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Possible nanomachines: nanotube walls as movable elements

Yu. E. Lozovik[1], *A. V. Minogin*, *A. M. Popov*[1]

Institute of Spectroscopy, RAS, 142190, Troitsk, Moscow reg., Russia

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Possible types of nanomachines based on many-wall carbon nanotube and their operation modes are considered. Potential relief, energy barriers for nanotube wall relative motion are studied. Principally new nanomachines based on thread-like relative motion of nanotube walls are proposed.

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1. Introduction. The progress in nanotechnology in last decades give rise the possibility to manipulate with nanometer size objects [1]. The principal schemes of nanometer size machines (nanomachines) where the controlled motion can be realized are considered [2]. Thus the search of nanoobjects that can be used as movable elements of nanomachines is a very actual challenge for development of nanomechanics. The low frictional relative motion of carbon nanotube walls [3 – 5] and unique elastic properties [6] of these walls allows to consider them as promising candidates for such movable elements. The set of nanomachines based on relative sliding of walls along nanotube axis or their relative rotation is proposed [5, 7 – 10].

All these nanomachines correspond to the case where the corrugation of interwall interaction energy has little or no effect on relative motion of nanotube walls. However all of carbon nanotube walls have the helical symmetry [11, 12] and this gives the possibility for neighbour walls of nanotube to be bolt and nut pair. The present work is devoted to principally new type of nanomachines where the relative motion of nanotube walls occurs along helical "thread" lines. The possibility to control this motion by the potential relief of interwall interaction energy is considered. The theory for dynamics of relative motion of nanotube walls is developed. Possible types of these nanomachines are discussed. Two operation modes for these nanomachines are analyzed: Fokker-Planck operation mode, where a relative motion of walls is diffusion with drift under the action of external forces and accelerating operation mode, where a relative motion of walls is controlled by external forces. The values of controlling forces corresponding to these modes are estimated.

2. Barriers for relative motions of walls along line of thread. By potential relief we mean the dependence of interwall interaction energy U of two neighbour nanotube walls on coordinates describing wall relative position. Such coordinates are the angle ϕ of wall relative rotation about nanotube axis and the length z of wall relative displacement along it. Several types of potential relief including the type where the valleys form a helical lines were considered by Dresselhaus et al. for a set of double-wall nanotubes [12]. However the barriers for relative motions of walls along the helical "thread" lines and for transitions on neighbour "thread" lines were not calculated until now. Here we present the first calculation of such barriers. Moreover the "thread-like" potential relief is firstly found for nanotube with commensurate walls. As it is discussed below, such nanotubes have some advantages of applying in nanomachines.

The interwall interaction is adopted here to be 6–12 Lenard-Jones potential $U = 4\epsilon((\sigma/r)^{12} - (\sigma/r)^6)$ with parameters $\epsilon = 2.968\,\mathrm{meV}$ and $\sigma = 3.407\,\mathring{A}$ (see [12]). The walls are considered as rigid. Account of the deformation of walls is not essential for the shape of potential relief both for double-wall carbon nanotubes [13] and nanoparticles [14]. The length of longer inner wall is chosen so that all pairs of atoms with interatomic distances within cutoff distance are taken into account.

The walls of double-wall nanotube are commensurate if ratio of wall unit cell lengths is a rational fraction and incommensurate otherwise. We have studied here the "thread-like" potential relief for the set of nanotubes with both commensurate and incommensurate walls. The thread-like pattern of potential relief arises due to the essential difference between barriers U_1 for relative motion of walls along the "thread" line and U_2 for transition of the system to neighbour "thread" line ($U_1 \ll U_2$). "Thread-like" potential relief for (6,4)@(16,4) nanotube is plotted on Fig.1.

The barriers for any kind of relative motion of incommensurate walls fluctuate near their average value analogeously to the sum of functions $\cos l$, where l is integer [13]. The dependencies of barriers U_1 and U_2 on the outer wall length are shown on Fig.2 and Fig.3,

[1]e-mail: lozovik@isan.troitsk.ru, popov@isan.troitsk.ru

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Fig.1. The potential relief of interwall interaction energy of (6,4)@(16,4) nanotube as the function of wall relative displacement along nanotube axis and wall relative rotation angle about nanotube axis; $\mathbf{b}_1$ and $\mathbf{b}_2$ are the unit vectors of the lattice formed by minima of potential relief. The energy is measured from its minimum. The equipotential lines are drawn with interval 10^{-2} meV per atom

respectively. One can see that barriers change by order of magnitude for all nanotubes considered as the outer wall length changes by only few nanometers. Note that

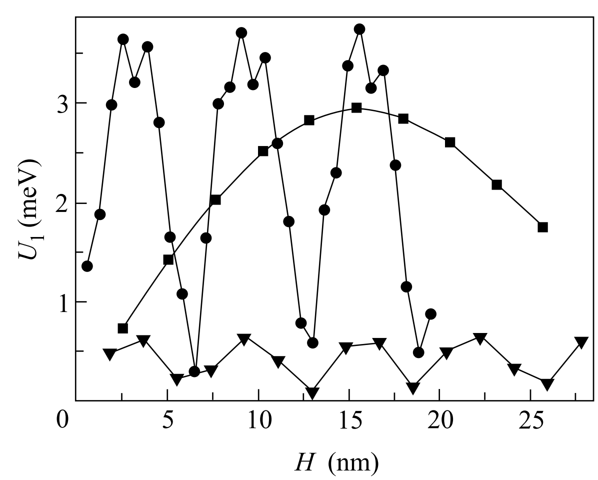

Fig.2. The dependence of the barrier U_1 for relative motion of walls along the "thread" line on the length H of outer wall for nanotubes with incommensurate walls. Filled circles, filled triangles and filled squares correspond to (6,4)@(16,4), (8,2)@(12,8) and (8,2)@(17,2) nanotubes, respectively

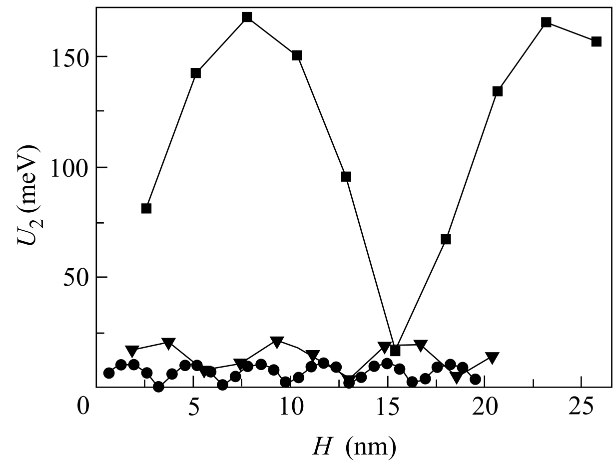

Fig.3. The dependence of the barrier U_2 for transition of the system on neighbour "thread" line on the length H of outer wall. Filled circles, filled triangles and filled squares correspond to (6,4)@(16,4), (8,2)@(12,8) and (8,2)@(17,2) nanotubes, respectively

these dependencies for both barriers at least for two of three considered nanotubes are quasiperiodic functions.

However the quantity that characterize the possibility for double-wall nanotube to have thread-like pattern of potential relief is not barrier itself but rather barriers ratio $\gamma = U_2/U_1$. It is naturally to call this ratio as relative thread depth. The dependence of relative thread depth on outer wall length is shown on Fig.4. If average periods of mentioned quasiperiodic functions are close

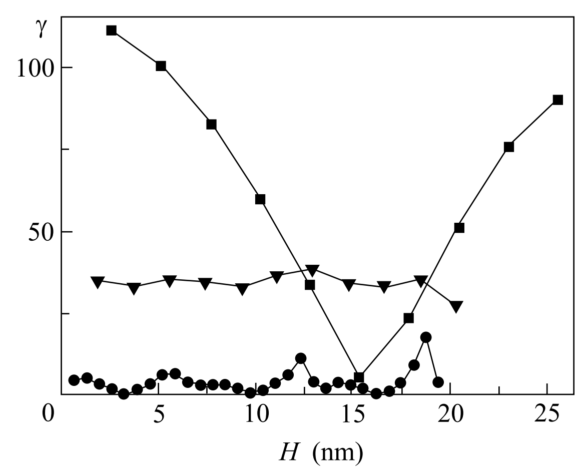

Fig.4. The dependence of the ratio $\gamma = U_2/U_1$ characterizing the "thread" depth on the length H of outer wall. Filled circles, filled triangles and filled squares correspond to (6,4)@(16,4), (8,2)@(12,8) and (8,2)@(17,2) nanotubes, respectively

and oscillations of functions are in phase for both barriers then the relative thread depth γ can be large for essential changes of outer wall length. The example of such a possibility is (8,2)@(12,8) nanotube.

The barriers for any kind of relative motion of commensurate walls with lengths corresponding to integer number of nanotube elementary cells are given by the relation $U_a = U_u N_u$, where U_u is the barrier per unit cell of the nanotube, N_u is a number of unit cells in the nanotube (the interaction with atoms on the edge of wall is disregarded here). Thus the barrier U_a for sufficiently long nanotube is proportional to its length and can be possible to obtain the given value of barrier by choice of nanotube length. To systemize the search of double-wall nanotubes with commensurate walls that can be bolt and nut pair the notion of equivalence class of walls can be introduced [15]. The analysis show that for some two-wall nanotubes with integer number of elementary cells the barriers can be extremely small in comparison with total interwall interaction energy. The reason of the fact is following. The potential field produced by each wall can be expanded in the basis of harmonics invariant under symmetry group of the wall [16]. Only harmonics with symmetry compatible with both walls can contribute in the interwall interaction potential relief $U(\phi, z)$. Therefore it was found that barrier for relative wall rotation for this nanotube is less than calculation accuracy [17]. The analogous results one can expect for majority of nanotubes with chiral commensurate walls.

3. Dynamics of relative motions of walls Let us study now the dynamics of relative motion of double-wall nanotube interacting walls under the action of external forces. One wall is treated as fixed and the motion of second wall relative to the first is examined. The external forces $\mathbf{F}_i^a$ acting on movable wall atoms does not cause its deformation if these forces have equal magnitudes for each atom and can be divided into two components $\mathbf{F}_z^a$ and $\mathbf{F}_L^a$ directed along the wall axis and the tangent to it circumference, respectively. The forces of considered types can have, for example, electrostatic nature [10] or can be applied by the nanomanipulator [5] or by laser electric field [7,8]. The analysis shows that for case considered the motion of one wall of double-wall carbon nanotube relative to fixed wall is equivalent to two-dimensional motion of particle with mass equals to that of movable wall in the potential field $U(\mathbf{r})$ and under the action of external force $\mathbf{F}$, where $\mathbf{r} = (z, L)$, $L = \phi R_1$, R_1 is radius of movable wall and $\mathbf{F} = (N_a F_z^a, N_a F_L^a)$, N_a is the number of movable wall atoms.

We consider the ensemble of "particles" with the motion described by this effective equation of motion, where force $\mathbf{F}$ have all properties described above and potential $U(\mathbf{r})$ correspond to the lattice, for example, as it is shown on Fig.1. The relative motion of walls can be diffusion with drift only in the case $kT \ll U_1, U_2$, where U_1 and U_2 are the barriers between minima of U for motion along lattice vectors $\mathbf{b}_1$ and $\mathbf{b}_2$, respectively. We restrict ourselves by the case of $U_1 \ll U_2$, where diffusion is one-dimensional. The probabilities w_1 and w_2 of displacements between neighbour minima in the line of diffusion direction and against it, respectively, are given approximately by Arrhenius formula

$$\begin{aligned} w_1 &= \Omega \exp\left(-\frac{U_1 - F_x\delta/2}{kT}\right), \\ w_2 &= \Omega \exp\left(-\frac{U_1 + F_x\delta/2}{kT}\right), \end{aligned} \tag{1}$$

where Ω is a frequency which has the same order of magnitude as oscillation frequency of the particle near the minimum, F_x is the projection of $\mathbf{F}$ on motion direction, δ is the distance between neighbour minima in the motion direction. Then the first term of exponents expansion (therefore the condition $F_x\delta/2 \ll kT$ is also necessary) is used to obtain the Fokker-Planck equation for particle concentration n:

$$\frac{\partial n}{\partial t} = D\frac{\partial n}{\partial x} + nBF_x. \tag{2}$$

Here D and B are, respectively, diffusion coefficient and mobility of particles given by

$$D = \frac{1}{2}\Omega\delta^2 \exp\left(-\frac{U_1}{kT}\right), \tag{3}$$

$$B = \frac{\Omega\delta^2}{2kT} \exp\left(-\frac{U_1}{kT}\right). \tag{4}$$

Note, that Einstein ratio $D = kTB$ is fulfilled.

4. Discussion We consider here two types of nanomachines based on relative motion of nanotube walls. Let us discuss firstly possible advantages of application of nanotubes with thread-like potential relief of interwall interaction energy in nanomachines where the direction of forces applied on movable wall does not correspond to desirable kind of wall motion. In the case where the potential relief has negligible effect on relative motion of walls, the directions of forces applied on movable wall must correspond to direction of relative motion of walls. Namely, if the relative motion of walls is sliding along nanotube axis, as it take place in constant-force nanosprings [5], gigahertz oscillators [9], and mechanical nanoswitch [10], than the forces applied on movable wall are bound to be directed along nanotube axis (first type forces). If the relative motion of walls is relative rotation, as it take place in nanobearings [7] and nanogears

[8] than the forces applied on movable wall must to be directed along the tangent to its circumference (second type forces).

However the presence of thread-like potential relief of interwall interaction energy remove the restriction on directions of forces applied on movable wall. The analysis above shows that relative motion of walls along helical line of "thread" is possible for both discussed types of external forces and any their superposition. Therefore the first type forces produce not only a relative sliding of walls along axis but also their relative rotation. Therefore a nanomachine based on wall motion can operate as a *nanowhirligig*. The proposed way to convert the forces directed along nanotube axis into relative rotation of walls can be used in nanobearings and nanogears. The second type forces producing a rotational moment gives rise not only a relative rotation but also a relative motion of walls along nanotube axis. This effect provides a possibility to construct a nanomachine based on carbon nanotube that is analogeous to old-desinged *faucet* where rotation of handle converts into forward motion of rod.

We propose here also principally new type of nanomachines that may be based on nanotubes with only thread-like potential relief of interwall interaction energy. The using of alternating-sign force to operate the relative position of walls can produce a motion of walls that is analogeous to the motion of auger in a perforating drill. Such a *perforating nanodrill* can be used for modification of surface in nanometer size.

Another new type of nanodevices which we propose here based on relative motion of nanotube walls are electromechanical nanodevices. For example, the conductivity of system consisting of two carbon nanotubes and a fullerene between them [18] can be tuned within orders of magnitude by rotation of a one nanotube or its displacement along the axis. This tuning can be controlled with the help of nanodevice based on relative motion of nanotube walls. In result a *variable nanoresistor* can be constructed, where wall of nanotube is both movable element and element of electric circuit.

Let us discuss possible operation modes of nanomachines based on relative motion of nanotube walls along line of thread. As we have shown above, in the case, when conditions $kT \ll U_1, U_2$ and $F_x\delta/2 \ll kT$ are fulfilled, the relative motion of carbon nanotube walls is described by Fokker-Planck equation (2). The operation mode of nanomachine based on such a motion is called here Fokker-Planck operation mode. This mode is worthwhile to use in nanomachine if average distance $x_{dr} = BF_xt$ passed by a wall along a helical line of "thread" in result of drift is greater than average distance $x_{dif} = \sqrt{2Dt}$ passed by this wall in result of diffusion. This condition is fulfilled for displacements $x_{dr} \gg \delta$, that is, e.g., for tens of relative jumps of wall along a helical "thread" line between minima of interwall potential $U(\mathbf{r})$. Such displacement along a helical line corresponds to less than one revolution of wall about the nanotube axis or displacement by nanometeres along this axis. Although Fokker-Planck operation mode does not allow the precise control of relative positions of walls, this mode can be used, for example, in perforating nanodrill for perforation of layers with thickness less than average displacement x_{dr} of wall (that plays the role of auger) in result of drift.

For forces $F_x\delta/2 \gg kT$ the stochastic contribution in relative motion of walls can be neglected. In this case the relative motion of walls is accelerated and as it is discussed above equivalent to two-dimensional motion of one particle . The operation mode of nanomachine based on such a motion is called here the accelerating operation mode. In this mode the controlled relative displacement of walls along a helical line of "thread" for distance that is less than δ is possible. This mode can be used, for example, in variable nanoresistor.

Let us estimate the range of forces that can be used to control the relative motion of carbon nanotube walls in nanomachine operating in Fokker-Planck and in accelerating operation modes. Our estimations are made for nanotube (8,2)@(12,8). The ratio of barriers $\gamma = U_1/U_2$ of this nanotube conserves within the range 25-40 for all considered lengths of outer wall. The conditions $kT \ll U_1, U_2$ and $F_x\delta/2 \ll kT$ give the maximal force F_{FP} corresponding to Fokker-Planck mode $F_{FP} \ll 2U_1/\delta$, where

$$\delta = \frac{a_0}{2}\sqrt{\left(\frac{R_2}{R_1}\right)^2 \cos^2\chi + \sin^2\chi}. \qquad (5)$$

Here R_1 and R_2 are radii of inner and outer wall, respectively, χ is the angle between helical line of "thread" and wall circumference.

For nanotube (8,2)@(12,8) we have: 1) value of χ equal to that of chiral angle $\theta = 10.89^o$ and 2) magnitude of $U_1 \approx 0.6$ meV corresponding to outer wall length that equals to the length of unit cell of the wall. In result we get $\delta = 1.86$ Å and $F_{FP} \ll 10^{-12}$ N.

The using of too high force controlling relative motion of walls at accelerating mode can give rise twist-off. The twist-off can occur only if the projection F_y of external controlling force on the direction normal to "thread" line will satisfy to the inequality

$$F_y > \left\langle \frac{\partial U(y)}{\partial y} \right\rangle_y \approx \frac{2U_2}{\delta_y} \qquad (6)$$

where y is wall relative displacement in the direction normal to "thread" line and δ_y is the distance between neighbour lines of "thread"

$$\delta_y = \frac{\sqrt{3}a_0}{2}\sqrt{\left(\frac{R_2}{R_1}\right)^2 \cos^2\chi + \sin^2\chi}. \qquad (7)$$

For controlling forces greater than $F_{ac} = 2U_2/\delta_y$ the relative motion of walls in the direction normal to "thread" line must be taken into account. For controlling forces less than F_{ac} it is sufficiently to consider the relative motion of walls only along the "thread" line. for nanotube (8,2)@(12,8) on substituting in Eq. (6) $\delta_y = 2.23$ Å, $U_2 = 20$ meV and magnitude of χ equal to chiral angle θ we get $F_{ac} \approx 3 \cdot 10^{-11}$ N.

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