SIMULATION OF NANOTUBE-BASED NEMS CONTROLLED BY NONUNIFORM ELECTRIC FIELD

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The set of nanoelectromechanical systems (NEMS) based on relative motion of the walls of nanotubes has been suggested recently [1-3]. Thus elaboration of methods to control the motion of nanotube walls is an actual problem of nanomechanics.

We propose new method to control the motion of nanotube-based NEMS. It is based on the chemical adsorption of atoms and molecules on the open edges of the single-walled carbon nanotube, which results in the appearance of electric dipole moment. In this case the functionalized nanotube can be actuated by non-uniform electric field. Semi-empirical method of molecular orbitals with PM3 parameterization of Hamiltonian [4] has been used to calculate the electric dipole moments of functionalized (5,5) nanotubes [5].

Potential of the proposed method of controlling the motion of nanotube-based NEMS is demonstrated by the example of the gigahertz oscillator based on relative sliding of carbon nanotube walls. The scheme, operational principles and theory of such oscillator were considered recently [2]. The molecular dynamics simulations show that the Q-factor of the gigahertz oscillator is about Q = 100–1000 and the frequency of its free vibrations increases with time [3]. Therefore to keep constant frequency of oscillator it is necessary to compensate the energy dissipation by an external force. Here we consider the possibility to compensate the energy dissipation by application to the movable wall of the control force $F(t) = F_0 \cos \omega t$, where ω is the desirable oscillation frequency. The analysis of the energy balance shows that the critical amplitude F_0^{cr} of control force which is necessary for the exact loss compensation is the smallest in the case of the oscillator with the walls of the same length and equals to $F_0^{cr} = \pi F_W/32Q$, where F_W is the force retracting the inner wall into the outer one. If the amplitude F_0 greater than F_0^{cr}, the stationary mode of operation with constant frequency is possible. For the functionalized (5,5) nanotubes [5] the amplitude F_0^{cr} is estimated to be 0.1–1 pN. The voltage 2–10 V is sufficient to apply such force to the wall in a cylindrical or spherical capacitor. The parameters of the system and control forces enabling to obtain the stationary operation are determined by the analysis of the equation of motion. We have found that oscillation amplitude is varied with time since the switching on of the control force and the stationary mode of operation is achieved in tens nanoseconds (see Fig.1). The dependencies of the parameters which characterize the establishment of the stationary mode on the amplitude F_0 and Q-factor are obtained. At the stationary mode the phase shift $\Delta\varphi$ between control force $F(t) = F_0 \cos \omega t$ and oscillation amplitude $A(t) = A_0 \cos(\omega t - \Delta\varphi)$ has been established so that the oscillation energy dissipation is exactly compensated by the work of the control force (see Fig.2). The condition $F_0 \geq F_0^{cr}$ of the possibility of the stationary mode is obtained for the case where the phase shift $\Delta\varphi = 0$ and the frequency ω of the control force coincides with the initial oscillation frequency ω_0 at the moment of control force switching on. The start conditions where the stationary mode is possible are shown on Fig. 3.

We perform the molecular dynamics simulations of (5,5)@(10,10) nanotube-based oscillator and have found the considerable Q-factor fluctuations. The influence of the Q-factor fluctuations on the parameters of the system and control forces enabling to obtain the stationary operation is studied.

This work has been partially supported by the RFBR (AMP, YEL and OVE grants 05-02-17864 and 06-02-81036-Bel) and BFBR (grant No. F06R-075).

References:

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Figures:

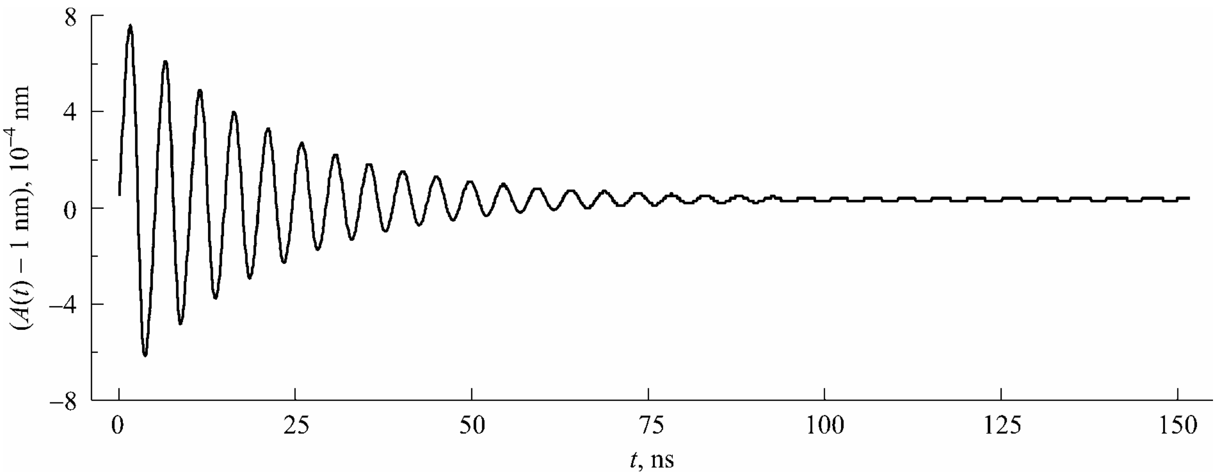

Fig. 1. Dependence of the oscillation amplitude on the time since the switching on of the control force with the amplitude $F_0 = 1.01F_0^{cr}$ for the system with $Q = 1000$

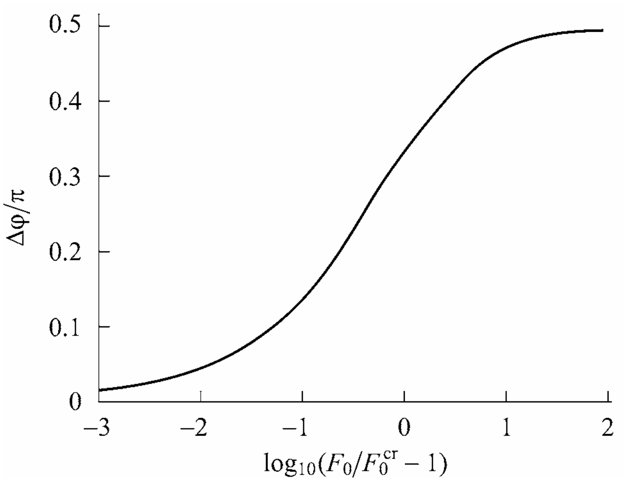

Fig. 2. Phase shift at the stationary mode between the control force and the oscillation amplitude as a function of $\log_{10}(F_0/F_0^{cr} - 1)$

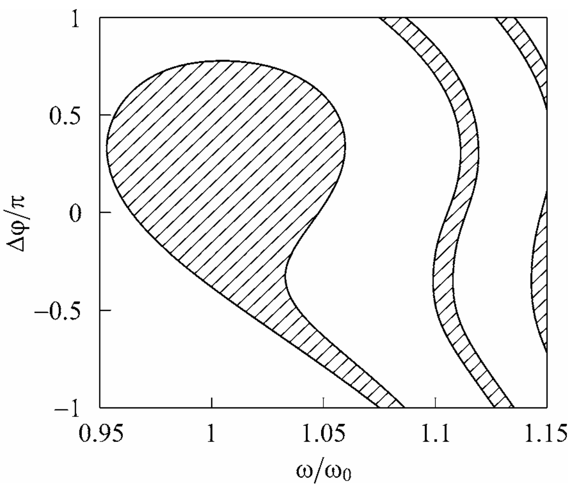

Fig. 3. Start phase shift $\Delta\varphi$ and the frequency ratio ω/ω_0 where the stationary mode is possible in the case of system with Q = 100 and control force amplitude $F_0 = 2F_0^{cr}$ are hatched