

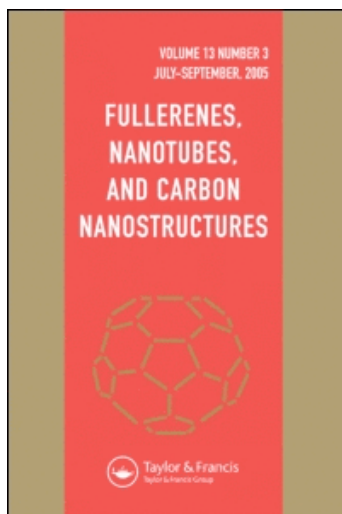
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## Fullerenes, Nanotubes and Carbon Nanostructures

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## Electromechanical Nanothermometer Based on Carbon Nanotubes

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**Abstract:** Electromechanical nanothermometer based on the interaction and relative motion walls of the (n,n)@(m,m) double-walled carbon nanotubes (DWNTs) is considered. Temperature measurements are carried out through the measurements of the conductivity. The dependence of the interwall interaction energy on the relative displacement of the walls of the DWNTs is computed *ab initio* using density functional theory. The conductivity of the DWNTs is calculated within the Huckel-Hubbard model. The operational characteristics of the nanothermometer are calculated.

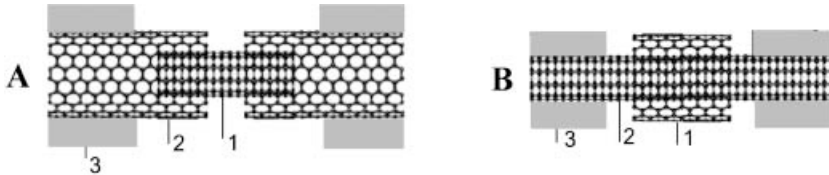
**Keywords:** NEMS, Nanotube, Nanodevice, Nanothermometer

With considerable progress in nanotechnology techniques, a number of feasible designs of nanoelectromechanical systems (NEMS) have recently evolved, in which the elements of electric circuits represent nanoobjects of progressively smaller scale (1, 2). Recently we have proposed a new concept of an electromechanical nanothermometer based on the interaction and relative motion of the components of a nanosystem (3, 4). It rests on the measurements of the conductivity of the components which, under the certain conditions, depends on their relative positions. The total conductivity of a system then changes significantly with the temperature due to the thermal vibrations of the components. The possibility of the

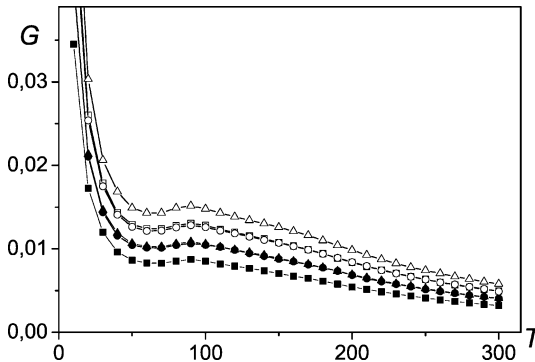
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general concept was considered on example of (6,6)@(11,11) double-walled nanotube (DWNT) (3, 4). Figure 1 is a schematic that shows a shuttle nanothermometer with a short movable outer wall (the shuttle) (1A) and a telescopic nanothermometer with a movable inner wall (1B). Here we calculate the operational characteristics of the nanothermometers based on (n,n)@(m,m) DWNTs.

Conductivity of the DWNTs with fixed relative positions of walls is calculated within the Huckel-Hubbard model (see details of calculations in (5)). A very weak temperature dependence of the conductivity above 50K was found (see Figure 2). This implies that the contributions to the



**Figure 1.** Schematic of an electromechanical nanothermometer. **A:** the shuttle nanothermometer with the movable outer wall, **B:** the telescopic nanothermometer with the movable inner wall. The movable wall is indicated as (1), the fixed wall as (2) and the attached electrodes as (3).



**Figure 2.** The conductivity  $G$  (in  $\text{Sm/m}$ ) as a function of the temperature  $T$  (in Kelvin degrees) calculated for different (n,n)@(m,m) DWNTs: (4,4)@(10,10) DWNT (filled squares), (5,5)@(10,10) DWNT (filled circles) (5,5)@(11,11) DWNT (filled triangles), (6,6)@(11,11) DWNT (open squares), (6,6)@(12,12) DWNT (open circles) and (7,7)@(12,12) DWNT (open triangles). The length of the movable wall is equal to 100 lengths of the unit cell of the DWNT.

total conductivity from phenomena other than the thermal vibration of the walls are insignificant.

For the shuttle nanothermometer design (Figure 1A), the displacement  $d$  of the shuttle (1) must be less than the distance  $L_{es}$  between the electrode (3) and the shuttle in any given time  $t$  of the operation of the nanothermometer, that is,

$$d = \sqrt{2Dt} < L_{es} \quad (1)$$

where  $D$  is the diffusion coefficient for the motion of the shuttle along the fixed wall (2). Expression for the diffusion coefficient  $D$  has been given in (6) as follows

$$D = A \exp\left(-\frac{BL}{kT}\right), \quad A = \pi \delta_z \sqrt{\frac{\Delta U_z}{2m}}, \quad B = \frac{\Delta U_z N_a}{l_m}, \quad (2)$$

where  $m$  is the mass of carbon atom,  $\Delta U_z$  and  $\delta_z$  are the energy barrier and period of sliding of the walls between the equivalent positions,  $N_a$  is the number of atoms in the unit cell of the shuttle,  $l_m$  is the length of the unit cell of the shuttle and  $L$  is the length of the shuttle. Thus, the length  $L$  of the shuttle can be estimated as

$$L = \frac{T}{B} \ln\left(\frac{2At}{L_{es}^2}\right), \quad (3)$$

and the total length  $L_{nt}$  of the nanothermometer between the electrodes as

$$L_{nt} = \frac{T}{B} \ln\left(\frac{2At}{L_{es}^2}\right) + 2L_{es}, \quad (4)$$

The total length of the nanothermometer is minimal if  $L_{es} = T/B$ . This condition for the minimum total length of the nanothermometer does not depend on the time of its operation.

The barriers  $\Delta U_z$  are computed *ab initio* using density functional theory (see details of calculations in (7)). The parameters  $A$  and  $B$  for the considered DWNTs are calculated using the *ab initio* values of the barriers. The dimensions of the nanothermometer have been estimated using equations (3) and (4).

Table 1 presents the lengths of the construction units of the nanothermometer, which operates at the temperatures  $T = 100\text{K}$  and  $T = 300\text{K}$  in two different regimes: the permanent mode of the operation during 100 years and the pulse mode with the time of the operation of  $10^{-6}$  sec. Table 1 shows that the nanothermometers are of a true nanometer size, which is governed merely by the length needed to attach the electrodes.

**Table 1.** Characteristic sizes of the nanothermometers based on the (n,n)@(m,m) DWNTs with the movable outer wall (shuttle):  $L_{nt}$  is the minimal total lengths between the electrodes,  $L_{es}$  is the distance between the electrode (3) and the shuttle and  $L$  is the length of shuttle.  $T$  is the temperature of the operation and  $t$  is the time of the operation

T=100k					
Nanotube	$L_{es},nm$	$t=10^{-6}$ sec		$t=100$ years	
		$L,nm$	$L_{nt},nm$	$L,nm$	$L_{nt},nm$
(4,4)@(10,10)	$2.9 \pm 1.1$	$15 \pm 7.0$	$21 \pm 7.0$	$120 \pm 45$	$125 \pm 45$
(5,5)@(11,11)	$2.0 \pm 0.5$	$12 \pm 3$	$16 \pm 3$	$80 \pm 21$	$85 \pm 21$
(6,6)@(12,12)	$1.4 \pm 0.3$	$10.1 \pm 2.0$	$12.9 \pm 2.0$	$60 \pm 11$	$63 \pm 11$
(5,5)@(10,10)	$0.36 \pm 0.02$	$4.2 \pm 0.2$	$4.9 \pm 0.2$	$17.0 \pm 0.8$	$18.0 \pm 0.8$
(6,6)@(11,11)	$0.27 \pm 0.01$	$3.2 \pm 0.1$	$3.8 \pm 0.1$	$12,8 \pm 0.5$	$13.0 \pm 0.5$
(7,7)@(12,12)	$0.19 \pm 0.01$	$2.50 \pm 0.07$	$2.90 \pm 0.07$	$9.7 \pm 0.3$	$10.0 \pm 0.3$

T=300k					
Nanotube	$L_{es},nm$	$t=10^{-6}$ sec		$t=100$ years	
		$L,nm$	$L_{nt},nm$	$L,nm$	$L_{nt},nm$
(4,4)@(10,10)	$8.8 \pm 3.4$	$27.1 \pm 15.1$	$44 \pm 15$	$340 \pm 130$	$350 \pm 130$
(5,5)@(11,11)	$5.9 \pm 1.5$	$24 \pm 8$	$35 \pm 8$	$240 \pm 60$	$240 \pm 60$
(6,6)@(12,12)	$4.2 \pm 0.8$	$21 \pm 4.5$	$29 \pm 4.5$	$170 \pm 30$	$180 \pm 30$
(5,5)@(10,10)	$1.10 \pm 0.05$	$10.2 \pm 0.5$	$12.4 \pm 0.5$	$49.4 \pm 2.4$	$51.6 \pm 2.4$
(6,6)@(11,11)	$0.80 \pm 0.02$	$7.9 \pm 0.3$	$9.5 \pm 0.3$	$36.6 \pm 1.3$	$38.2 \pm 1.3$
(7,7)@(12,12)	$0.6 \pm 0.2$	$6.4 \pm 0.2$	$7.6 \pm 0.2$	$27.8 \pm 0.7$	$29.0 \pm 0.7$

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