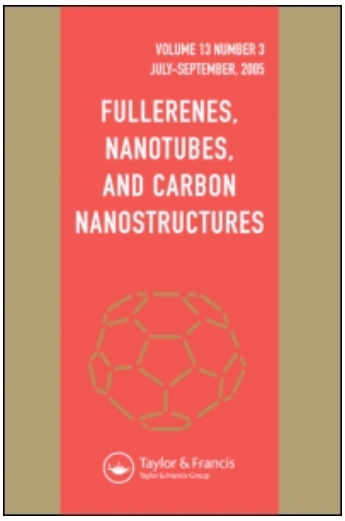

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Nanorelay Based on Multi-walled Nanotubes

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Abstract: New type of nanotube-based electromechanical nanorelay with first, second and control electrodes made of carbon nanotubes is considered. *Ab initio* and semi-empirical calculations have been used to estimate switching time and switching voltage of the nanorelay.

Keywords: NEMS, Nanotube, Nanodevice, Nanorelay, Memory cell, On-line storage

Unique properties of carbon nanotubes, such as ability of free relative sliding and rotation of the walls and metallic conductivity, allow using the walls of nanotubes as movable elements and elements of electric circuit in nanoelectromechanical systems (NEMS). An example of such an application is the nanotube-based nanomotor, which has been recently produced (1). A number of nanorelays with one electrode made of a carbon nanotube have been considered: two-terminal (2) and three-terminal (3) nanorelays based on the bending of nanotube and a two-terminal nanorelay based on relative motion of nanotube walls (4).

We propose some new schemata of two-terminal and three-terminal electromechanical "all carbon" nanorelay based on the relative motion of nanotube walls with all electrodes made of nanotubes (5). The condition that allows one to use the nanorelays as a memory cell of external or on-line storage was considered (5). In the present paper the switching voltage and switching time between position "on" and "off" for three-terminal nanorelays have been calculated (see Figure 1A).

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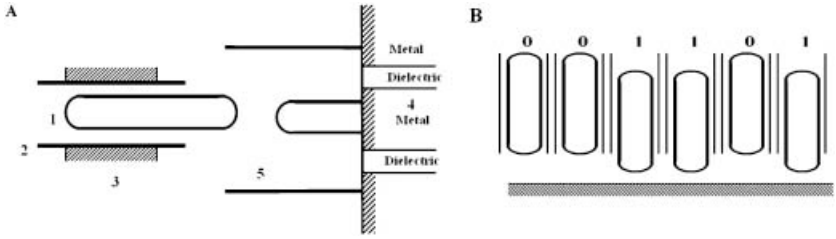

Figure 1. **A** is schematics of the three-terminal memory cells based on DWNTs in position 'on'. 1 is the movable inner wall; 2 is the fixed outer wall; 3, 4 and 5 are the first, second and control electrodes, respectively. **B** shows an example of the storage produced from the two terminal memory cells.

The density functional AIMPRO supercell code within the local density approximation has been used to calculate the capillary force F_c which retracts the inner wall of the nanotube inside the outer one [the details of the method can be found in (6)]. The structure of the caps of the nanotubes used as the electrodes of a nanorelay has been obtained using the Q-Chem 2.1 quantum chemistry package. The 6-12 Lennard-Jones potential with parameters σ =3.44 E, $\varepsilon = 2.62 \cdot 10^{-3}\ eV$ (7) has been used for calculations of the interaction between the nanotube caps as electrodes of a nanorelay.

To estimate the switching voltage we consider the inner movable wall of the first electrode and the control electrode as armatures of cylindrical capacitor. The electrostatic force acting on the movable wall can be estimated as

$$F_e = \frac{dE_{cap}}{dz} = \frac{d}{dz}\frac{CU_a^2}{2} = \frac{d}{dz}\frac{\pi\varepsilon_0 z U_a^2}{\ln R_c/R_m} = \frac{\pi\varepsilon_0 U_a^2}{\ln R_c/R_m}, \qquad (1)$$

where E_{cap} is the electrostatic energy of the capacitor, C is the capacity, U_a is the applied voltage, z is the length of the overlap of the movable wall and control electrode, ε_0 is the vacuum permittivity, R_m and R_c are radii of the movable wall and control electrode. Assuming the friction force is negligible and $R_c/R_m \sim 5$, the voltage of the switching between positions off and on can be determined by the condition $F_e > F_c$ and estimated to be about 6 V. In this case, the voltage needed to hold the nanorelay in position on is about U_h = 4.8 V.

According to the semiempirical calculation (8) the interwall interaction energy per one atom E_a is approximately the same for all considered pairs of neighboring wall with the interwall distance about 3.4 E and does not depend on the radius of the walls. The capillary force is given as

$$F_c = \frac{dE_a S}{dz_1} = \frac{dE_a 2\pi R_m dz_1}{dz_1} = 2\pi R_m E_a, \quad (2)$$

where S and z_1 are the surface and length of the overlap of the movable and fixed walls of the first electrode. Thus the capillary force is approximately proportional to the radius of the movable wall. We use equation (2) to estimate the dependence of switching voltage on the radius of the movable wall assuming that the interwall distance between movable and fixed walls of the first electrode is 3.4 E and the gap between the first and control electrodes $R_c - R_m$ = 1nm and using ab initio value of E_a. The dependence of the switching voltage on the radius of the movable wall is presented on Figure 2a. Figur 2a shows that the increase of the movable wall radius does not lead to a considerable increase of switching voltage.

The mechanical switching time can be estimated as the time required for the movable wall to move from one equilibrium position to another when the total van der Waals and electrostatic forces act. Here we estimate the switching time of the nanorelay with the (5,5) nanotube as the inner wall of the first and the second electrode by solving the motion equation. The following switching voltage pulse $U(t)$ was considered: $U(t) = U_p$ for $0 < t < t_p$, $U(t) = U_h = 4.8$ V for $t > t_p$. The dependence of pulse time t_p on voltage U_p is shown in Figure 2b. The time of switching between positions off and on is calculated to be in the range 10–30 ps.

A considerable progress has been achieved in nanotechnology techniques in the field of production of NEMS. This give us cause for optimism that the proposed all-carbon nanorelay will be produced in the near future.

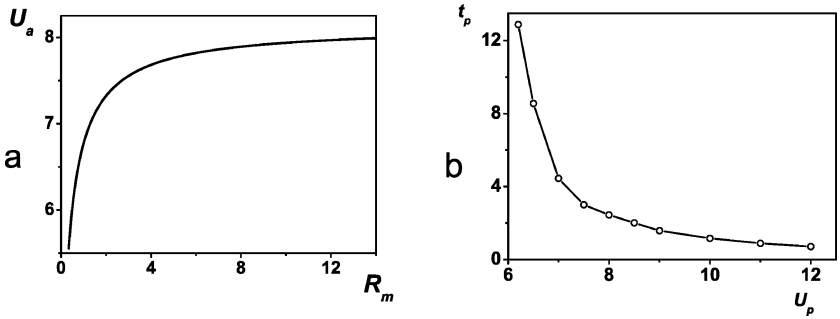

Figure 2. **a)** The dependence of the switching voltage U_a (in V) applied to the control electrode of the nanorelay shown on Figure 1A on the radius R_m (in Å) of the movable wall of the first electrode. **b)** The dependence of the pulse time t_p (in ps) on the voltage U_p (in V) applied to the control electrode for switching between positions 'off' and 'on' of the nanorelay.

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