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Modelling interwall interactions in carbon nanotubes: fundamentals and device applications

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Carbon nanotubes are the most commonly used 'building blocks' of modern nanotechnology. Their unique mechanical and electronic properties, stability and functionality show great promise in creating functional devices on the nanometre scale. One of the great challenges in using this scale is the ability of physical manipulation of the components, such as their positioning and assembling. Strong correlation between the structure and mechanical interactions of the walls of carbon nanotubes provides self-regulation of their relative motion. This can be further exploited in low-friction and high-stiffness devices. In this paper, we present a condensed overview of the recent progress in fundamental understanding of nanomechanical and nanoelectromechanical behaviour of carbon nanotubes and their applications in nanodevices.

Keywords: carbon nanotubes; interwall interactions; nanoelectromechanical devices; incommensurability defects; Frenkel–Kontorova model

1. Introduction

Nanoelectromechanical systems (NEMS) are built from the components which are integrated or organized on the nanometre scale. This transfers us into the truly small world. One nanometre is one billionth of a metre, approximately 10 atomic diameters. Thus, the nanometre scale is of the order of the size of individual molecules. NEMS involve using the properties of submicrometre scale machines which move atoms and molecules and create new artificial structures, performing work in this small nanoworld.

The unique electronic properties of carbon nanotubes make them excellent candidates in the electronic industry for replacing silicon-based technologies with those based on nanocarbons. One of the greatest current challenges of nanoscience is building a molecular electronic computer. The existing technologies for data storage and computer memory, such as magnetic hard disks and silicon-based microelectronics, cannot be reliably used in submicrometre scale machines and will soon reach their fundamental physical limitations. Progressive minds already design, through molecular nanoengineering, universal memory devices capable of non-volatile, long-term data storage as well as

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high-speed temporary data processing storage (Rueckes *et al.* 2000; Choi *et al.* 2004; Kish & Ajayan 2005). Recently, Nantero, Inc. presented a nanoelectromechanical memory array based on suspended nanotubes (Ward *et al.* 2004) called nanotube random access memory (NRAM).

Furthermore, carbon nanotubes continue to provide opportunities for using their mechanical properties in NEMS. Several impressive experimental reports have been recently published, which use sliding and rotation of the walls of nanotubes in novel nanodevices. Fennimore *et al.* (2003) demonstrated a rotational nanoactuator in which a multi-walled carbon nanotube (MWNT) serves as both an electrical wire and a rotational bearing. The interwall sliding force in a MWNT has been successfully measured using a nanomanipulation system that combines a controlled electrical breakdown process with a manipulation process using a scanning electron microscope (Akita & Nakayama 2003). Owing to their well-defined structure, carbon nanotubes are particularly attractive for theoretical and simulation studies. A variety of NEMS based on the relative motion of the walls of double-walled carbon nanotubes (DWNTs) have been suggested theoretically. New designs of a nanogear (Srivastava 1997), an artificial gigahertz oscillator (Zheng & Jiang 2002), a variable nanoresistor and a perforating nanodrill (Lozovik *et al.* 2003; Lozovik & Popov 2004), and an electromechanical nanothermometer (Bichoutskaia *et al.* 2007) have been proposed for realization.

In this paper, we discuss the possibilities of using the self-regulation of the relative motion of the walls of MWNTs in nanodevices. We start with an overview of NEMS based on the controlled and reversible telescoping motion of MWNTs, with particular emphasis on the physics that defines this process. We then discuss how the interaction of the walls in nanotubes affects their structural and elastic properties, show that the incommensurability defect (ID) can be formed on the interacting walls and explain how the ID can be used in NEMS.

2. Electromechanics based on telescoping carbon nanotubes

Initial construction of the first bearings and mechanical switches (Cumings & Zettl 2000) out of MWNTs with diameters of a few tens of nanometres represented an important step towards the controlled manipulation of the components of molecular devices. Using a manipulator inside a high-resolution electron microscope, they are able to pull out a few inner layers of the MWNT fixed at one end and move it back and forth. This experiment demonstrates near-ideal low-friction and low-wear linear and rotational nanobearing, where the outer layers of the MWNT form a sleeve and the inner core forms a shaft. The interacting surfaces are atomically perfect, and the spacing between the sleeve and the shaft is just the van der Waals distance in graphite. Consequently, there is no grit between them and the problem of wear can be avoided. Such bearing could be a very efficient part of future nanodevices.

Theoretical calculations (Kolmogorov & Crespi 2000) indicate that the interwall interaction energy in a MWNT is indeed very small and favours such an easy bearing. However, the sleeve and the shaft move without difficulty only if they have different chiralities and, therefore, incommensurate. Lack of commensurability between the sleeve and the shaft implies very low barriers to their relative motion and a dramatic weakening of the corrugation in the

interwall interaction potential. What is more, the barriers to the relative motion of incommensurate walls do not increase with the length of a nanotube, but fluctuate near the average value (Damnjanović *et al.* 2002). Such incommensurate walls, even if they contain thousands of carbon atoms, have barriers to the relative motion of the walls comparable to those of a single unit cell.

The walls of a nanotube are commensurate if the ratio of the lengths of their unit cells is a rational fraction. Barriers to the relative motion of commensurate walls of a sufficiently long nanotube are proportional to the nanotube length: $\Delta U = \Delta U_{\mathrm{uc}} n_{\mathrm{uc}}$, where ΔU_{uc} is the barrier per unit cell and n_{uc} is a number of unit cells in a nanotube. Conceivably, there is a possibility of fabrication of, say, a DWNT with commensurate walls and custom-ordered values of barriers to the relative motion of the walls.

The route towards an electromechanical nanoswitch based on the controlled and reversible telescopic extension of MWNTs was first reported by Forro (2000). The inner core of a MWNT after being pulled out of the sleeve by a manipulator, after release, could be completely pushed back into the sleeve by capillary forces restoring a MWNT to its original condition. Such a telescoping process was found to be fully reversible and could be repeated a number of times without apparent damage to the sliding surfaces (Cumings & Zettl 2000). Forro (2000) suggested a simple electronic control of such back-and-forth movement. If the nanoswitch is charged, due to the Faraday cage effect the electrons are located only on the surface of the nanoswitch. The density of the charge can be changed through an electric contact attached to the fixed non-moving part of the MWNT. The change in the electrostatic energy due to the increase in the surface charge density acts in the opposite direction of the van der Waals force restoring the extruded MWNT. The nanoswitch could be opened and closed by altering the amount of charge. Several internal forces are associated with telescoping MWNTs. However, what mainly defines the process of extending and retracting the core of the MWNT is the balance between the restoring capillary force and the threshold forces to the relative motion of the core (Bichoutskaia *et al.* 2006*a*).

(*a*) *Threshold and capillary forces determining the telescoping motion of the walls in MWNTs*

The telescopic process of extending and retracting the core of the MWNT can take place only if the restoring capillary force, F_{cap}, acting between the core and the sleeve is greater than the threshold forces for the sliding and the rotation of the core, F_{z} and F_{ϕ}, respectively. The threshold forces have been previously defined for DWNTs (Bichoutskaia *et al.* 2005) and can be written as

$$F_{\mathrm{z}} = \frac{\pi \Delta U_{\mathrm{z}} N_{\mathrm{c}} l}{\delta_{\mathrm{z}} t_{\mathrm{cs}}} \quad \text{and} \quad F_{\phi} = \frac{\pi \Delta U_{\phi} N_{\mathrm{c}} l}{\delta_{\phi} R_{\mathrm{c}} t_{\mathrm{cs}}}, \tag{2.1}$$

where N_{c} is the number of carbon atoms in the unit cell of the outer wall of the telescoping core, l is the length of overlap between the core and the sleeve, R_{c} is the radius of the outer wall of the core and t_{cs} is translational length of the unit cell of a DWNT which comprises the outer wall of the core and the inner wall of the sleeve. The remaining values in equation (2.1) are global characteristics of the energy surface which defines the interaction between the core and the sleeve:

ΔU_z and ΔU_ϕ are the energy barriers and δ_z and δ_ϕ are periods of the sliding and rotation of the core between the equivalent positions, respectively. The threshold forces are proportional to the barriers to the sliding and rotation of the core. In this formalism, the barriers are traversed in adiabatic manner without a local expansion or contraction of the interacting walls. It is also assumed that for a sufficiently large overlap between the core and the sleeve, contributions from the edges are small and can be neglected.

The capillary force, however, is independent of the core extension or, equivalently, independent of a contact area l and can be defined as

$$F_{\mathrm{cap}} = \frac{\mathrm{d}U}{\mathrm{d}l} = \frac{U_{\mathrm{cs}}^{\mathrm{int}} N_{\mathrm{c}}}{t_{\mathrm{cs}}}, \tag{2.2}$$

where $U_{\mathrm{cs}}^{\mathrm{int}}$ is the interaction energy between the core and the sleeve of a MWNT (per atom of the outer wall of telescoping core).

Maximum contact area between the core and the sleeve, for which the threshold forces do not hinder the retraction of the core, can therefore be found from the balance of the forces $F_{\mathrm{cap}} = F_{\mathrm{z}}$ as

$$l_{\max} = \frac{\delta_{\mathrm{z}} U_{\mathrm{cs}}^{\mathrm{int}}}{\pi \Delta U_{\mathrm{z}}}. \tag{2.3}$$

Bichoutskaia *et al.* (2006*a*) explored the relative motion of the walls in DWNTs with different radii and chiralities. The interwall interaction energy surfaces have been computed using density functional theory with periodic boundary conditions and Gaussian basis set for carbon which has been optimized to reproduce basal plane binding energy and elastic constants for basal shear in graphite. It was found that the barriers to the relative rotation of the walls in excess of the accuracy of calculations can be found only for DWNTs with compatible rotational symmetry of the walls. DWNTs with incompatible rotational symmetry of the walls have extremely small barriers to the relative rotation of the walls. This suggests the possibility of orientational melting in such DWNTs, i.e. a sudden rotational diffusion of the walls or even free rotation at quite low (room) temperatures.

Barriers to the relative sliding of the walls are usually greater than that to their relative rotation. For armchair DWNTs, the barrier to the relative sliding of the walls increases as their radius grows. For example, the computed value of ΔU_z is 0.143 meV per atom for the (5, 5)@(10, 10) DWNT and 0.220 meV per atom for the (7, 7)@(12, 12) DWNT (Bichoutskaia *et al.* 2006*a*). For the overlap of the walls of 100 nm, which corresponds to the experimental conditions (Cumings & Zettl 2000), the threshold force F_z for the relative sliding of the walls can be estimated, using equation (2.1), as 9.7 nN for the (5, 5)@(10, 10) DWNT and 17.8 nN for the (7, 7)@(12, 12) DWNT. Furthermore, maximum overlap of the walls $l_{\max}$, for which threshold force F_z is greater that the restoring capillary force, can be estimated using equation (2.3), as 6.43 nm for the (5, 5)@(10, 10) DWNT and 4.24 nm for the (7, 7)@(12, 12) DWNT. Both the (5, 5)@(10, 10) DWNT and the (7, 7)@(12, 12) DWNT belong to the same family of DWNTs, namely, the (n, n)@$(n+5, n+5)$ family. It has been shown (Bichoutskaia *et al.* 2006*a*) that within the same family of DWNTs, say, (n, n)@$(n+5, n+5)$ or (n, n)@$(n+6, n+6)$, $l_{\max}$ decreases with an increase in the radius of the walls.

It has been further concluded that if the outer wall of the telescopically pulled out core of a MWNT and the inner wall of the sleeve comprise a non-chiral commensurate pair, the maximum overlap of these walls, for which threshold forces remain greater than the capillary forces, is always significantly smaller than the experimental value of an order of 100 nm. Therefore, for such pairs of neighbouring walls, the core cannot be fully pushed back by the capillary forces, and the experiment of Cumings & Zettl cannot be successfully performed.

However, if the interacting walls of the core and the sleeve are incommensurate then the barriers to their relative motion, and hence the threshold forces, do not increase with the length of the overlap. As a result, these forces will never prevent the retraction of the core. Another possibility is a chiral commensurate pair of neighbouring walls, say, the (8, 2)@(16, 4) DWNT. For this DWNT, the interwall interaction energy and the barrier to the relative sliding of the walls have been computed (Bichoutskaia *et al.* 2005), and the reported values are $U^{\mathrm{int}} = 17.5$ meV per atom and ΔU_z is less than 0.001 meV per atom, respectively. Using a method described elsewhere (Damnjanović *et al.* 2002), the period of the relative sliding of the walls can readily be calculated as $\delta_z = 0.046$ nm. From equation (2.3), maximum overlap $l_{\max}$ of the walls of the (8, 2)@(16, 4) DWNT, for which the controlled reversible telescoping can be achieved, is estimated to be greater than 250 nm. This is the lowest estimate of $l_{\max}$, and in principle this value can be orders of magnitude greater!

Since the experiment of Cumings & Zettl will fail only if the outer wall of the core and the inner wall of the sleeve are a non-chiral commensurate pair, reversible telescopic extension of MWNTs could be used for selecting and identifying pairs of non-chiral commensurate walls.

(*b*) *Nanorelays*

The experiment of Cumings & Zettl demonstrates that extremely light, mechanically and chemically resistant MWNTs hold great promise for NEMS applications. In the future, they will play a major role in manufacturing nanomachines with low-friction and low-wear springs, bearings and switches as their essential components.

In transistor technology, several concepts of logic memory and storage devices based on carbon nanotubes have been developed recently. In the device architecture of an ultra-high density transistor based on a vertical array of carbon nanotubes (Choi *et al.* 2004), each nanotube is electrically attached to the bottom source and upper drain electrodes, and the gate electrode is positioned around the nanotube. Such a device requires fabrication of a nanoscale array which consists of hundreds of vertical nanotubes working as memory elements. Rueckes *et al.* (2000) proposed the first integrated device that fully exploits single-walled carbon nanotubes (SWNTs) for storing, reading and writing information. In a SWNT-based cantilever nanorelay, the key components are a movable part containing a SWNT or MWNT and a fixed ground plane modelled by a graphite bulk. When the voltage is applied, the tube deflects and comes in contact with the ground plane (the ON state). When the potential is released, the tube and the ground plane are separated (the OFF state). However, the short-range and van der Waals forces have significant influence on the characteristics of such a device and introduce some design constraints. Nanorelays with

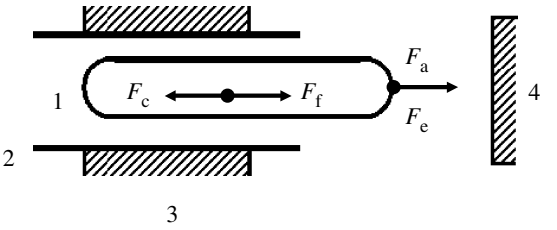

Figure 1. Schematic of a memory cell with a flat electrode based on a conducting DWNT: 1 is a moving capped inner wall; 2 is a fixed outer wall; 3 and 4 are the electrodes. F_a is the attraction force of the van der Waals interaction between the wall 1 and electrode 4, and F_e is the electrostatic force between the electrodes 3 and 4. The forces of the interwall interaction are F_c, the capillary force which retracts the inner wall back and F_f, the static friction force. The balance of forces is shown for the ON state.

small-diameter nanotubes have the stiction and the adhesion problems. If the gap between the cantilever nanotube and the plane is very small, then even without the voltage applied the tube can stick to the ground plane owing to the van der Waals forces. Furthermore, these forces will keep the tube and the plane together making their separation after the contact difficult (Aluru *et al.* 2002). NEMS based on suspended nanotubes are effectively applied to memory devices without both the stiction and the adhesion problems because the tensions of the suspended nanotubes are higher than those of the cantilevered ones. An excellent example of such NEMS is a NRAM composed of drain, source, gate and nanotube bridges, freely suspended between source and drain electrodes, in the vicinity of a gate (Ward *et al.* 2004).

Maslov (2006) suggested a new highly integrated, fast and macroscopically addressable data storage device which can be used as non-volatile random access memory, as well as terabit solid-state storage. A simple schematic of the memory cell in the ON state is shown in figure 1. This device is based on a conducting DWNT and essentially represents a nanorelay, a three-terminal device which acts as a switch in the gigahertz regime. We further developed the general design and operation principles of such memory cells. Popov *et al.* (2007) suggested schematics of 'all-carbon' memory cells with a carbon nanotube attached to the second electrode and with a control electrode made of a carbon nanotube. The essential working condition for any nanosystem to operate as a relay is the presence of two minima in the interaction energy of its components (the ON and OFF states), or so called bistability. Four kinds of forces are involved in the operation of these devices. First, there is a van der Waals attraction, F_a, between the cap of the inner nanotube 1 and the electrode 4. When the inner wall 1 is in the extended position, the memory cell stays in the ON state due to the van der Waals forces between the wall 1 and the electrode 4. This provides their permanent contact after the power is switched off and yields the non-volatile capability of the memory cell. The second force required for operation of the memory cell is the electrostatic force, F_e, which is also applied to the inner wall 1. This force pushes the inner wall back and forth providing a controlled motion between the ON and OFF states. The force based on the weak van der Waals interaction between the walls is the restoring capillary force, F_c, which retracts the inner wall 1 back inside the fixed outer

wall 2. When no voltage is applied, this force provides a permanent gap between the cap of the inner wall 1 and the electrode 4, thus keeping the memory cell in the OFF state. Another force based on the interwall interaction of the walls of a DWNT is the static friction force, F_f. The balance of these forces in all-carbon nanorelays made of a DWNT with non-chiral commensurate walls has been recently analysed by Popov *et al.* (2007), as well as the incommensurate and chiral cases.

The nanorelay is only one of many examples of using mechanical characteristics of nanotubes in NEMS. Industrial realization of these NEMS cannot be achieved without full understanding of the fundamental science giving rise to the properties of carbon nanotubes. Furthermore, one such fundamental question remains unanswered.

3. Can double-walled carbon nanotubes be commensurate?

Owing to the effects of curvature, the bond length in carbon nanotubes is slightly different to that in graphite. It also changes with the size and chirality of a nanotube. Additionally, the interaction of the walls of a nanotube (or other influences) may lead to a local contraction or expansion of the walls and a subsequent change in the bond length. As a result, a phase transition from commensurate to incommensurate structure may occur, and the tube acquires a periodic structure of alternating long 'near-commensurate' regions and short regions of IDs.

Recent high-resolution transmission electron microscopy experiments on DWNTs (Hashimoto *et al.* 2005) showed that the walls of a DWNT can indeed elastically deform to produce commensurate segments between the defects. It is important to be able to recognize whether the walls of a DWNT have commensurate or incommensurate structure, as these structures show very different fundamental mechanical behaviour and will find applications in distinctly different components of nanodevices. A DWNT with commensurate walls can be used only in devices in which a precise control of the relative motion of the walls is required, for example in variable nanoresistors (Lozovik *et al.* 2003). A DWNT with incommensurate walls holds best promise for applications in mechanical elements which require perfect bearing and fast relative motion of the walls.

(*a*) *Incommensurability defects in DWNTs: Frenkel–Kontorova model*

A historic approach to describe incommensurate systems is the model of Frenkel and Kontorova (FK), which was first introduced to describe the dynamics of dislocations in crystals (Frenkel & Kontorova 1938). In a more general context, the FK model describes a system of interacting particles subjected to a periodic substrate potential. In the past, this model was successfully applied to describe such problems as a closely packed row of atoms in crystals (Paneth 1950), a chain of ions in a channel of one-dimensional conductors (Boyce & Huberman 1979) and hydrogen atoms in hydrogen-bonded systems (Pnevmantikos *et al.* 1991).

We used the FK model to investigate the effects of expansion and contraction of the walls of a DWNT (Bichoutskaia *et al.* 2006*b*). The possibility of expansion of a SWNT as a result of the interaction with a graphite substrate was first suggested by Kolmogorov *et al.* (2004). However, we made the first attempt to

quantify these effects and combine an analytical FK approach with *ab initio* studies of the interaction of the walls to calculate the length and the energy of formation of the ID in DWNTs (Bichoutskaia *et al.* 2006*b*).

The one-dimensional discrete FK model consists of a linear harmonic chain of particles coupled with springs of elastic constant k_0 and natural length l_0 subject to an external spatially periodic potential of period λ and amplitude W. The Hamiltonian for the particles is commonly written as

$$H = \sum_j \left\{ \frac{k_0}{2} (x_{j+1} - x_j - l_0)^2 + \frac{1}{2} W(1 - \cos(2\pi x_j/\lambda)) \right\}, \tag{3.1}$$

where x_j is the coordinate of particle j.

This standard discrete FK model can be extended to the case of two interacting harmonic chains which represent two interacting walls of a DWNT. If one of the chains gets expanded (denoted by a superscript e) and another contracted during the interaction (denoted by a superscript c), the Hamiltonian (3.1) can be rewritten as follows:

$$H = \sum_j \left\{ \frac{k^{\mathrm{e}} k^{\mathrm{c}}}{2(k^{\mathrm{e}} + k^{\mathrm{c}})} \left(x^{\mathrm{e}}_{j+1} - x^{\mathrm{e}}_j - l^{\mathrm{e}}_0 - x^{\mathrm{c}}_{j+1} + x^{\mathrm{c}}_j + l^{\mathrm{c}}_0\right)^2 + \frac{1}{2} W\left(1 - \cos\left(2\pi\left(x^{\mathrm{c}}_j - x^{\mathrm{e}}_j\right)/\lambda\right)\right) \right\}. \tag{3.2}$$

After having introduced a new dimensionless coordinate $u_j = \left(x^{\mathrm{e}}_j - x^{\mathrm{c}}_j\right)/\lambda$ and having defined $k = (k^{\mathrm{e}} k^{\mathrm{c}})/(k^{\mathrm{e}} + k^{\mathrm{c}})$ and $l_{\mathrm{d}} = (l^{\mathrm{e}}_0 - l^{\mathrm{c}}_0)/\lambda$, the Hamiltonian (3.2) can be simplified as

$$H = \sum_j \left\{ \frac{k\lambda^2}{2} (u_{j+1} - u_j - l_{\mathrm{d}})^2 + \frac{1}{2} W(1 - \cos(2\pi u_j)) \right\}. \tag{3.3}$$

By solving the equilibrium equations $\partial H/\partial u_{\mathrm{j}} = 0$ for all j values, we find solutions with no forces on the particles and thus obtain

$$u_{j+1} - 2u_j + u_{j-1} = -\frac{W\pi}{k\lambda^2} \sin(2\pi u_j). \tag{3.4}$$

In the continuum limit, equation (3.4) can be written as

$$\frac{\mathrm{d}^2 u}{\mathrm{d}n^2} = -\frac{W\pi}{k\lambda^2} \sin(2\pi u). \tag{3.5}$$

The solution $u(n) = 0$ to equation (3.5) corresponds to the commensurate phase of the system. In the incommensurate phase, the structure of the system comprises a lattice of near-commensurate sectors separated by narrow IDs. It has been shown (Bichoutskaia *et al.* 2006*b*) that if the commensurability parameter h is introduced as

$$h = \sqrt{\frac{W}{2k(\lambda l_{\mathrm{d}})^2}}, \tag{3.6}$$

the system remains in the commensurate phase if h is greater than the critical value $h_{\mathrm{c}} = \pi/4$, and the incommensurate phase is defined by the condition $h < h_{\mathrm{c}}$.

When $h \to h_c$, only one ID remains, namely, the defect described by the following solution of equation (3.5):

$$u(n) = \frac{2}{\pi}\arctan\left(\exp\left(\pi n\sqrt{\frac{2W}{k\lambda^2}}\right)\right). \tag{3.7}$$

Analytical solution $\mathrm{d}u/\mathrm{d}n$ of equation (3.7) can be viewed as a single static soliton which represents strain distribution in the system. If $h > h_c$, equation (3.7) describes the ID which occurs in the commensurate phase of the system. The length of the ID should exceed the effective value given by the expression

$$l_{\mathrm{ID}} = \lambda\left(\left(\frac{\mathrm{d}u}{\mathrm{d}n}\right)_{n=0}\right)^{-1}. \tag{3.8}$$

The formation of such ID is analogous to the formation of dislocations in ideal crystals.

If we consider the case of interacting walls of a DWNT, the difference between natural lengths of two springs $\lambda l_{\mathrm{d}} = l_0^{\mathrm{e}} - l_0^{\mathrm{c}}$ in equation (3.6) can be redefined as the difference Δt between the lengths of the unit cells of two SWNTs comprising a DWNT, which corresponds to the translational length of the unit cell of a DWNT t_{d}. The amplitude W of the substrate potential in (3.6) can be extracted from the interwall interaction energy surface of a DWNT. As a result, the commensurability parameter h takes the following form for a DWNT:

$$h = \sqrt{\frac{\Delta U_z N_c}{2k_{\mathrm{d}}\Delta t^2}}. \tag{3.9}$$

In equation (3.9), k_{d} is defined in the same way as the elastic constant k of the interacting springs with the only difference that k corresponds to the period λ of the substrate potential, whereas k_{d} corresponds to the translational length of the unit cell of a DWNT t_{d}.

Similarly, equation (3.7) can be rewritten for a DWNT as

$$u(x) = \frac{2}{\pi}\arctan\left(\exp\left(\frac{2\pi x}{t_{\mathrm{d}}}\sqrt{\frac{\Delta U_z N_c}{k_{\mathrm{d}} t_{\mathrm{d}}}}\right)\right), \tag{3.10}$$

taking into consideration that $\lambda = \delta_z = t_{\mathrm{d}}/2$ (Belikov *et al.* 2004). The effective length of the ID formed on the walls of a DWNT can be obtained from equation (3.8) as

$$l_{\mathrm{ID}} = \frac{t_{\mathrm{d}}}{2}\sqrt{\frac{k_{\mathrm{d}} t_{\mathrm{d}}^2}{2\Delta U_z N_c}}. \tag{3.11}$$

For a specific case of $l_0^{\mathrm{e}} = l_0^{\mathrm{c}}$, the minimum energy required to form the ID in the commensurate phase can be derived analytically (Frenkel & Kontorova 1938)

$$U_{\mathrm{ID}} = \frac{2\sqrt{2k^2 W}}{\pi} = \frac{\sqrt{2k_{\mathrm{d}} t_{\mathrm{d}}^2 \Delta U_z N_c}}{\pi}. \tag{3.12}$$

The energy of the ID formation remains the same whether the inner wall of a DWNT is compressed and the outer wall is expanded or vice versa.

The results of calculations of the main characteristics of IDs in a variety of DWNTs are presented in table 1. These data are obtained using a combined

Table 1. Characteristics of the incommensurability defect in DWNTs: the commensurability parameter h defines a phase of a DWNT; U_{ID} (in eV) is the energy of formation of the ID; l_{ID} (in nm) is its length.

DWNT	h	phase	U_{ID}	l_{ID}
(4, 4)@(10, 10)	0.07	incommensurate	—	87.0
(5, 5)@(11, 11)	1.36	commensurate	0.42	74.0
(6, 6)@(12, 12)	4.36	commensurate	0.54	70.0
(5, 5)@(10, 10)	3.32	commensurate	0.95	31.7
(6, 6)@(11, 11)	10.72	commensurate	1.22	29.8
(7, 7)@(12, 12)	17.03	commensurate	1.51	27.5
(9, 0)@(18, 0)	5.84	commensurate	6.03	11.2
(10, 0)@(20, 0)	3.99	commensurate	3.75	28.6

approach which incorporates *ab initio* computations of the energetics and structural properties of DWNTs with analytical estimations within the FK model of the energy of formation and length of the ID, using equations (3.11) and (3.12), and of the commensurability parameter h that defines a phase of a DWNT, using equation (3.9). Barriers to relative sliding of the walls of DWNTs, ΔU_{z}, and the translational lengths of the unit cells of DWNTs, t_{d}, are taken from Bichoutskaia *et al.* (2006*a*).

Among the DWNTs presented in table 1, all conventionally known as commensurate pairs of the walls, only the (4, 4)@(10, 10) DWNT has the calculated commensurability parameter smaller than the critical value of $\pi/4=0.7854$. This implies that due to the combination of a small barrier to relative sliding of the walls (ΔU_{z} in the nominator of equation (3.9)) and notable difference between the lengths of the unit cells of the (4, 4) and (10, 10) SWNTs (Δt in the denominator of equation (3.9)), the (4, 4)@(10, 10) DWNT has an incommensurate structure of the walls. This effect becomes greater if the DWNT has larger diameter of the outer wall, and hence weaker interwall interaction, smaller value of ΔU_{z} and a greater discrepancy in the lengths of the unit cells of their walls Δt. It can be also readily concluded from equation (3.9) that, in general, DWNTs with extremely small barriers to relative sliding of the walls and/or large difference in the lengths of the unit cells of the walls have incommensurate structure of the walls. Furthermore, the interaction of the walls in DWNTs with commensurate structure or other external influences may lead to the commensurate–incommensurate structural phase transition, which manifests itself in a DWNT acquiring the ID with the length and energy of formation also tabulated in table 1.

(*b*) *Strain nanosensor*

Bichoutskaia *et al.* (2006*b*) elaborated a new NEMS, called a strain nanosensor, based on a change in the structural phase of a DWNT (figure 2). The nanosensor is designed to measure the critical strain (tension) and strain distribution in any solid medium or surface. It can be embedded in the medium or mounted on the surface. It comprises a DWNT with the long outer wall with some defects of atomic structure on both ends in order to make a better adhesion between the sensor and the medium. Both ends of the outer wall provide the transfer of strain from the medium to the

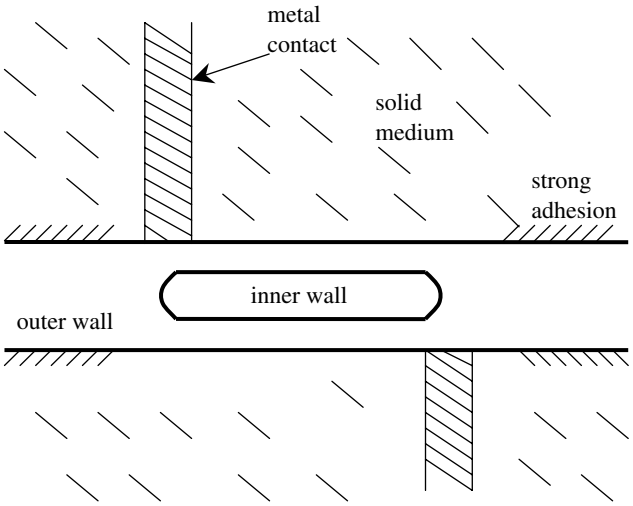

Figure 2. Schematic of strain nanosensor.

sensor. The central part of the sensor registers the critical strain. The central part of the outer wall and the short capped inner wall require perfect structure. The inner wall should be short and well separated from the defected ends of the outer wall in order to avoid their interactions.

The operation of the nanosensor requires the commensurability parameter h of the DWNT being close to the critical value h_c. In the absence of strain applied to the nanosensor, this corresponds to the DWNT being near the commensurate–incommensurate phase transition. The strain of the medium transferred to the DWNT causes extension (or contraction) of its central part and, as a result, the increase (or decrease) in the parameter Δt. At some critical value Δt_c, which corresponds to the critical strain of medium, the commensurate–incommensurate phase transition takes place. The nanosensor can be further adjusted to a given critical strain of medium by changing the length of the inner wall and therefore the value of Δt. To study the strain distribution, a number of nanosensors can be embedded into the sample, which are adjusted to different critical values of the strain.

Since the length of the outer wall is fixed, the commensurate–incommensurate phase transition takes place only in the inner wall. In this case, k_d in equation (3.9) is replaced by the elastic constant of the inner wall, k_{in}, and the critical difference, Δt_c defining the phase transition is obtained as

$$\Delta t_c = \frac{2\sqrt{2}}{\pi}\sqrt{\frac{\Delta U_z N_c}{k_{in}}}. \tag{3.13}$$

The minimum strain of the medium is then estimated as $\epsilon_c = \Delta t_c / t_d$, and the nanosensor measures values of the strain which exceed this critical value. A possible method of registration of the commensurate–incommensurate phase transition can be achieved through the measurements of conductance of DWNT. At the phase transition, the relative displacement of the walls and conductance of DWNT undergo a sudden simultaneous change. The change in conductance can be registered with the contacts attached to the outer wall.

4. Conclusions

Significant advances in nanoengineering and nanotechnology are required before the nanodevices reviewed in this paper become reality and can be mass produced outside the laboratory. There are solid grounds for optimism. Already, a nanomanipulator can be routinely attached to a MWNT and move individual walls, the caps of nanotubes can be removed, nanotubes can be cut into pieces of desirable length and the techniques for unambiguous determination of chirality of the walls have been successfully demonstrated.

However, the following areas need further developments: high-yield and low-cost synthesis techniques for production of defect-free and high-purity nanotubes; precise measurements performed on well-characterized individual nanoscale objects; establishment of new techniques for quantifying the number of defects, their type and position in the nanotube structure; and effective purification techniques for the metal particles within nanotubes, which reduce them to the level below parts per million.

Furthermore, an understanding and accurate assessment of the properties of nanomaterials at an atomic level can be achieved through theoretical and computational modelling. Such insight should aid further technological developments. Modelling is exploited throughout chemistry and materials for its ability to explain the underlying chemistry and provide a detailed picture of the fundamental interactions that underpin the studied properties. It allows further prediction of the properties and fundamental behaviour of new materials.

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References

Akita, S. & Nakayama, Y. 2003 Interlayer sliding force of individual multiwall carbon nanotubes. *Jpn. J. Appl. Phys.* **42**, 4330–4833. (doi:10.1143/JJAP.42.4330)

Aluru, N. R., Leburton, J.-P., McMahon, W., Ravaioli, U., Rotkin, S. V., Staedele, M., van der Straaten, T., Tuttle, B. R. & Hess, K. 2002 Modeling electronics on the nanoscale. In *Handbook of nanoscience, engineering and technology* (eds W. Goddard, D. Brenner, S. Lyshevski & G. J. Iafrate), pp. 11-1–11-33. Boca Raton, FL: CRC Press.

Belikov, A. V., Lozovik, Y. E., Nikolaev, A. G. & Popov, A. M. 2004 Double-wall nanotubes: classification and barriers to walls relative rotation, sliding and screwlike motion. *Chem. Phys. Lett.* **385**, 72–79. (doi:10.1016/j.cplett.2003.12.049)

Bichoutskaia, E., Popov, A. M., El-Barbary, A., Heggie, M. I. & Lozovik, Y. E. 2005 *Ab initio* study of relative motion of walls in carbon nanotubes. *Phys. Rev. B* **71**, 113 403. (doi:10.1103/PhysRevB.71.113403)

Bichoutskaia, E., Heggie, M. I., Popov, A. M. & Lozovik, Y. E. 2006*a* Interwall interaction and elastic properties of carbon nanotubes. *Phys. Rev. B* **73**, 045435. (doi:10.1103/PhysRevB.73.045435)

Bichoutskaia, E., Heggie, M. I., Lozovik, Y. E. & Popov, A. M. 2006*b* Multi-walled nanotubes: commensurate–incommensurate phase transition and NEMS applications. *Fuller. Nanotub. Carbon Nanostruct.* **14**, 131–140. (doi:10.1080/15363830600663412)

Bichoutskaia, E., Popov, A. M., Lozovik, Y. E., Ivanchenko, G. S. & Lebedev, N. G. 2007 Electromechanical nanothermometer. *Phys. Lett. A* **366**, 480–486. (doi:10.1016/j.physleta.2007.01.077)

Boyce, J. B. & Huberman, B. A. 1979 Superionic conductors: transitions, structures, dynamics. *Phys. Rep.* **51**, 189–265. (doi:10.1016/0370-1573(79)90067-X)

Choi, W. B., Bae, E., Kang, D., Chae, S., Cheong, B.-H., Ko, J.-H., Lee, E. & Park, W. 2004 Aligned carbon nanotubes for nanoelectronics. *Nanotechnology* **15**, S512–S516. (doi:10.1088/0957-4484/15/10/003)

Cumings, J. & Zettl, A. 2000 Low-friction nanoscale linear bearing realized from multiwall carbon nanotubes. *Science* **289**, 602–604. (doi:10.1126/science.289.5479.602)

Damnjanović, M., Vuković, T. & Milošević, I. 2002 Super-slippery carbon nanotubes—symmetry breaking breaks friction. *Eur. Phys. J. B* **25**, 131–134.

Fennimore, A. M., Yuzvinsky, T. D., Han, W. Q., Fuhrer, M. S., Cumings, J. & Zettl, A. 2003 Rotational actuators based on carbon nanotubes. *Nature* **424**, 408–410. (doi:10.1038/nature01823)

Forro, L. 2000 Beyond gedanken experiments. *Science* **289**, 560–561. (doi:10.1126/science.289.5479.560)

Frenkel, Y. & Kontorova, T. 1938 On theory of plastic deformation and twinning. *Phys. Z. Sowjetunion* **13**, 1–7.

Hashimoto, A., Suenaga, K., Urita, K., Shimada, T., Sugai, T., Bandow, S., Shinohara, H. & Iijima, S. 2005 Atomic correlation between adjacent grapheme layers in double-wall carbon nanotube. *Phys. Rev. Lett.* **94**, 045504. (doi:10.1103/PhysRevLett.94.045504)

Kish, L. B. & Ajayan, P. M. 2005 TerraByte flash memory with carbon nanotubes. *Appl. Phys. Lett.* **86**, 0931061. (doi:10.1063/1.1874304)

Kolmogorov, A. N. & Crespi, V. H. 2000 Smoothest bearings: interlayer sliding in multiwalled carbon nanotubes. *Phys. Rev. Lett.* **85**, 4727–4730. (doi:10.1103/PhysRevLett.85.4727)

Kolmogorov, A. N., Crespi, V. H., Schleier-Smith, M. H. & Ellenbogen, J. C. 2004 Nanotube–substrate interactions: distinguishing carbon nanotubes by the helical angle. *Phys. Rev. Lett.* **92**, 085503. (doi:10.1103/PhysRevLett.92.085503)

Lozovik, Y. E. & Popov, A. M. 2004 Nanomachines based on carbon nanotubes walls motion: operation modes and control forces. *Fuller. Nanotub. Carbon Nanostruct.* **12**, 485–492. (doi:10.1081/FST-120027211)

Lozovik, Y. E., Minogin, A. V. & Popov, A. M. 2003 Nanomachines based on carbon nanotubes. *Phys. Lett. A* **313**, 112–121. (doi:10.1016/S0375-9601(03)00649-2)

Maslov, L. 2006 Concept of nonvolatile memory based on multiwall carbon nanotubes. *Nanotechnology* **17**, 2475–2482. (doi:10.1088/0957-4484/17/10/007)

Paneth, H. R. 1950 The mechanism of self-diffusion in alkali metals. *Phys. Rev.* **80**, 708–711. (doi:10.1103/PhysRev.80.708)

Pnevmantikos, S., Savin, A. V., Zolotaryuk, A. V., Kivshar, Y. S. & Velgakis, M. J. 1991 Nonlinear transport in hydrogen-bonded chains: free solitonic excitations. *Phys. Rev. A* **43**, 5518–5536. (doi:10.1103/PhysRevA.43.5518)

Popov, A. M., Bichoutskaia, E., Lozovik, Y. E. & Kulish, A. S. 2007 Nanoelectromechanical systems based on multi-walled nanotubes: nanothermometer, nanorelay, and nanoactuator. *Phys. Stat. Sol. A* **204**, 1911–1917. (doi:10.1002/pssa.200675322)

Rueckes, T., Kim, K., Joselevich, E., Tseng, G. Y., Cheung, C.-L. & Lieber, C. M. 2000 Carbon nanotube-based nonvolatile random access memory for molecular computing. *Science* **289**, 94–97. (doi:10.1126/science.289.5476.94)

Srivastava, D. W. 1997 A Phenomenological model of the rotation dynamics of carbon nanotube gears with laser electric fields. *Nanotechnology* **8**, 186–192. (doi:10.1088/0957-4484/8/4/005)

Ward, J. W., Meinhold, M., Segal, B. M., Berg, J., Sen, R., Sivarajan, R., Brock, D. K. & Rueckes, T. 2004 In *Proc. Non-Volatile Memory Technol. Symp., 15–17 November 2004*, pp. 34–38.

Zheng, Q. & Jiang, Q. 2002 Multiwalled carbon nanotubes as gigahertz oscillators. *Phys. Rev. Lett.* **88**, 045503. (doi:10.1103/PhysRevLett.88.045503)

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Elena Bichoutskaia, born in St Petersburg, Russia, studied at St Petersburg State University where she graduated with an MSc degree in physics in 1993, and obtained her PhD in physics and mathematics in 2000. She was granted a United Nations Educational, Scientific and Cultural Organization (UNESCO) Anniversary Award in 1996. In 1997, she moved to the UK after being awarded a President Yeltzin's Research Scholarship, which she held at the Queen's University of Belfast. In 2000, she was appointed as a Royal Society/NATO postdoctoral fellow at Queen's University, followed by postdoctoral appointments at the Universities of Nottingham, Sussex and Cambridge. In 2007, she received a Royal Society UK Relocation Fellowship and moved back to Nottingham. Here, she welcomed the birth of her daughter Emily Anna. The highlight of her career break was the Royal Garden Party at Buckingham Palace. Elena spent summer 2007 at the Australian National University, Canberra as an academic visiting research fellow.