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Diffusion of Walls in Double-Walled Carbon Nanotubes

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Abstract: Possibility of rigid and non-rigid diffusion of the walls in double-walled carbon nanotubes with armchair and zigzag walls is considered. Diffusion coefficients and mobilities are calculated using ab initio values of the barriers to relative motion of the walls. Operation modes for possible nanodevices based on relative motion of the walls are discussed.

Keywords: Carbon nanotubes, interwall interaction, incommensurability defects, diffusion

A wide range of electromechanical nanodevices based on relative motion of the walls of carbon nanotubes has been recently proposed (see for example (1–5)). Theoretical modelling of orientation and relative motion of the walls holds the key to success of these applications. Our previous work (6, 7) has been concerned with the study of interwall interaction in double walled carbon nanotubes (DWNTs) and computation of barriers to relative motion of their walls using density functional theory (DFT). In present letter, we extend this study to investigating relative diffusion of the walls for DWNTs with non-chiral commensurate walls which are based on ab initio values for the barriers to relative motion of the walls computed in

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(6, 7). Cases of compatible and incompatible rotational symmetries of zigzag and armchair walls are considered.

Possibility of formation of incommensurability defect (*ID*) in DWNTs with non-chiral commensurate walls has been proposed in (6, 8). Similarly to the motion of dislocations in crystals, the *ID* can travel between the ends of a DWNT causing relative displacement of the walls. However, formation of the *ID* can only occur if the length of the wall is greater than the length of the *ID*, l^{ID}. This compares favourably with dislocation structure of submonolayer film near commensurate-incommensurate phase transition for which dislocations can be only formed in sufficiently large islands (9)

If the movable wall is short, $l < l^{ID}$, its motion corresponds to the case of rigid concerted diffusion and all barriers to relative motion of the walls in a DWNT are traversed in commensurate way. In this case, barrier to relative diffusion of the walls is proportional to the length of the movable wall. In principle, two types of relative motion of the walls are possible and these depend on length of the movable wall. Rigid diffusion of the walls can be achieved for very short walls. If the movable wall is long enough, non-rigid incommensurate diffusion occurs as a result of the *ID* motion. These two modes of relative diffusion of the walls in DWNTs are explained in Figure 1. Calculations (8) show that formation of the *ID* requires the energy of several eV and the length of the *ID* of tens of nanometers. These values of the energy of formation and the length of the *ID* allow us to conclude that for short movable walls, rigid diffusion takes place at room temperature

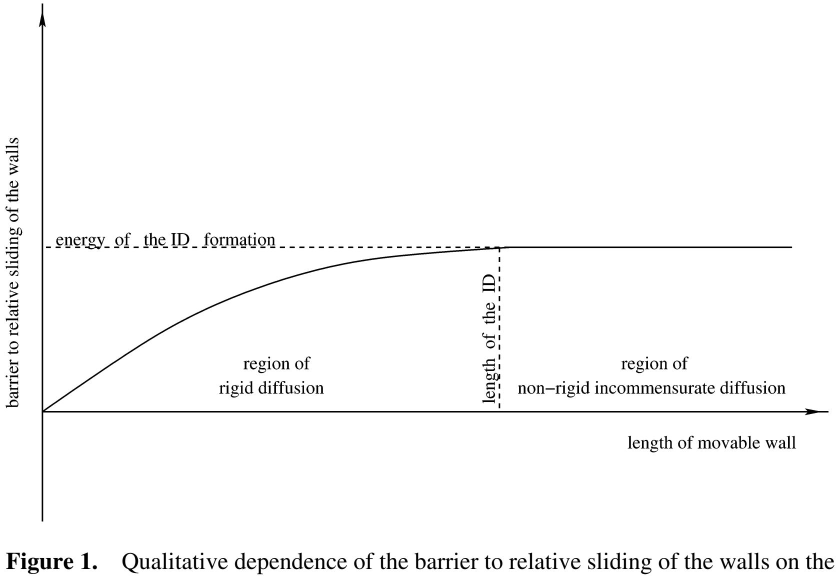

Figure 1. Qualitative dependence of the barrier to relative sliding of the walls on the length of movable wall: two modes of relative diffusion of the walls in DWNTs.

(conditions at which formation of the *ID* is highly unlikely) and can be considered as a valid process in mechanical nanodevices.

For DWNTs, the Fokker–Planck equation has been obtained in (2, 3) for diffusion and drift of the walls along the helical line in rigid mode at temperatures $kT \ll \Delta U$ (ΔU is the barrier to relative motion of the walls). The following expressions for diffusion coefficients corresponding to diffusion along the nanotube axis, D_z, and about the nanotube axis, D_φ, are given in (6)

$$D_x = a_x \exp\left(\frac{b_x l}{T}\right) \quad x = z, \varphi \tag{1}$$

$$a_z = \pi\delta_z\sqrt{\frac{\Delta U_z}{2m}} \quad a_\varphi = \frac{\pi\delta_\varphi}{R}\sqrt{\frac{\Delta U_\varphi}{2m}} \tag{2}$$

$$b_x = \frac{\Delta U_x N}{tk} \quad x = z, \varphi \tag{3}$$

where ΔU_z and ΔU_φ are the barriers to relative sliding and rotation of the walls, δ_x is a distance between two neighbouring minima of the interwall interaction energy surface, *m* is the mass of carbon atom, *N* is the number of atoms in the unit cell of the movable wall, *R* is the radius of the movable wall, and *t* is the translational length of the unit cell of the movable wall. Mobility for sliding along the axis, B_z, can be easily obtained from the diffusion coefficient, D_z, using the Einstein ratio $D_z = kTB_z$. To characterize the rotational drift we introduce the rotational mobility as

$$B_\varphi = \frac{w}{F} = \frac{D_\varphi R}{kT} \tag{4}$$

where *w* is the angular velocity of the movable wall and *F* is the sum of tangential components of forces acting on atoms of the movable wall. The values of parameters a_x and b_x calculated for a set of DWNTs are presented in Table 1.

Two operation modes for possible mechanical nanodevices based on relative motion of the walls have been suggested in (2, 3) for the case when external forces do not cause deformation of a nanotube. Under zero time-average acceleration, if $kT \ll \Delta U$, the motion of the walls is controlled by diffusion, and if $F_x\delta_x/2 \ll \Delta U$, this motion is controlled by drift (F_x is a projection of the force causing drift in the direction of motion). In the latter case, motion of the walls can be described by the Fokker-Planck equation. The Fokker–Planck operation mode (for forces $F_x\delta_x/2 \ll kT$) is based on relative drift of the walls. For example, a mechanical nanoswitch (5) or nanodrill (2–4) can operate in the Fokker–Planck mode. However, the Fokker-Planck mode does not allow a precise control of relative positions of the walls. The second type of the operation mode is the accelerating mode (for forces $F_x\delta_x/2 \gg kT$). In this mode, the controlled relative displacement of the walls within the distances less than δ_x is possible, and

Table 1. Characteristics of relative diffusion and drift of the inner wall of DWNTs

Nanotube	$a_z \times 10^{-8}$ m^2/s	$a_\varphi \times 10^{10}$ rad^2/s	b_z Kelvin/nm	b_φ Kelvin/nm	l_z nm	l_φ nm
(4,4)@(10,10)	0.21 ± 0.07		34 ± 13		330 ± 140	
(5,5)@(11,11)	0.23 ± 0.05		51 ± 13		220 ± 60	
(6,6)@(12,12)	0.25 ± 0.03	1.8 ± 0.7	71 ± 13	23 ± 13	160 ± 30	400 ± 230
(5,5)@(10,10)	1.30 ± 0.04	16.6 ± 0.3	273 ± 13	774 ± 13	43.6 ± 2.0	12.81 ± 0.25
(6,6)@(11,11)	1.39 ± 0.03		372 ± 13		31.9 ± 1.1	
(7,7)@(12,12)	1.49 ± 0.03		502 ± 13		23.7 ± 0.6	
(9,0)@(18,0)	7.90 ± 0.01		3475 ± 8		3.48 ± 0.01	
(10,0)@(20,0)	4.39 ± 0.02		1192 ± 8		9.98 ± 0.06	

this operation mode can be suggested if the barriers to relative motion of the walls are high enough to prevent the diffusion. A variety of nanoresistors and electrical nanoswitches operating in the accelerating mode have been suggested in (2–4).

In order to identify which DWNT considered in this letter can be possibly used in nanodevices based on the two operation modes discussed, we first calculate l_φ and l_z corresponding to relative rotation and sliding of the walls (see Table 1). These lengths are characterized by one displacement of the walls between the two neighbouring minima of the interwall interaction energy surface, on average, say, during 24 hours at room temperature. In experiment (1), the controlled motion of the walls has been realized with MWNTs of hundreds nanometers in length. Our estimations show that for the armchair (n,n)@(n + 5,n + 5), zigzag (9,0)@(18,0) and (10,0)@(20,0) DWNTs, diffusion of the walls is possible in principle for relative sliding of the walls, but only if the movable wall is impracticably short. For the armchair (5,5)@(10,10) DWNT, in addition to relative sliding, relative rotation is also unlikely. These DWNTs, for which relative diffusion along the nanotube axis and rotational diffusion of the walls is unfeasible, can be used in nanodevices based on the accelerating operation mode, where there is no risk of diffusion of the walls to hinder the operation of a nanodevice. Otherwise, relative diffusion of the walls is conceivable at room temperatures if the walls are hundreds nanometers in length.

For the (4,4)@(10,10) DWNT which corresponds to the incommensurate phase (8), a non-rigid diffusion of the walls along the nanotube axis is possible as a result of the *ID* motion. DWNTs of this type can be used in nanodevices in either operation mode depending on the temperature and length of the movable wall.

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