Control of NEMS Based on Carbon Nanotube

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ABSTRACT

A new method is proposed for controlling the motion of nanoelectromechanical systems (NEMS) based on carbon nanotubes. In this method chemical adsorption of atoms and molecules at open ends of a single-walled carbon nanotube leads to the appearance of an electric dipole moment. In this case the nanotube can be actuated by a non-uniform electric field. Possibility of the proposed method is shown on the example of the gigahertz oscillator based on a carbon nanotube. Molecular dynamics simulations of the oscillator operation are performed. The simulations reveal for this NEMS considerable thermodynamic fluctuations. The influence of thermodynamic fluctuations on the possibility of controlling the motion of NEMS is investigated.

Keywords: gigahertz oscillator, DWNT, Q-factor, nanotube

1 INTRODUCTION

Ability of free relative sliding and rotation of walls in carbon nanotubes [1], [2] allows using nanotube walls as moveable elements in nanoelectromechanical systems (NEMS). Among these devices there are rotational [3] and plain [2] nanobearings, a nanogear [4], a mechanical nanoswitch [5], a nanoactuator [6], a Brownian motor [7], a nanorelay [8], a nanobolt-nanonut pair [9]–[11], and a gigahertz oscillator [12], [13]. The crucial issue in nanotechnology is actuation of NEMS components in a controllable way. Several methods to control relative sliding of nanotube walls have been proposed recently: by magnetic field in the case of metallic moveable wall [14]; by electric field in the case of moveable wall with metallic ions inside [15]; by pressure of heated gas enclosed between moveable and fixed walls [16].

We propose new method for controlling the motion of NEMS based on carbon nanotubes. More specifically, if electron donors or/and acceptors are adsorbed at the ends of a nanotube wall, the wall has an electric dipole moment. The motion of such a functionalized wall can be controlled by a nonuniform electric field. The possibility of the proposed method is confirmed by molecular dynamics (MD) simulations of the controlled operation of the (5,5)@(10,10)nanotube-based gigahertz oscillator.

As compared to microelectromechanical systems, the principal feature of NEMS connected with the small number of atoms in these systems is that thermodynamic fluctuations in NEMS are significant. These fluctuations can essentially influence the operation of NEMS. Thermodynamic fluctuations were considered in the case of directional motion in NEMS with ratchet (Brownian motors) [7]. Here we present the study of influence of thermodynamic fluctuations on the processes of energy dissipation in NEMS. The controlled motion of the oscillator is examined by MD simulations and using the mechanical model. These investigations indicate a critical influence of thermodynamic fluctuations on the possibility of controlling the NEMS operation.

2 CONTROL OF OSCILLATOR OPERATION

The scheme, operational principles and theory of the gigahertz oscillator based on relative sliding of carbon nanotube walls were considered recently [12], [13]. Upon the telescopic extension of the inner wall outside the outer wall, the Van der Waals force F_W draws the inner wall back into the outer wall. The dependence of the Van der Waals force $F_W(x)$ on the distance x between the centers of the nanotube walls can be approximated by the following relationship [12], [13]:

$$F_W(x) = \begin{cases} F_W, |L-l|/2 < |x| < |L+l|/2 \\ 0, |x| < |L-l|/2 \\ 0, |x| > |L+l|/2, \end{cases} \quad (1)$$

where L and l are the lengths of the outer and inner nanotube walls, respectively. The frequency of the gigahertz oscillator strongly depends on the oscillation amplitude [12]:

$$\omega = \sqrt{\frac{2F_W s}{m}} \frac{\pi}{(L-l)+4s}, \quad (2)$$

where m is the mass of the movable wall and s is the maximum telescopic extension. The molecular dynamics simulations of the gigahertz oscillator show that the oscillation energy dissipates [17]. Thus, the oscillation

amplitude decreases with time and the frequency increases with time. To provide the stationary operation of the gigahertz oscillator, it is necessary to compensate the energy dissipation by the work of some external force.

We considered the possibility to compensate the energy dissipation by applying to the moveable wall an external harmonic force $F(t) = F_0 \cos \omega t$ directed along the axis of the oscillator, where ω is the desirable oscillation frequency. In particular, this force can be applied to the wall which has an electric dipole moment using a nonuniform electric field. Let us now assume that, at the instant of time $t = 0$ the inner wall is at the center of the outer wall and moves at its maximum velocity $V_{max} = \sqrt{2F_W s/m}$. The work done by the force F over the oscillation period is given by the integral

$$A_c = \int_0^T V(t)F(t)dt = \frac{4F_W F_0}{m\omega^2} \cos\left(\frac{\omega t_{in}}{2}\right), \qquad (3)$$

where $V(t)$ is the time dependence of the velocity of the inner wall, $t_{in} = (L - l)\sqrt{m/2F_W s}$ is the time of the motion of the inner wall inside the outer wall from one end to the other end without the telescopic extension. The work done by the frictional force over the same time is given by $A_f = -F_W s/Q$, where Q is the Q-factor of the oscillator, which is the ratio of the oscillation energy E to the oscillation energy loss ΔE over one oscillation period. The critical amplitude F_{0c} of the external control force, that is the minimum amplitude for which the motion controlling is possible, can be found from the condition $A_c + A_f = 0$. As a result, we obtain the critical amplitude of the control force

$$F_{0c} = \frac{ms\omega^2}{4Q \cos\left(\frac{\omega t_{in}}{2}\right)}. \qquad (4)$$

The detailed analysis shows that the critical amplitude F_{0c} of the control force is minimum if the lengths of inner and outer walls are equal $L = l$. In this case the critical amplitude of the control force is given by

$$F_{0c} = \frac{\pi^2 F_W}{32Q}. \qquad (5)$$

The estimations of characteristics of the electric field required for controlling the operation of NEMS were performed on the example of the gigahertz oscillator based on the (5,5)@(10,10) double-walled carbon nanotube with the equal lengths of inner and outer walls: $L = l = 3.1$ nm. One end of the inner wall is capped and hydrogen atoms are adsorbed on all dangling bonds at the opposite open end of the inner wall. The electric dipole moment of the inner wall in this case equals $4.5 \cdot 10^{-29}$ C·m [18].

The value of Van der Waals force for the (5,5)@(10,10) nanotube calculated using the Lennard-Jones 12-6 potential [19] is about $F_W = 1100$ pN. For this value of Van der Waals force and the Q-factor Q lying in the range $50 - 250$ (see Table 2) the critical amplitude of the control force is $F_{0c} = 1.4 - 6.8$ pN. This corresponds to voltages from 10 to 80 V at the plates of a spherical capacitor with the radii of 100 and 110 nm.

3 Q-FACTOR CALCULATIONS

As it is shown in section 1, the critical amplitude of the control force depends on the Q-factor of the gigahertz oscillator. We performed microcanonical MD simulations of free oscillations to study Q-factors of gigahertz oscillators. The in-house MD-kMC code was used. The interaction between the atoms of the inner and outer walls was described by the Lennard-Jones 12-6 potential with the parameters obtained from the AMBER database [19]. The parameters for the Lennard-Jones 12-6 potential are $\varepsilon_{\mathrm{CC}} = 3.73$ meV and $\sigma_{\mathrm{CC}} = 3.40$ Å for carbon-carbon interaction and $\varepsilon_{\mathrm{CH}} = 0.65$ meV and $\sigma_{\mathrm{CH}} = 2.59$ Å for carbon-hydrogen interaction. The cut-off distance of the Lennard-Jones potential is 12 Å. The empirical Brenner potential was used to describe the covalent carbon-carbon and carbon-hydrogen interactions [20]. The time step was 0.2 fs. At the beginning of the MD simulations the inner wall was pulled out at about 30% of its length and then released with zero initial velocity. The outer wall was kept fixed during the simulations. Nanotubes with walls of equal length were considered.

If no control force is applied, the oscillations are damped because of the interwall friction (see Fig. 1). The frequencies of damped oscillations of the (5,5)@(10,10) nanotube-based oscillator $2.4 - 4.6$ nm in length are $55 - 105$ GHz (see Table 1). This result is in agreement with other MD simulations [14], [17], [21]–[23].

We estimated the instantaneous Q-factor for every half-period $Q_{T/2} = 0.5E/\Delta E_{T/2}$, where E is the oscillation energy and $\Delta E_{T/2}$ is the oscillation energy loss over a half period. Significant fluctuations of Q-factor $Q_{T/2}$ are observed. Thus, $Q_{T/2}$ should be regarded as a statistically distributed quantity. $Q_{T/2}$ is singular for $\Delta E_{T/2} = 0$. Therefore, to obtain the average value of the Q-factor over the full simulation time we averaged the inverse Q-factor $Q^{-1}_{T/2}$. The root-mean-square deviation σ of the inverse Q-factor was also calculated.

The calculated values of the Q-factor and the relative deviation $\delta = \sigma/Q^{-1}_{T/2}$ of the inverse Q-factor at different temperatures and for the oscillators of different length are listed in Tables 1, 2. The considerable decrease of the Q-factor is found for the oscillator that is less than 3 nm in length. For the oscillators of greater length the Q-factor only slightly depends on length (see Table 1). According to Table 2, the Q-factor of the os-

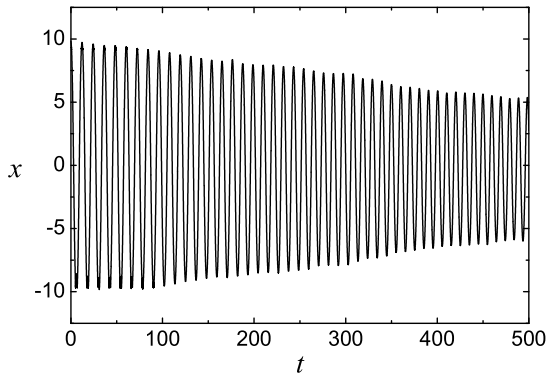

Figure 1: Distance x (in Å) between the mass centers of the walls as a function of time (in ps). The free oscillations of the (5,5)@(10,10) nanotube-based oscillator 3.1 nm in length at temperature 300 K.

cillator strongly increases with decreasing the temperature, which is in agreement with the result in [23].

Table 1: Calculated frequencies, Q-factors and relative deviations δ of the inverse Q-factor of the (5,5)@(10,10) nanotube-based oscillators of different length at temperature 150 K. The both ends of the inner wall are open and not functionalized.

length (nm)	frequency (GHz)	Q	δ
2.4	105	66 ± 9	1.20
3.1	80	120 ± 21	1.32
3.8	65	105 ± 19	1.19
4.6	55	112 ± 17	0.94

4 SIMULATIONS OF CONTROLLED OSCILLATIONS

We also performed the MD simulations of the controlled operation of a nanotube-based oscillator. In these simulations the temperature of the outer wall was kept constant by means of the Berendsen thermostat. The harmonic electric field of the spherical capacitor described in section 1 acted on the inner moveable wall with one end capped and the other end terminated by hydrogen atoms. The frequency of the field was equal to the oscillation frequency at the initial moment of the simulation. The result which confirms the possibility of the operation mode with steady frequency is shown in Fig. 2. The MD simulation predicts that the critical amplitude of the control voltage is less than the value given by Eq. (5). This is because Eq. (5) is derived for a long oscillator with a high oscillation amplitude. In this case

Table 2: Calculated Q-factors and relative deviations δ of the inverse Q-factor of the (5,5)@(10,10) nanotube-based oscillator at different temperatures. The oscillator is 3.1 nm in length. The inner wall has one end capped and the other end terminated by hydrogen atoms.

T (K)	Q	δ
50	253 ± 33	1.19
100	162 ± 25	1.41
150	135 ± 19	1.45
300	55 ± 8	1.45

the expression (1) for the Van der Waals force is adequate. For the oscillator of 3.1 nm length considered here the Van der Waals force can not be taken constant and has less average value.

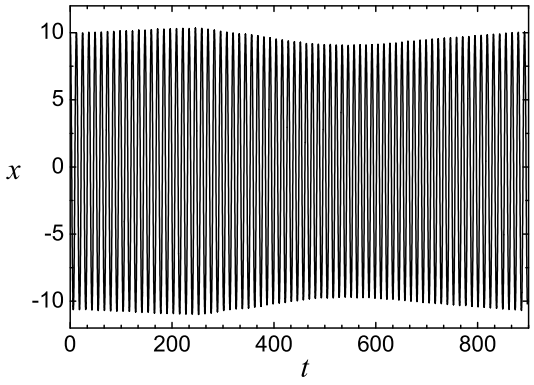

Figure 2: Distance x (in Å) between the mass centers of the walls as a function of time (in ps). The MD simulation of the controlled oscillations of the (5,5)@(10,10) nanotube-based oscillator 3.1 nm in length at temperature 50 K. The voltage 10.9 V is applied.

The MD simulations allow one to study the system behavior only for times of few nanoseconds. To reach longer simulation times and to investigate the influence of the Q-factor fluctuations on the possibility of controlling the oscillator operation the mechanical model was used. The motion equation for the moveable inner wall of the gigahertz oscillator with the fixed outer wall was solved semi-analytically. The frictional force was considered to be proportional to the relative velocity $F_f = -\gamma V$ of the walls. In this case the motion equation for the moveable wall is given by

$$\ddot{x} + \gamma\dot{x} + a\,\mathrm{sign}(x) = b\cos(\omega t), \qquad (6)$$

where $a = F_W/m$, $b = F_0/m$ and the frictional coeffi-

cient

$$\gamma = \frac{3}{8Q}\sqrt{\frac{F_W}{2sm}}. \quad (7)$$

The value of inverse Q-factor Q^{-1} was changed randomly each half period. The Gaussian distribution was used for the inverse Q-factor. This distribution was cut for the values less than $-9\langle Q^{-1}_{T/2}\rangle$ and greater than $11\langle Q^{-1}_{T/2}\rangle$. Smaller values of the relative deviation δ of inverse Q-factor Q^{-1} should correspond to greater sizes of NEMS (Table 2).

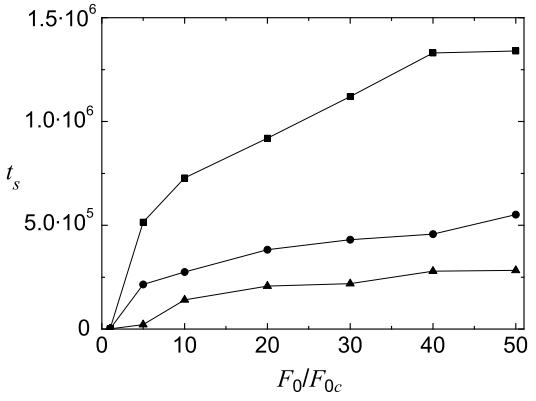

Figure 3: The dependence of the lifetime t_s (in oscillation periods) of the operation mode with steady frequency of the oscillator with Q-factor $Q = 253$ at temperature $T = 50$ K on the ratio of the control force amplitude to critical control force amplitude. The squares, circles and triangles correspond to relative deviations $\delta = 0.4$, $\delta = 0.5$ and $\delta = 1.6$, respectively.

Due to the Q-factor fluctuations the lifetime of the operation mode with steady frequency is not infinite. However, the performed simulations show that for the amplitude of the control force $F_0/F_{0c} \geq 2.0$ and the relative deviation $\delta \leq 0.2$ the lifetime t_s is greater than 10^8 oscillations periods. As can be seen in Fig. 3, the lifetime t_s decreases with increasing δ and only slightly depends on the amplitude F_0 for $F_0/F_{0c} > 20$.

5 CONCLUSIONS

We proposed a new method of controlling the operation of NEMS based on carbon nanotubes by a non-uniform electric field. The molecular dynamics simulations showed the possibility of the method on the example of the nanotube-based gigahertz oscillator. The simulations revealed considerable thermodynamic fluctuations of the oscillator Q-factor. The influence of the Q-factor fluctuations on the possibility of controlling the oscillator operation was investigated with the help of semi-analytical solution of the oscillator motion equation. It was demonstrated that an increase of the Q-factor fluctuations causes a decrease of the average lifetime of the operation mode with steady oscillation frequency. Thermodynamic fluctuations can impose restrictions on sizes and operational temperatures for which the controllability of NEMS is possible.

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