1. INTRODUCTION

Nanotube walls are promising for the use as movable elements in nanoelectromechanical systems owing to the arbitrary motion [1, 2] and controlled (with manipulators) relative motion [3] executed by walls in multiwalled carbon nanotubes [4], as well as to the extraordinary elastic properties exhibited by nanotubes [5, 6]. A number of devices that hold great promise for applications in nanoelectromechanical systems and are based on the use of the relative motion of the walls in carbon nanotubes have been proposed in recent years. Among these devices are plain [7] and rotational [3] nanobearings, a nanogear [8], a nanoswitch [9], a gigahertz oscillator [10, 11], a Brownian nanomotor [12], a nanorelay [13], and a nanobolt–nanonut pair [14–17]. Moreover, nanomotors in which walls of the multiwalled carbon nanotubes serve as a shaft and a sleeve have been implemented in the experiments [18, 19].

In our previous papers [15–17], the double-walled carbon nanotube, which is a nanobolt–nanonut pair, was proposed to use for transforming the force applied to one of the walls and directed along the nanotube axis into the relative rotation of the walls. This nanobolt–nanonut pair can also be used in a nanoactuator (i.e., the device intended for driving a nanoelectromechanical system), for which the principle of operation is similar to the principle of spinning of a whirligig [20]. In the present paper, we propose a concept of a nanoactuator and perform the calculations that confirm the possibility of implementing this device in practice. This paper is organized as follows. In Section 2, we describe the schematic diagrams of the nanoactuator, consider a number of possible nanotubes that can be used for fabricating this device, and perform an analytical description of the principle embodied in the operation of the nanoactuator. Section 3 is devoted to numerical calculations of the relative motion of the walls in the nanotube used in the design of the nanoactuator. The possible methods for driving the nanoactuator are discussed in Section 4.

2. SCHEMATIC DIAGRAMS AND PRINCIPLE OF THE OPERATION OF THE NANOACTUATOR

The schematic diagrams of the nanoactuators are shown in Fig. 1. In the schematic diagram depicted in Fig. 1a, the inner wall (wall 1) serves as a stator and is fixed in position. The next two walls (walls 2, 3) form a rotor. The relative positions of these walls should be fixed. The stator and rotor make up a rotational nanobearing. The outer walls serve to transform the force which is applied to wall 4 and directed along the nano-
tube axis into rotation of the rotor. This transformation is possible in the case where walls 3 and 4 make up a nanobolt–nanonut pair. The schematic diagram shown in Fig. 1b differs from the schematic diagram depicted in Fig. 1a in that the walls are arranged in the reverse order: the stator (wall 1) is the outer wall, and the nanobolt–nanonut pair (walls 3, 4) is formed by the inner walls.

Walls 1 and 2 represent a rotational nanobearing when the following condition is satisfied: \( E_\phi \ll E_z \), where \( E_\phi \) and \( E_z \) are the barriers to the relative rotation of walls 1 and 2 and their sliding along the nanotube axis, respectively. This condition is very well satisfied in the case where walls 1 and 2 are nonchiral commensurate walls [walls 1 and 2 form a double-walled nanotube with either the “armchair” type \((n, n)@ (m, m)\) or the “zigzag” type \((n, 0)@ (m, 0)\)]. The calculations demonstrate that, in these nanotubes, the barriers \( E_\phi \) to the relative rotation of the walls are very low (i.e., they are less than 0.005 meV/atom for the density-functional calculations [21] and less than \( 10^{-11} \) meV/atom for the calculations performed with the use of semiempirical potentials [22]) and at least several orders of magnitude lower than the barriers \( E_z \) to the relative sliding of the walls (the exception is provided by the \((5, 5)@ (10, 10)\) and \((9, 0)@ (18, 0)\) double-walled nanotubes, which are characterized by considerable barriers to the relative rotation of the walls). On this basis, it was proposed to use these double-walled nanotubes as rotational bearings with an exactly fixed position along the rotation axis [22, 23].

In order to investigate the characteristics of the relative motion of the nanotube walls, it is necessary to calculate the dependence of the energy \( U \) of the interaction between two neighboring walls on the coordinates that describe the relative position of the walls, namely, the angle \( \phi \) of the relative rotation of the walls around the nanotube axis and the length \( z \) of the relative displacement of the walls along this axis. The potential relief of the interaction energy of nanotube walls \( U(z, \phi) \) can be conveniently represented in the form of the development of the cylindrical surface. In principle, the double-walled nanotube can be used as a nanobolt–nanonut pair when the potential relief has valleys located along the helical line similar to the thread on the lateral surface of the bolt. In what follows, these potential reliefs will be referred to as thread-like reliefs. The thread can be quantitatively characterized by the potential barrier \( E_t \) to the relative rotation of the nanotube walls along the thread line and the potential barrier \( E_s \) to the thread stripping (the motion across the thread), as well as by the threshold forces for the relative motion along the threshold line and thread stripping. The thread can be qualitatively characterized not only by the potential barriers but also by the ratio \( \beta = E_s/E_t \). This ratio is referred to as the relative thread depth [15, 16].

In the general case, the nanotube wall has screw symmetry [24]. Therefore, the thread-like relief can be observed for the majority of double-walled nanotubes. However, in the cases where double-walled nanotubes with walls without defects can have a thread-like relief, the low barrier to the thread stripping associated with the incommensurability of the screw symmetries of the walls makes it impossible to use these nanotubes as nanobolt–nanonut pairs in nanoelectromechanical systems [15, 16, 20, 25]. In our previous studies [20, 22, 25], it was demonstrated that double-walled nanotube with commensurate walls, of which one wall is chiral and the other wall contains regularly arranged atomic structural defects, are the most promising objects for the use as nanobolt–nanonut pairs in nanoelectromechanical systems.

The barrier \( E_\phi \) to the relative rotation of nonchiral walls 1 and 2 is low only when both walls do not contain atomic structural defects. As was shown in [20, 25], the nonchiral wall without defects cannot be used for fabricating a nanobolt–nanonut pair. Consequently, the same wall cannot be a component of a nanobearing and a nanobolt–nanonut pair. Therefore, the nanoactuator can be prepared from a nanotube containing no less than four walls: two walls form a rotational nanobearing and two walls represent a nanobolt–nanonut pair. For an adequate operation of the nanoactuator, it is desirable that the relative position of walls 2 and 3 would be fixed. The relative displacement of walls 2 and 3 along the nanotube axis will be prevented if wall 3 will be a nonchiral wall commensurate with wall 2. In order to avoid the relative rotation of walls 2 and 3, we propose to produce atomic structural defects in wall 3. The same defects regularly arranged at identical points of unit cells in wall 3 can be used for fabricating the nanobolt–nanonut pair from walls 3 and 4. A chiral wall commensurate with wall 3 is conveniently used as wall 4. In this case, the barriers to the relative motion along the thread line and thread stripping are proportional to the total number of defects per length of overlapping of walls 3 and 4 [20, 25]. Therefore, the barriers with heights necessary for operating the nanoactuator can be produced by varying the length of wall 4 or the defect concentration in wall 3.

Thus, the nanoactuator under consideration consists of three sequential commensurate nonchiral inner walls and one commensurate chiral wall.

In our recent works [22, 26], we proposed a classification of double-walled nanotubes with commensurate walls. According to this classification, the double-walled nanotubes under consideration make up a family whose all members are characterized by identical interwall distances and identical chiral angles of the inner and outer walls. The proposed classification is also a classification of possible pairs of commensurate neighboring walls. In particular, the interwall distance for nonchiral commensurate walls corresponds to experi-
mental distances in the case of the following chiral indices of walls 1, 2, and 3:

\[(k, 0) @ (k + 9, 0) @ (k + 18, 0), \quad k \geq 4 \quad (1)\]

\[(k, k) @ (k + 5, k + 5) @ (k + 10, k + 10), \quad k \geq 2. \quad (2)\]

The interwall distance is equal to 3.50 Å in the former case and 3.37 Å in the latter case.

Walls 3 and 4 can be represented by nanotubes of all families with one nonchiral and one chiral commensurate walls. We selected these families from the total list of double-walled commensurate nanotubes presented in [22, 26]. All possible double-walled carbon nanotubes suitable for fabricating a nanobolt–nanonut pair appropriate for using in the nanoactuator are listed in the table. The four-walled nanotube that can be used to

<table>
<thead>
<tr>
<th>No.</th>
<th>((n_3, m_3) @ (n_4, m_4))</th>
<th>(H, \text{ Å})</th>
<th>(\theta, \text{ deg})</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>((26 + 7n, 0) @ (25 + 5n, 15 + 3n))</td>
<td>29.82</td>
<td>21.79</td>
</tr>
<tr>
<td>2</td>
<td>((30 + 13n, 0) @ (24 + 8n, 21 + 7n))</td>
<td>55.38</td>
<td>27.80</td>
</tr>
<tr>
<td>3</td>
<td>((29 + 19n, 0) @ (32 + 16n, 10 + 5n))</td>
<td>80.94</td>
<td>13.17</td>
</tr>
<tr>
<td>4</td>
<td>((22 + 31n, 0) @ (24 + 24n, 11 + 11n))</td>
<td>132.06</td>
<td>17.90</td>
</tr>
<tr>
<td>5</td>
<td>((28 + 37n, 0) @ (33 + 33n, 7 + 7n))</td>
<td>157.62</td>
<td>9.43</td>
</tr>
<tr>
<td>6</td>
<td>((34 + 43n, 0) @ (35 + 35n, 13 + 13n))</td>
<td>183.18</td>
<td>15.18</td>
</tr>
<tr>
<td>7</td>
<td>((40 + 49n, 0) @ (39 + 39n, 16 + 16n))</td>
<td>208.74</td>
<td>16.43</td>
</tr>
<tr>
<td>8</td>
<td>((58 + 67n, 0) @ (45 + 45n, 32 + 32n))</td>
<td>285.42</td>
<td>24.43</td>
</tr>
</tbody>
</table>

Stator in the form of an inner zigzag wall (Fig. 1a)

<table>
<thead>
<tr>
<th>No.</th>
<th>((n_3, m_3) @ (n_4, m_4))</th>
<th>(H, \text{ Å})</th>
<th>(\theta, \text{ deg})</th>
</tr>
</thead>
<tbody>
<tr>
<td>9</td>
<td>((16 + 7n, 16 + 7n) @ (33 + 11n, 6 + 2n))</td>
<td>17.22</td>
<td>8.21</td>
</tr>
<tr>
<td>10</td>
<td>((21 + 13n, 21 + 13n) @ (44 + 22n, 2 + n))</td>
<td>31.97</td>
<td>2.20</td>
</tr>
<tr>
<td>11</td>
<td>((14 + 19n, 14 + 19n) @ (26 + 26n, 11 + 11n))</td>
<td>46.73</td>
<td>16.83</td>
</tr>
<tr>
<td>12</td>
<td>((26 + 31n, 26 + 31n) @ (46 + 46n, 13 + 13n))</td>
<td>76.24</td>
<td>12.10</td>
</tr>
<tr>
<td>13</td>
<td>((32 + 37n, 32 + 37n) @ (47 + 47n, 26 + 26n))</td>
<td>91.00</td>
<td>20.57</td>
</tr>
</tbody>
</table>

Stator in the form of an inner armchair wall (Fig. 1a)

<table>
<thead>
<tr>
<th>No.</th>
<th>((n_3, m_3) @ (n_4, m_4))</th>
<th>(H, \text{ Å})</th>
<th>(\theta, \text{ deg})</th>
</tr>
</thead>
<tbody>
<tr>
<td>14</td>
<td>((5 + 5n, 3 + 3n) @ (16 + 7n, 0))</td>
<td>29.82</td>
<td>21.79</td>
</tr>
<tr>
<td>15</td>
<td>((8 + 8n, 7 + 7n) @ (16 + 7n, 0))</td>
<td>55.38</td>
<td>27.80</td>
</tr>
<tr>
<td>16</td>
<td>((16 + 16n, 5 + 5n) @ (28 + 19n, 0))</td>
<td>80.94</td>
<td>13.17</td>
</tr>
<tr>
<td>17</td>
<td>((24 + 24n, 11 + 11n) @ (40 + 31n, 0))</td>
<td>132.06</td>
<td>17.90</td>
</tr>
<tr>
<td>18</td>
<td>((33 + 33n, 7 + 7n) @ (46 + 37n, 0))</td>
<td>157.62</td>
<td>9.43</td>
</tr>
<tr>
<td>19</td>
<td>((35 + 35n, 13 + 13n) @ (52 + 43n, 0))</td>
<td>183.18</td>
<td>15.18</td>
</tr>
<tr>
<td>20</td>
<td>((39 + 39n, 16 + 16n) @ (58 + 49n, 0))</td>
<td>208.74</td>
<td>16.43</td>
</tr>
<tr>
<td>21</td>
<td>((45 + 45n, 32 + 32n) @ (76 + 67n, 0))</td>
<td>285.42</td>
<td>24.43</td>
</tr>
</tbody>
</table>

Stator in the form of an outer zigzag wall (Fig. 1b)

<table>
<thead>
<tr>
<th>No.</th>
<th>((n_3, m_3) @ (n_4, m_4))</th>
<th>(H, \text{ Å})</th>
<th>(\theta, \text{ deg})</th>
</tr>
</thead>
<tbody>
<tr>
<td>22</td>
<td>((11 + 11n, 2 + 2n) @ (12 + 7n, 12 + 7n))</td>
<td>17.22</td>
<td>8.21</td>
</tr>
<tr>
<td>23</td>
<td>((22 + 22n, 1 + n) @ (18 + 13n, 18 + 13n))</td>
<td>31.97</td>
<td>2.20</td>
</tr>
<tr>
<td>24</td>
<td>((26 + 26n, 11 + 11n) @ (24 + 19n, 24 + 19n))</td>
<td>46.73</td>
<td>16.83</td>
</tr>
<tr>
<td>25</td>
<td>((46 + 46n, 13 + 13n) @ (36 + 31n, 36 + 31n))</td>
<td>76.24</td>
<td>12.10</td>
</tr>
<tr>
<td>26</td>
<td>((47 + 47n, 26 + 26n) @ (42 + 37n, 42 + 37n))</td>
<td>91.00</td>
<td>20.57</td>
</tr>
</tbody>
</table>

Stator in the form of an outer armchair wall (Fig. 1b)

<table>
<thead>
<tr>
<th>No.</th>
<th>((n_3, m_3) @ (n_4, m_4))</th>
<th>(H, \text{ Å})</th>
<th>(\theta, \text{ deg})</th>
</tr>
</thead>
</table>

Note: For each family, the index \(n = 0\) corresponds to the nanoactuator with the minimum possible radius. The table includes all families of double-walled nanotubes for which the minimum possible radius of wall 4 meets the condition \(R_4 \leq 100\) Å, the chiral indices of wall 4 satisfy the inequalities \(n_4 < 50\) and \(m_4 < 50\), and the distance between the walls is given by \(R_{34} \in [3.3, 3.7] \text{ Å}\). Designations: \(H\) is the unit cell length of the double-walled nanotube, and \(\theta\) is the chiral angle of wall 4. 
design the nanoactuator is chosen as follows: after selecting the chiral indices of walls 3 and 4 (the nanobolt–nanonut pair) in the table, the chiral indices of walls 1 and 2 are determined from relationships (1) and (2).

Let us consider the operation of the nanoactuator in which the force \( \mathbf{F} \) directed along the nanotube axis is applied to wall 4. As was shown in our earlier works [15, 16], the motion of wall 4 with respect to wall 3 under the action of the force directed along the nanotube axis is described by the equation identical to the equation of motion of a particle in the plane in a potential field corresponding to the interaction energy between walls 3 and 4; that is,

\[
M_4 \ddot{r} = - \frac{dU(r)}{dr} + \mathbf{F}. \tag{3}
\]

Here, \( M_4 \) is the mass of wall 4, \( U(r) \) is the interaction energy between walls 3 and 4, \( r \) is the vector with the components \( z \) and \( L = \phi R_4 \) (where \( z \) and \( \phi \) are the cylindrical coordinates describing the position of wall 4 with respect to wall 3), and \( R_4 \) is the radius of wall 4. In the plane of particle motion under consideration, the thread lines are straight lines that intersect the \( L \) coordinate axis at a thread angle \( \chi \). Therefore, the relative helical motion of walls 3 and 4 is similar to the motion of a particle along a straight–light potential valley of the thread line under the action of the force \( \mathbf{F} \) directed at an angle to the valley.

Now, we consider a short impulse of force \( \mathbf{P} = \mathbf{F} \Delta t \), when the time \( \Delta t \) of the action of the force \( \mathbf{F} \) is considerably shorter than the time of particle motion to the neighboring minimum of the potential relief. The velocity \( \mathbf{V} \) that the particle acquires under the action of the impulse of force \( \mathbf{P} \) can be decomposed into the mutually perpendicular components \( V_\parallel = V \sin \chi \) and \( V_\perp = V \cos \chi \), which are directed along and across the thread line, respectively. The particle will move along the thread line (correspondingly, wall 4 will move in a helical way with respect to wall 3) when the following conditions will be satisfied.

1. The initial kinetic energy of the particle for the motion along the thread line is higher than the barrier \( E_1 \) to this motion; that is,
   \[
   \frac{M_4 V^2 \sin^2 \chi}{2} > E_1. \tag{4}
   \]

2. The initial kinetic energy of the particle for the motion across the thread line is higher than the barrier \( E_2 \) to thread stripping; that is,
   \[
   \frac{M_4 V^2 \cos^2 \chi}{2} < E_2. \tag{5}
   \]

It is easy to show that conditions (4) and (5) can be simultaneously fulfilled only in the case where

\[
\cot^2 \chi \leq \frac{E_2}{E_1} = \beta. \tag{6}
\]

This condition determines the possibility of fabricating the nanoactuator based on the given nanobolt–nanonut pair. Note that, according to condition (6), nanobolt–nanonut pairs with a small relative thread depth and a thread angle larger than 45° can be used to fabricate the nanoactuator.

The time dependence of the particle velocity \( V_\parallel(t) \) along the thread line can be found by integrating Eq. (3). The rotational velocity of wall 4 is given by the formula \( V_\parallel(t) = V_\parallel(t) \cos \chi \). Since the force \( \mathbf{F} \) is directed along the rotation axis of the movable walls of the nanoactuator, the angular momentum of the system composed of walls 2, 3, and 4 after the action of this force remains equal to zero; that is,

\[
M_4 V_\parallel(t) \cos \chi R_4 + M_2 V_\parallel(t) R_2 + M_3 V_\parallel(t) R_3 = 0, \tag{7}
\]

where \( M_2 \) and \( M_3 \) are the masses of walls 2 and 3, respectively; \( V_\parallel(t) \) and \( V_\parallel(t) \) are the time dependences of the rotational velocities of walls 2 and 3; and \( R_2 \) and \( R_3 \) are the radii of walls 2 and 3. In Eq. (7), the velocities \( V_\parallel(t) \) and \( V_\parallel(t) \) can be replaced by the angular velocity \( \omega_\parallel(t) = V_\parallel(t) R_2 = V_\parallel(t) R_3 \) of rotation of walls 2 and 3, whose relative positions are fixed. From Eq. (7), we found that the angular velocity \( \omega_\parallel(t) \) of the rotor consisting of walls 2 and 3 is determined by the relationship

\[
\omega_\parallel(t) = \frac{M_4 V_\parallel(t) \cos \chi R_4}{M_2 R_2^2 + M_3 R_3^2} = \frac{M_4 \omega_\parallel(t) R_4}{M_2 R_2^2 + M_3 R_3^2}, \tag{8}
\]

where \( \omega_\parallel = V_\parallel(t) \cos \chi R_4 \) is the angular velocity of wall 4.

The angle \( \xi_3 \) through which the rotor is rotated for the time \( t_0 \) after applying the impulse of force \( \mathbf{P} \) to wall 4 is defined by the expression

\[
\xi_3 = \int_0^{t_0} \omega_\parallel(t) dt. \tag{9}
\]

The angular rotation of the rotor at the instant of time \( t_0 \) can be terminated by applying an oppositely directed impulse of force \( -\mathbf{P} \) to wall 4. Therefore, the proposed nanoactuator can be used for rotating the rotor through a specified angle or a specified number of revolutions.

We determine the minimum rotor length \( L_4 \) at which the rotor in our actuator can be rotated through the angle \( \xi_3 \). The maximum number of revolutions of wall 4 with respect to wall 3 is equal to the ratio of the difference between the length of wall 3 and the length \( L_4 \).
sheets have never been investigated in detail to date. As a result, the maximum rotation angle ξ4 of wall 4 with respect to wall 3 can be written in the form

$$\xi_4 = \frac{L_4 - L_3}{R_4 \sin \chi}$$

(11)

At any instant of time $t_0$ after applying the impulse of force $P$ to wall 4, the ratio between the angles $\xi_3(t_0)$ and $\xi_4(t_0)$ is determined by the relationship

$$\frac{\xi_3(t_0)}{\xi_4(t_0)} = \frac{\int_0^{t_0} \omega_3(t) dt}{\int_0^{t_0} \omega_4(t) dt}.$$  

(12)

Substitution of expressions (8) and (11) into relationship (12) gives

$$\xi_3 = \frac{(L_4 - L_3)M_3R_4}{(M_3R_3^2 + M_4R_4^2)\sin \chi}. $$

(13)

The ratio of the above barriers $\beta_3 = \frac{E_3}{E_4}$ for the potential relief were obtained by different computational methods for the (5, 5)@[(10, 10) double-walled nanotube. In particular, the ratios $\beta_3 = 2.08$ [21], $\beta_3 = 2.85$ [23], and $\beta_3 = 2.50$ [29] were determined using the density-functional calculations and the ratio $\beta_3 = 3.50$ was obtained by the tight-binding method [30]. The ratios $\beta_3 = 3.10$ [14] and $\beta_3 = 2.90$ [22] were obtained in the case where the interwall interaction was described by the Lennard-Jones potential $U = 4\epsilon((\sigma/r)^{12} - (\sigma/r)^6)$ with the parameters $\epsilon_0 = 2.968$ meV and $\sigma_0 = 3.407$ Å. Note that the calculations were carried out upon annealing of the wall structure in [14] and under the assumption that the walls are rigid in [22]. Furthermore, the use of the Lennard-Jones potential [22] and other semiempirical potentials [28, 31] allowed one to obtain an important qualitative result: the potential relief for all double-walled nanotubes with commensurate walls of which even if one wall is chiral is extremely flat. Therefore, we believe that the simple Lennard-Jones potential enables us to obtain adequate qualitative characteristics of the potential relief. Moreover, the number of atoms in the unit cells of the double-walled nanotubes with commensurate walls of which even if one wall is chiral is too large for the interwall interaction to be studied using first-principles calculations.

According to both experimental data and results of different calculations, the interaction energies between graphite sheets can differ by two orders of magnitude (see [27] and references therein). No chiral indices of the walls were determined in experiments devoted to the measurement of the threshold forces for the relative motion of the walls along the nanotubes [1–3]. Consequently, the data of these experiments cannot be used for verifying the calculations of the relative motion of the walls. Only for the (5, 5)@[(10, 10) double-walled nanotube with a small number of atoms in the unit cell, the barriers to the relative motion of nanotube walls were calculated not only with the use of semiempirical potentials [14, 22, 28] but also from first principles [21, 23, 29, 30]. Different methods for calculating the (5, 5)@[(10, 10) double-walled nanotube result in different barriers $E_3$ and $E_4$ to the relative sliding of the walls along the nanotube axis and to the relative rotation of the walls, respectively. However, close qualitative characteristics (the ratio of the above barriers $\beta_3 = \frac{E_3}{E_4}$ for the potential relief were obtained by different computational methods for the (5, 5)@[(10, 10) double-walled nanotube. In particular, the ratios $\beta_3 = 2.08$ [21], $\beta_3 = 2.85$ [23], and $\beta_3 = 2.50$ [29] were determined using the density-functional calculations and the ratio $\beta_3 = 3.50$ was obtained by the tight-binding method [30]. The ratios $\beta_3 = 3.10$ [14] and $\beta_3 = 2.90$ [22] were obtained in the case where the interwall interaction was described by the Lennard-Jones potential $U = 4\epsilon((\sigma/r)^{12} - (\sigma/r)^6)$ with the parameters $\epsilon_0 = 2.968$ meV and $\sigma_0 = 3.407$ Å. Note that the calculations were carried out upon annealing of the wall structure in [14] and under the assumption that the walls are rigid in [22]. Furthermore, the use of the Lennard-Jones potential [22] and other semiempirical potentials [28, 31] allowed one to obtain an important qualitative result: the potential relief for all double-walled nanotubes with commensurate walls of which even if one wall is chiral is extremely flat. Therefore, we believe that the simple Lennard-Jones potential enables us to obtain adequate qualitative characteristics of the potential relief. Moreover, the number of atoms in the unit cells of the double-walled nanotubes with commensurate walls of which even if one wall is chiral is too large for the interwall interaction to be studied using first-principles calculations.

In this respect, the Lennard-Jones potential with the above parameters was used in the present work to describe the pair interaction of atoms located in neighboring walls. These parameters of the potential were fitted to the interlayer distance and elastic moduli of graphite. Note that the Lennard-Jones potential was successfully used to investigate the ground state and phase transitions in a C60 crystal [32], the potential relief of the interwall interaction energy in double-walled nanotubes [14–17, 21, 33], and the relative motion of the walls in nanotubes without defects [10, 11]. In order to exclude the influence of the nanotube

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ends on the potential relief, we considered the double-walled nanotubes that consist of a long inner wall and a short outer wall. The length of the outer wall was taken equal to the equivalent length of the unit cell in the double-walled nanotube. The length of the inner wall was chosen so that all pairs of atoms with interatomic distances smaller than the potential cutoff radius equal to 40 \sigma_0 were taken into account. Previously, it was demonstrated that the wall deformation does not substantially affect the characteristics of the potential relief for both double-walled nanotubes [22, 31] and two-shell carbon nanoparticles [34, 35]. For example, the calculated barriers to the relative rotation and sliding of the walls in the (5, 5)@(10, 10) double-walled nanotube in the case of the walls with an unannealed structure [22] differ only by 14\% from those obtained by Dresselhaus et al. [14] for walls with an annealed structure. For this purpose, we considered the interaction of rigid walls. The wall structure was constructed by rolling up a graphite sheet in which the bond length is equal to 1.42 Å (the bond lengths in multiwalled nanotubes and graphite coincide to within an accuracy of ~0.01 Å in neutron diffraction measurements [36]).

According to the calculations performed with the use of semiempirical potentials, the potential relief for any double-walled nanotubes with commensurate walls of which even if one wall is chiral is extremely flat. This is explained by the incommensurability of screw symmetries of the walls [37]. Specifically, as follows from the calculations with the Lennard-Jones potential, the barrier to the relative rotation of the walls in the (8, 2)@(16, 4) double-walled nanotube is approximately equal to 5 \times 10^{-12} \text{meV per atom} and this is the sole revealed example when the barrier to the relative motion of chiral commensurate walls exceeds the accuracy in calculations [22]. The other barriers for several tens of the double-walled nanotubes with chiral commensurate walls under consideration are lower than the accuracy in calculations [22]. The calculations with the use of the Kolmogorov–Crespi potential [31] also demonstrated that the potential barrier is extremely flat for all the double-walled nanotubes under consideration with commensurate wall without defects of which even if one wall is chiral. The interwall interaction energy \( U_{\text{def}} \) for double-walled nanotubes with defects can be written in the form

\[
U_{\text{def}}(\phi, z) = U_{\text{per}}(f, z) + \sum_{i,j=1}^{N_p, j = N_d} (U_{ij, \text{lat}}(\phi, z) - U_{ij, \text{per}}(\phi, z)).
\]  

(17)

Here, \( U_{\text{per}} \) is the interwall interaction energy for perfect double-walled nanotubes; \( N_p \) is the number of atoms in a perfect wall; \( N_d \) is the number of atoms in a wall with defects (these atoms change their positions or electronic properties due to the defect formation); and \( U_{ij, \text{lat}}(\phi, z) \) and \( U_{ij, \text{per}}(\phi, z) \) are the pair interaction energies between atoms of the perfect wall and \( N_d \) atoms with modified properties in the wall with defects for double-walled nanotubes with and without defects, respectively. Since the potential relief for double-walled nanotubes with chiral commensurate walls without defects is extremely flat, i.e., \( U_{\text{per}}(\phi, z) = U_0 \) (where \( U_0 \) is a constant), the first term in relationship (17) does not contribute to the potential relief and, hence, to the barriers to the relative motion of the walls. Therefore, these barriers can be calculated with allowance made only for the pair interactions for \( N_d \) atoms corresponding to defects. This permits us to reduce significantly the computer time of calculating the potential relief for double-walled nanotubes with chiral commensurate walls containing defects. It should be noted that the given technique cannot be used for double-walled nanotubes consisting of two nonchiral commensurate walls, for which the potential reliefs with considerable barriers to the relative motion of the walls were also revealed in the case of perfect walls [22].

In our previous paper [20], we analyzed defects of different types, such as the single-atom vacancy and replacement of one carbon atom by a particle with modified parameters of the interaction between this particle and carbon atoms in a neighboring perfect wall. It was shown that the type and geometric characteristics of the defect and the parameters of the interaction potential between replaced atoms and atoms of the perfect wall do not affect the qualitative characteristic of the thread. In this respect, we investigated the relative motion of the walls in the nanobolt–nanonut pair for defects of one type, namely, single-atom vacancies.

4. RESULTS AND DISCUSSION

Earlier, the potential reliefs of the interaction energy between the walls of the double-walled nanotube used as a nanobolt–nanonut pair were calculated only in the case of identical positions of defects in each unit cell of the nanotube [20, 22, 25]. It was revealed that the lattice formed by minima of the potential relief \( U(r) \) (where, \( r \) is the vector with the components \( z \) and \( L = \phi R, z \) and \( \phi \) are the cylindrical coordinates describing the relative position of the walls, and \( R \) is the radius of the perfect wall) follows the structure of the development of the perfect wall; i.e., their unit cell coincide with each other.

In this paper, the potential reliefs for the (11, 2)@(12, 12) double-walled nanotube, which is the nanobolt–nanonut pair in the nanoactuator under investigation, were calculated for different numbers of positions of atom vacancies in the outer wall. When the vacancies in the unit cell of the double-walled nanotube are rather widely spaced, each unit cell of the nanotube can contain all vacancies with different positions in the (12, 12) wall. Otherwise, the condition for the applicability of the results obtained is the coincidence of the
According to our calculations, the relative thread depth characteristics of the thread are presented in Fig. 2. The potential relief for this case and the vacancies are located in the same straight line parallel to the nanotube axis. The potential relief shown in Fig. 2 is characterized by the development of the wall free from vacancies. Light circles correspond to the minima of the potential relief in the unit cell of the perfect (vacancy-free) wall.

It turned out that not only the relative thread depth but also qualitative characteristics of the potential relief, such as the thread angle and the number of thread lines, are determined by the number of vacancy positions in the unit cell of the double-walled nanotube. The largest relative thread depth was obtained in the case of seven different positions in the unit cell of the double-walled nanotube. Note that all these vacancies are located in the same straight line parallel to the nanotube axis. The potential relief for this case and the characteristics of the thread are presented in Fig. 2. According to our calculations, the relative thread depth $\beta = 5.812$ in this case is rather large. Furthermore, condition (6) for the calculated thread angle $\chi = 70.9^\circ$ is satisfied for any relative thread depth. Therefore, the nanoactuator can be fabricated using the $(11, 2)@(12, 12)$ nanotube with seven vacancies per unit cell of the double-walled nanotube (the nanobolt–nanonut pair) as a function of the relative displacement $z$ of the outer wall along the nanotube axis and the angle $\phi$ of the relative rotation of the outer wall around this axis. Designations: $\chi$ is the thread angle, $\Theta$ is the chiral angle of the wall free from vacancies, and $a_1$ and $a_2$ are the unit vectors of the unit cell of the development of the wall free from vacancies. Light circles correspond to the minima of the potential relief in the unit cell of the perfect (vacancy-free) wall.

Two types of correlations between the structure of the development of the perfect wall and the lattice formed by the minima of the potential relief of the interwall interaction energy for the double-walled nanotube used as the nanobolt–nanonut pair was found for nanotubes with short and long incommensurate chiral walls [15]. Only one of these types was revealed for double-walled nanotubes with commensurate walls and one identical defect in each unit cell of the nanotube [20, 25]. The potential relief shown in Fig. 2 is characterized by a new type of correlations: seven equivalent minima of the potential relief correspond to each unit cell of the development of the perfect wall.

Below, we will consider a number of techniques for driving the nanoactuator that can be used for both nanoactuators (with inner and outer wall 4) depicted in Fig. 2. The calculations of the charge distribution revealed that the dipole moment appears upon chemical adsorption of Br$_2$ [38] and H$_2$O [39] molecules at the ends of single-walled nanotubes. Moreover, the sign of the charge transferred to the end depends on atoms adsorbed on the open ends of nanotubes [40]. Therefore, we propose to increase the dipole moment of wall 4 due to the adsorption of charge donors and charge acceptors at opposite open ends of the wall. In this case, the nanoactuator can be driven with the use of a nonuniform electric field. In the case where wall 4 is conducting, the nanoactuator can be driven with a nonuniform magnetic field directed along the nanoactuator axis [41].

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A number of methods developed for incorporating magnetic materials inside nanotubes are described in [45–47]. In this case, the motion of wall 4 filled with a magnetic material can be controlled by varying a magnetic field.

As follows from the calculations, the electrostatic potentials at open and capped ends of single-walled nanotubes differ significantly [48]. Consequently, wall 4, which is open from one end and closed from the other end, should have a dipole moment and the nanoactuator can be driven by a nonuniform electric field.

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Now, we discuss the possible ways of driving the nanoactuator. Initially we consider the methods that can be used for both nanoactuators (with inner and outer wall 4) depicted in Fig. 2. The calculations of the charge distribution revealed that the dipole moment appears upon chemical adsorption of Br$_2$ [38] and H$_2$O [39] molecules at the ends of single-walled nanotubes. Moreover, the sign of the charge transferred to the end depends on atoms adsorbed on the open ends of nanotubes [40]. Therefore, we propose to increase the dipole moment of wall 4 due to the adsorption of charge donors and charge acceptors at opposite open ends of the wall. In this case, the nanoactuator can be driven with the use of a nonuniform electric field. In the case where wall 4 is conducting, the nanoactuator can be driven with a nonuniform magnetic field directed along the nanoactuator axis [41].

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REFERENCES


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