect to the fixed shell, v is the relative velocity, U is the LJ potential, and F_m is the amplitude of driving force applied to the core with angular frequency ω and initial phase φ. The damped term is associated with a friction proportional to v^2, where the friction coefficient γ will be imposed constant values 1.48 pN ps^2/Å^2 [21]. We suppose the initial velocity is always equal to zero. The natural frequency of the oscillator is defined as the frequency of free oscillation without damping. If we omit the friction by taking γ=0 and calculate the time that the core tube with certain initial displacement returns to the initial position after one oscillatory period, we can get the period T and then get the natural angular frequency $\Omega=2\pi/T$. In order to obtain stable oscillation, the states of the oscillator and the driving force must return to the original states after one period T. So the angular frequency ω of the driving force has to be equal to the integral multiple of the angular frequency Ω for anharmonic oscillator,

$$\omega = n\Omega \tag{4}$$

Although these periods are only a small subset of total possible periods, the conditions are absolutely necessary. Limiting the solutions to this subset is not artificial. Outside this subset, the oscillatory system cannot always fully restore

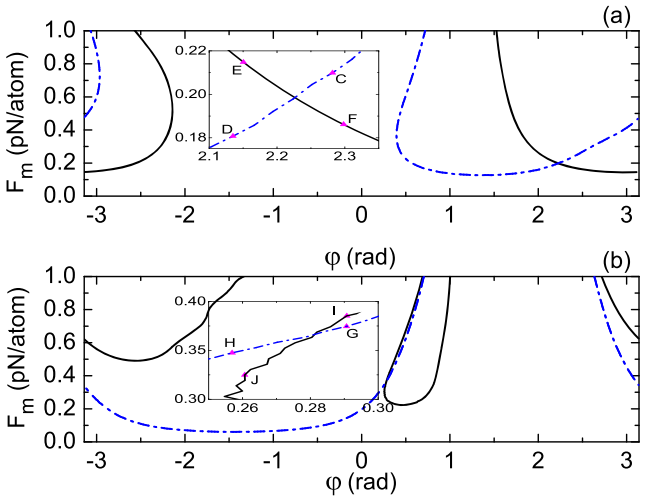

Fig. 4 The initial phase ϕ and the amplitude F_m of the driving force satisfying Eqs. (8) and (9), which correspond to the *solid and dotted lines*, respectively. The cross points of the curves give the solutions that the DWCNT oscillator can oscillate under stable conditions. The driving frequencies are taken to be ω=5 Ω for the shell lengths **a** 20 nm and **b** 30 nm. An enlarged view near the cross points is shown to emphasize the possibility of obtaining more choices to sustain persistent oscillation

in one period. Nevertheless, this limitation is not essential for a harmonic potential because the natural frequency Ω is not dependent on the initial displacement.

If the initial conditions are proper, the energy that the periodical driving force afford is equal to the dissipation of oscillation energy due to the frictional force in a period T, then we have

$$\int_0^T \left\{ F_m \sin(n\Omega t + \varphi) - \gamma \mathrm{sgn}[v(t)]|v(t)|^2 \right\} v(t)dt = 0 \qquad (5)$$

The displacement at time t is dependent on many parameters, including the shape of the potential, the initial displacement, the friction coefficient, and the frequency, initial phase,

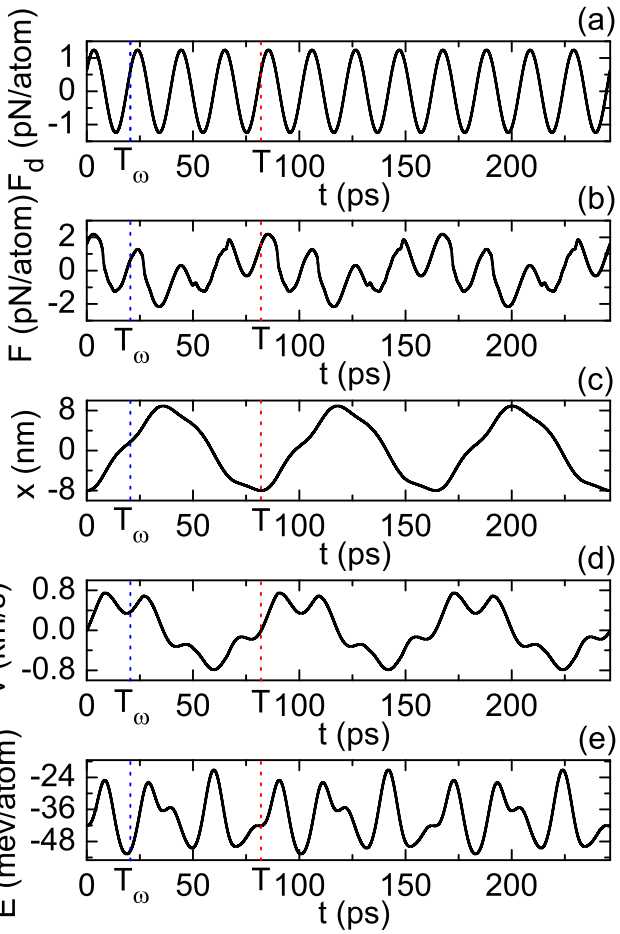

Fig. 6 **a** Driving force, **b** total force, **c** displacement, **d** velocity, and **e** total energy of the moving tube as a function of time for the shell length 20 nm. The driving frequency is taken to be ω=4 Ω. T and T_ω are oscillation period and driving period, respectively

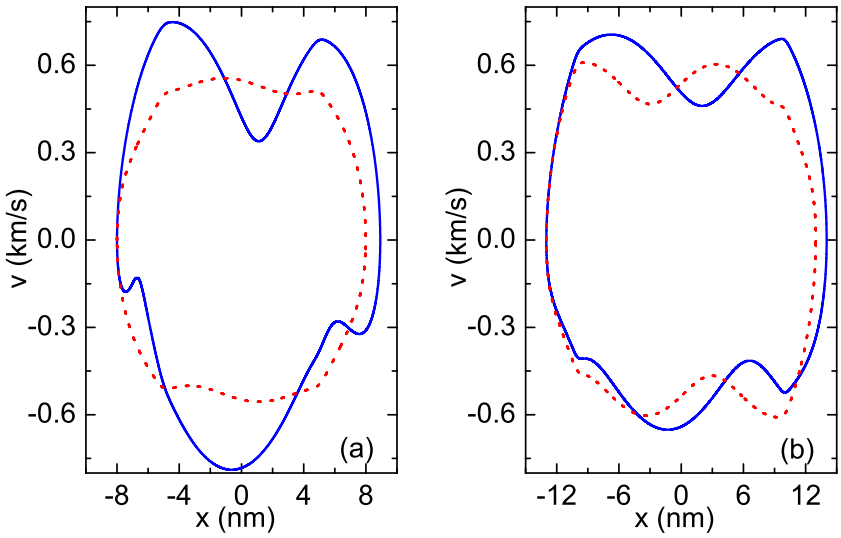

Fig. 5 The resulting phase space trajectories for the shell lengths **a** 20 nm and **b** 30 nm. The *blue (solid) lines* and the *red (dotted) lines* correspond to the driving frequency ω=4 Ω and ω=5 Ω, respectively

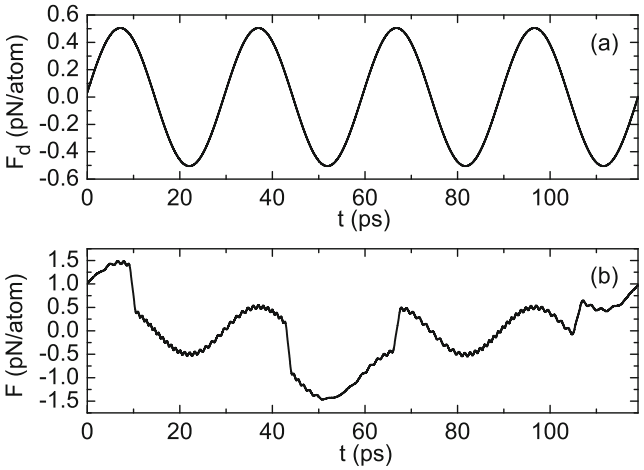

Fig. 7 **a** Force and **b** total force of the moving tube as a function of time for the shell length 30 nm. The driving frequency is taken to be ω=4 Ω

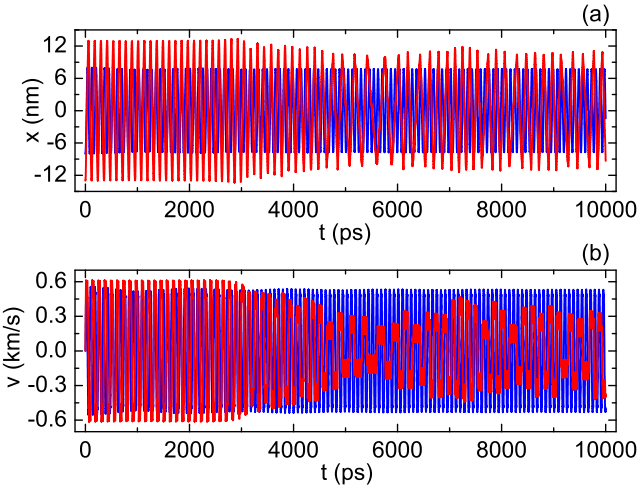

Fig. 8 **a** Displacement and **b** velocity of the moving tube as a function of time. The *blue lines* and the *red lines* correspond to points E and I of Fig. 4, respectively

and amplitude of the driving force, namely $x[t; U(x), x(0), \gamma, \omega, \varphi, F_m]$. In order to sustain the stable oscillation, the displacement and the velocity must return to the initial values after one period T. It follows that

$$x[t = T; U(x), x(0), \gamma, \omega, \varphi, F_m] = x(0) \tag{6}$$

$$v[t = T; U(x), x(0), \gamma, \omega, \varphi, F_m] = v(0) \tag{7}$$

To obtain a stable solution, it is necessary to solve the combination of Eqs. (6) and (7). However, it is difficult to determine the conditions concerning multiple parameter operation for sustained oscillator. If the driving frequency satisfies Eq. (4), then the conditions of the stable oscillation are determined by the initial phase and the amplitude of the controlled force. Thus, we should solve the following combination of equations:

$$x(F_m, \varphi; t = T) = x(0) \tag{8}$$

$$v(F_m, \varphi; t = T) = v(0) \tag{9}$$

Each equation of the combination gives a curve in the $\varphi - F_m$ plane. From this, we can obtain the solutions for the combination of Eqs. (8) and (9). Here, the Verlet velocity algorithm and steepest descent method were used to solve them.

In order to investigate the operating conditions of the DWCNT oscillator controlled by the driving force, we firstly analyze the solutions to the equations of motion when the initial overlap is 7 nm between the movable core and the outer nanotube. The frequency of free oscillation of the system depends on the initial extrusion of the moving tube for the anharmonic oscillator. We find that, for the shell lengths 20 and 30 nm, the frequencies of the oscillator in the case with the absence of the driving force and frictional force are Ω= 0.0765 and Ω= 0.0527 rad/ps, respectively.

As demonstrated above, to sustain stable oscillation, the driving frequency must be equal to the integral multiple of the oscillatory frequency once the core is released from an initial displacement. We take ω=5Ω as the frequency of the periodical harmonic driving force. The curves that satisfy Eqs. (8) and (9) are shown in Fig. 4, where (a) and (b) are the case of the shell lengths 20 and 30 nm, respectively. The black (solid) lines correspond to Eq. (8), while the red (dotted) lines correspond to Eq. (9). There are many solutions that satisfy Eq. (8) or (9), and one initial phase φ corresponds to several amplitudes F_m, same if vice versa. However, there is only one solution within the range $-2\pi \sim 2\pi$ for the initial phase φ. The cross points of the curves in the $\varphi - F_m$ plane are (φ, F_m)=(2.22652, 0.19854) for (a) and (φ, F_m)=(0.28132, 0.36646) for (b), respectively. Therefore, the oscillator operation requires a smaller amplitude of the driving force. As increasing the shell length, the amplitude F_m of the driving force needed to sustain the stable oscillation increased and the initial phase φ decreased. In the cases of both large and small driving frequencies, we obtain similar results. The amplitudes

Table 1 Calculated percentage reduction of the displacement amplitude and velocity amplitude corresponding to the points of Fig. 4

Point	C (%)	D (%)	E (%)	F (%)	G (%)	H (%)	I (%)	J (%)
Δx	3.12	4.44	3.13	4.50	12.31	19.82	17.03	20.54
Δv	5.14	5.80	4.46	6.40	34.33	50.83	45.17	51.50

of the driving force are the same order of magnitude (56.56~106.42 pN) that was reported through using thermal gradients [21, 33].

The analysis has been performed with reference to the phase space, examples of which are shown in Fig. 5. We consider that the trajectories of interest are those that form a closed loop in one oscillation cycle, as these will show the least harmonic artifacts, a desirable aspect for any driven oscillator system. It is found that every solution for the combination of Eqs. (8) and (9) corresponds to a closed loop. The simulation results indicate that the phase diagram of each oscillator is not a standard ellipse but a smooth loop. Consequently, the oscillator is anharmonic vibration periodically. Interestingly, the oscillation amplitude is equal for the frequency $\omega=5\Omega$ and unequal for the frequency $\omega=4\Omega$. Furthermore, the phase trajectories are asymmetric. So the choice of the driving frequency has great influence on the behavior of the considered oscillator.

The results of the controlled stable oscillations are presented in Fig. 6. In the case of shell length 20 nm, the driving frequency is taken to be $\omega=4\Omega$. It is indicated that the amplitudes of net force and total energy are approximately equal to 2.2 pN and 15.9 meV/atom, respectively. The driving frequency is four times that of net force, displacement, velocity, and total energy. However, for the periodic driving force applied on the carbon nanotubes, the net force is not exactly zero after a driving period T_ω. With regard to the same initial displacement and different driving force, the displacement may be positive or negative, and the oscillator may even move backward at $t=T_\omega$. This state is the initial condition of next driving period, which has great effect on the following movement. Consequently, the conditions to sustain the stable oscillation of DWCNTs are very rigorous. Furthermore, we found that in the cases of both small and large shell lengths, we obtained similar results. As are explicitly plotted in Figs. 6 and 7, the choice of the shell length has little influence on the behavior of the considered oscillator, although the fluctuations of the total force for the shell length 30 nm are frequent. Accordingly, only if the driving frequency is equal to the integral multiple of the oscillatory frequency and the initial phase and amplitude of the controlled force satisfy certain conditions which are determined by the combination of Eqs. (8) and (9), we can conveniently choose different shell length to sustain stable oscillation.

Furthermore, we calculated percentage reduction of the displacement amplitude and velocity amplitude of the moving tube corresponding to the points near the cross points of Fig. 4, as depicted in Table 1. We found that the percentage reduction of the displacement amplitude is small within 10 ns. The interesting feature lies in that the percentage reductions of the displacement amplitude and velocity amplitude are only a few percent for the shell length 30 nm. Two concrete examples of these are shown in Fig. 8 for the displacement and velocity of the moving tube as a function of time. The blue lines and the red lines correspond to points E and I near the cross points of Fig. 4, respectively. It is also interesting to see that, after a short time, the oscillation comes to a steady state. So, we can obtain more choices to sustain persistent and stable oscillation for the small range near the cross points of Fig. 4.

4 Conclusion

The present work has focused on the controlled conditions under which the carbon nanotubes can present sustained stable oscillation driven by periodic harmonic force. Using numerical simulations, we demonstrate that the use of proper driving force can be an effective and convenient approach to control and tune CNT-based oscillators. The parameters and characteristics corresponding to the controllable operating conditions for the stable oscillators are determined. From the simulation, we find that, if we choose the amplitude and the initial phase of the periodic harmonic driving force satisfy the conditions of the combination of Eqs. (8) and (9), we can obtain the stable oscillation of the DWCNT-type oscillator.

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