Operating Characteristics of Nanotube-Based Bolt/Nut Pairs for Nanoelectromechanical System

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Potential surfaces of interwall interaction energy is calculated for double-walled carbon nanotubes (DWNTs) with chiral commensurate walls and atomic scale defects of structure. The calculated surfaces are used to obtain the dependencies of characteristics of the DWNTs as bolt/nut pairs on the structure parameters: radius and chirality angles of the walls and interwall distance. It is found that a quality of the thread of the DWNT-based bolt/nut pair improves with the decrease of the DWNT radius, only slightly depends on the chirality angles of the walls and does not correlate with the interwall distance. DWNTs with the smallest radii which can be used as the best bolt/nut pairs are selected. The expression which approximately describes the calculated potential surfaces for all considered DWNTs is also introduced.

Keywords: Nanotube, Nanoelectromechanical System, Bolt/Nut Pair, Actuator, Interwall Interaction.

1. INTRODUCTION

The possibility of relative motion of walls in multi-walled carbon nanotubes¹,² allows to use these walls as movable elements of nanoelectromechanical systems (NEMS), see Ref. [3] for a review. At present, nanomotors in which walls of a multi-walled nanotube play the role of the shaft and the bush⁴–⁷ and memory cells operating on relative sliding of the walls along the nanotube axis⁸–⁹ have been implemented. It has been proposed that double-walled nanotube (DWNT) can operate as a bolt/nut pair⁶,¹⁰–¹³ and thus it can be used in a nanoactuator in which the force directed along the nanotube axis is transformed into rotational motion of the walls.¹⁴–¹⁶

The recent experimental study of relative motion of nanotubes walls in the nanotube-based nanomotor driven by a thermal gradient had revealed both relative sliding of the walls along the nanotube axis and pure relative rotation of the walls.⁶ Although, as it is particularly emphasized in Ref. [6], relative motion of nanotube walls is in the general case a helical motion, such a motion had not been observed. The mentioned success in the nanomotor elaboration poses an actual problem on search of nanotubes which can easily operate as bolt/nut pairs. The aim of the present paper is to study characteristics of the nanotube-based bolt/nut pairs as functions of their structural parameters and to select nanotubes with the best characteristics.

To study the relative motion of the nanotube walls, the dependence of the interwall interaction energy $U$ of two neighbouring nanotube walls on their relative position needs to be calculated. It is convenient to visualize the potential surface of the interwall interaction energy $U(\phi, z)$ as a map plotted on a cylindrical surface, where $z$ is the wall relative displacement along the nanotube axis and $\phi$ is the angle of the wall relative rotation about this axis. In principle, DWNT can operate as the bolt/nut pair if the potential surface have valleys directed along a helical line by analogy with a thread on a bolt lateral surface (so-called thread-like potential surface).¹¹,¹² The quantitative characteristics of this thread are the potential barriers $E_1$ and $E_2$ to the relative motion of the DWNT walls along the thread line and across it ($E_2$ is the barrier to twist-off or the thread depth). The quality of thread can be characterized not only by the potential barriers themselves but also by their ratio, the relative thread depth $\beta = E_2/E_1$.¹¹,¹² Evidently that high value of the relative thread depth $\beta$ implies low probability to give rise the twist-off using a force which is sufficient for the relative screw motion of the nanotube walls.

In general case, a nanotube wall has a helical symmetry (see, for example Ref. [17]). Therefore the relative screw motion of the walls can be expected for majority of DWNTs. However, as it was discussed in detail,
the symmetry-based characteristics of the relative screw motion of the walls for the DWNTs with the perfect walls do not allow to use such nanotubes as the bolt/nut pairs in NEMS.\textsuperscript{14, 18} Recently it was shown that an atomic scale design of the wall structure makes it possible to produce nanotubes that can operate as the bolt/nut pair with desirable characteristics of the relative screw motion of the DWNT walls. Namely, it was proposed to produce the DWNT that can operate as the bolt/nut pairs by creating artificial defects at identical positions for many unit cells of a nanotube with chiral commensurate walls.\textsuperscript{14, 18, 19} In this case, any barrier for the relative motion of the walls is proportional to the number of the unit cells with identical positions of the defects. Therefore such atomic scale design of the DWNT structure allows to obtain the bolt/nut pair with the desirable (sufficiently great) value of a barrier to twist-off. It was shown also that the relative thread depth $\beta$ does not depend on the type of the defects and number of unit cells with defects.\textsuperscript{14, 18} Thus the nanotube-based bolt/nut pair with a high value of the relative thread depth $\beta$ can be obtained by creating a single defect. Here the relative screw motion of the walls is studied by the example of DWNTs with chiral commensurate walls including a single vacancy with an identical position in each unit cell of the nanotube.

Up to now multi-walled nanotubes with the smallest radius of the inner wall about 1.4 Å were produced.\textsuperscript{20} Here we calculate the potential surfaces for DWNTs with the commensurate chiral walls and with the interwall distance close to the experimental value 3.4 Å for multi-walled nanotubes. The considered ranges of the wall radiiues are $R_1 = 1.8–9.0$ Å and $R_2 = 5.1–12.5$ Å for the inner and outer walls, respectively. The cases of a single vacancy per the unit cell of the inner wall and the perfect outer wall as well as a single vacancy per the unit cell of the outer wall and the perfect inner wall are considered. The dependencies of the barriers to the relative motions of the walls along the helical thread line and across it, the relative thread depth $\beta$ and threshold forces causing screw-like motion and twist-off on the structural parameters of DWNT are analyzed. The DWNTs with best operating characteristics as the bolt/nut pair are selected.

2. INTERWALL INTERACTION CALCULATION

The unit cells of the DWNTs with the commensurate chiral wall contain several hundreds of atoms. Moreover the calculations of the interwall interaction energy of the DWNTs show that the barriers to motion of the short wall relative to the long wall are very sensitive to the length of the long wall.\textsuperscript{19} Thus the size of the system is too large for \textit{ab initio} calculations of the potential surface of the interwall interaction energy for 15 DWNTs considered here. Therefore we describe the interaction between carbon atoms of the neighbor walls of the DWNT by empirical Lenard-Jones potential $U = 4\varepsilon((\sigma/r)^{12} - (\sigma/r)^6)$, where $r$ is the interatomic distance. The parameters of the potential, $\varepsilon = 2.968$ meV and $\sigma = 3.407$ Å, were fitted to reproduce the interlayer distance and and $c$-axis compressibility for graphite.\textsuperscript{10} The cut-off distance $r = r_c$ of the potential is taken equal to $r_c = 40\ell$. Lenard-Jones potential was used to study the potential surface of the interwall interaction energy for the DWNTs without defects,\textsuperscript{10–13, 19, 21} the dependencies of the ground state interwall interaction energy,\textsuperscript{22, 23} and the frequencies radial breathing mode\textsuperscript{23} on the radius and chiral angle of the wall of the DWNTs. Note also that the using of Lenard-Jones\textsuperscript{19} and other semiempirical potentials\textsuperscript{24, 25} allows to obtain the important and adequate qualitative result that the potential surface for all DWNTs with perfect commensurate chiral walls is extremely flat. The potential surface of the interlayer interaction energy for bilayer graphene calculated using Lenard-Jones potential and \textit{ab initio} method have the same shape and differ only in amplitude of the surface corrugations.\textsuperscript{26} Thus we believe that Lenard-Jones potential is suitable for qualitative calculations of physical quantities related with the interwall interaction, that is this potential is adequate to study the qualitative dependencies of the bolt/nut pair characteristics on the structural parameters of DWNTs and to select DWNTs which are the best bolt/nut pairs, i.e., for both aims of the present paper.

The structure of the walls is constructed by folding of a graphene layer with the bond length of 1.42 Å (the bond length of the multi-wall nanotubes coincides with the bond length of graphite within the accuracy of neutron diffraction measurements --0.01 Å). The walls are considered as rigid. Account of the deformation of the walls is not essential for the shape of the potential surface both for the interwall interaction energy of the DWNTs and the intershell interaction energy of the carbon nanoparticles.\textsuperscript{28, 29} For example, the barriers to the relative wall rotation and sliding of the walls for the $(5,5)@10(10,10)$ DWNT calculated for the walls with the unannealed structure\textsuperscript{19} coincide within 14% with the results of Dresselhaus et al. which were obtained using the annealed wall structure.\textsuperscript{10} In order to avoid the influence of the nanotube edge on the potential surface we consider the case of the long inner wall and the short outer wall. The length of the outer wall is chosen to be equal to the length of the DWNT unit cell. The length of the inner wall is taken so that all pairs of atoms with the interatomic distances smaller than the cutoff distance are considered. Since the relative sliding\textsuperscript{1, 2, 8, 9} and rotation\textsuperscript{4, 7} of walls have been realized for nanotubes which are hundreds nanometers in length, in the present paper we present all barriers in meV per 100 nm.

According to the theoretical consideration the potential surface for any DWNTs with perfect chiral commensurate walls should be extremely flat due to incompatibility of chiral symmetries of walls.\textsuperscript{30} Up to now, this assumption was confirmed by calculations only for the DWNTs
with the radius of the inner wall which exceeds 3.5 Å.\textsuperscript{19, 25} Namely, the barrier to the relative rotation of the walls of the (8, 2)@16, 4 DWNT calculated using the Lennard-Jones potential is about 8.61 $\cdot$ 10^{-8} meV per 100 nm and it is the only example found where any barrier to the relative motion of the walls for such nanotubes exceed the calculation accuracy.\textsuperscript{19} Magnitudes of other barriers for tens of the DWNTs with the perfect chiral commensurate walls are less than calculation accuracy.\textsuperscript{19, 25}

Up to now multi-walled nanotubes with the smallest radius of the inner wall about 1.4 Å were produced.\textsuperscript{20} The analysis of the DWNTs symmetry shows that the thread-like potential surface is in principle possible only for three DWNTs ((6, 3)@14, 7), (3, 2)@9, 6, and (4, 1)@(12, 3)) with the perfect chiral commensurate walls and the radius between 1.4 and 3.5 Å (which were not considered in Refs. [19, 25]). Here to test this possibility the potentials surfaces of these DWNTs are calculated. We have found that the (3, 2)@9, 6 DWNT has the extremely flat potential surface with the corrugations less than 10^{-7} meV per 100 nm. It is revealed that the rotation of the walls is the easiest relative motion of the walls of the (6, 3)@14, 7 DWNT. This DWNT has the barrier to the rotation $E_z = 6.7 \cdot 10^{-8}$ meV per 100 nm, whereas the barrier to the sliding of the walls along the nanotube axis is $E_x = 1.28 \cdot 10^{-5}$ per 100 nm. The potential surface of the (4, 1)@12, 3 DWNT is symmetric about two mirror planes passing through the nanotube axis. Therefore this DWNT has coinciding barriers to left-hand and right-hand thread-like relative motion of walls ($E_x = E_z = 1.83 \cdot 10^{-5}$ meV per 100 nm with the thread angle $\chi = 45^\circ$) and cannot be used as bolt/nut pair. Moreover the calculated values of the barriers are too small to use these DWNT in any applications based on the shape of the potential surface. Thus the results described above confirm that DWNT with the perfect chiral commensurate walls can not be used as the bolt/nut pairs.

The interwall interaction energy $U_{ij}$ for the DWNT with a vacancy in a one wall can be considered as

$$U_{ij}(\phi, z) = U_{\text{perf}}(\phi, z) + \sum_{i=1}^{N} U_{ij}$$

where $U_{\text{perf}}$ is the interwall interaction energy for the DWNT with the perfect walls, $U_{ij}$ are the pairwise interaction energies between the remote atom, corresponding the vacancy and atoms of neighboring wall, $N$ is the number of atoms in the perfect wall, and $j$ is the number of the atom corresponding to the vacancy. Here, we consider the DWNTs which have the extremely flat surface in the absence of defects $U_{\text{perf}}(\phi, z) \approx U_0$, where $U_0$ is constant. The constant first term $U_{\text{perf}}(\phi, z)$ in Eq. (1) has no influence on the potential surface shape and, therefore, does not contribute into any barrier to the relative motion of the walls. Thus, only the pairwise interaction energies $U_{ij}$ which contribute into the second term in Eq. (1) should be taken into account in the calculation of the potential surface shape. As a result, the number of the energies $U_{ij}$ which must to be calculated is decreased in $1/N$ times. Therefore the computation time for the calculation of potential surface for the DWNTs with defects under consideration can be considerably decreased. Note, that this method can not be used for the DWNTs with the nonchiral commensurate walls where the corrugation of the potential surface in the case of the perfect walls is considerable.\textsuperscript{19, 24}

3. RESULTS AND DISCUSSION

Examples of thread-like potential surfaces of the interwall interaction energy for the DWNTs with the chiral commensurate walls with one vacancy are shown in Figure 1. The minima of the potential surface form the lattice with the lattice vectors $a$ and $b$. Evidently, the lattice of this minima correlates with the lattice of perfect wall network. Such correlation is also observed for the DWNTs with the incommensurate walls, where the lattice of the potential surface minima correlates with the lattice of the longer wall structure.\textsuperscript{11} To consider this correlation in details let us convert the angle coordinate $\phi$ to the space coordinate $z$.
The envelope of the unit cell of the wall cut from graphene plane is shown as a rectangle with sides $c$ and $d$. $c$ is equal to the length of the wall circumference and $d$ is equal to the length of the wall unit cell. The possible directions of thread are shown by intersecting lines which are perpendicular to the hexagon sides.

$L$ as $L = \phi R_p$, where $R_p$ is the perfect wall radius. In this coordinate system $(L, z)$ the relative motion of the walls is analogous to the motion of the projection of a vacancy on the surface of the perfect wall. Two types of the potential surface minima lattices were found for the DWNTs with the incommensurate walls: the type I with the rectangular lattice of minima and the type II with the oblique lattice of minima.\(^1\) We have found that all calculated thread-like potential surfaces correspond to the type II with the lattice vectors $a$ and $b$ which have the lengths $a = b = a_0$, where $a_0 = 2.46 \text{ Å}$ is the length of the graphite lattice vector and the angle between the lattice vectors equals to 60°.

Let us consider the geometrical characteristics of the thread. Since the thread direction is determined by the lattice of the perfect wall, the thread angle $\chi$ between a thread line and the wall circumference in the coordinate system introduced above is determined by the chirality angle $\theta$ of the perfect wall

$$\chi = \theta + k \cdot 60^\circ$$  \hspace{1cm} (2)

where $k$ is equal to 0, 1, or 2. The chirality angle $\theta$ for any nanotube wall can be expressed as\(^3\)

$$\theta = -\arccos \frac{2n_1 + n_2}{\sqrt{h^2 + n_1^2 + n_2^2}}$$  \hspace{1cm} (3)

The chirality angle $\theta$ of the perfect wall, the thread angle $\chi$, the number of thread lines $N_t$, and the pitch $h$ of thread are tabulated in Table I. For all considered DWNTs the thread lies between 0° and 30° (that is $k = 0$ in Eq. (2)) and between 60° and 90° (that is $k = 1$ in Eq. (2)) for the cases of vacancy in the inner wall and in the outer wall, respectively.

The calculated values of the barriers $E_1$ and $E_2$ to the relative motion of the walls along thread line and twist-off, respectively, and the relative thread depth $\beta$ (the ratio of these barriers) which evaluate the quality of the bolt/nut pair are presented in Table II for all considered DWNTs. Figure 3 shows the relative thread depth $\beta$ versus the radius and the thread angle of the perfect wall. According to classification DWNTs with commensurate walls,\(^9\) these DWNTs make up families whose all members have identical interwall distances and identical chiral angles of the inner and outer walls. Therefore DWNTs from the same family differ only in their radius. Such DWNTs are shown

<table>
<thead>
<tr>
<th>DWNT</th>
<th>$N_t$</th>
<th>$\theta$</th>
<th>$\chi$</th>
<th>$h$</th>
<th>$N_t$</th>
<th>$\theta$</th>
<th>$\chi$</th>
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<td>12.78</td>
<td>1</td>
<td>23.41</td>
<td>83.41</td>
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<tr>
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<td>10.89</td>
<td>10.89</td>
<td>6.39</td>
<td>1</td>
<td>10.89</td>
<td>70.89</td>
<td>10.65</td>
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<tr>
<td>(4, 2)@12(6)</td>
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<td>19.11</td>
<td>12.78</td>
<td>2</td>
<td>19.11</td>
<td>79.11</td>
<td>12.78</td>
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<td>17.00</td>
<td>17.00</td>
<td>12.78</td>
<td>1</td>
<td>17.00</td>
<td>77.00</td>
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<tr>
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<td>19.11</td>
<td>19.11</td>
<td>14.91</td>
<td>3</td>
<td>19.11</td>
<td>79.11</td>
<td>19.17</td>
</tr>
<tr>
<td>(6, 4)@12(8)</td>
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<td>23.41</td>
<td>23.41</td>
<td>17.04</td>
<td>2</td>
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<td>83.41</td>
<td>21.30</td>
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<td>27.00</td>
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<td>21.05</td>
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<td>1</td>
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by the same symbols in Figure 3. Following interesting conclusions can be extracted from the results presented in Figure 3.

(1) The relative thread depth $\beta$ rapidly decreases with the increase of nanotube radius. This is an expected result, since $\beta = 1$ for infinite radius, i.e., for relative motion of flat graphene layers.

(2) The relative thread depth $\beta$ is typically greater for the DWNTs with vacancies in the inner wall than for the DWNT with the close radius and vacancies in the outer wall.

(3) The DWNTs with the thread angle close to $0^\circ$ and to $90^\circ$ for the cases of vacancies in the outer wall and in the inner wall, respectively, tends to have greater values of the relative thread depth $\beta$.

We do not observe any correlations between the relative thread depth $\beta$ and the interwall distance.

Figure 4 shows the barriers $E_1$ and $E_2$ to the relative motion of the walls versus the radius of the perfect wall for the $(4k,k)@(4(k + 2), k + 2)$ family of DWNTs. The analysis of results presented in Figure 4 allows us to draw the conclusion that for the DWNTs from the same family the barriers $E_1$ and $E_2$ only weakly depend on the DWNT radius. It is interesting that although the relative thread depth is typically greater for the DWNTs with vacancies in the inner wall, the barriers $E_2$ for twist-off (i.e., the absolute thread depth) are typically greater for the DWNTs with vacancies in the outer wall. It is not found correlations between the barriers $E_1$ and $E_2$ and the thread angle. Note also that DWNTs with smaller values of the interwall distance have greater values of the barriers $E_1$ and $E_2$ for the relative motion of the walls.

We have found that the calculated potential surfaces of the DWNTs with the small radius and the chiral commensurate walls with a vacancy per elementary cell of the wall can be described using the simple approximation containing only the first Fourier component

$$U(\varphi, z) = U(\varphi_{\text{min}}, z_{\text{min}}) + \frac{E_2}{2} \left(1 - \cos \left[ \frac{2\pi}{a_1 - b_2 - a_2 - b_1 (b_2 R_p [\varphi - \varphi_{\text{min}}] - b_1 [z - z_{\text{min}}])} \right] \right)$$
Fig. 3. Relative thread depth versus radius of the walls without vacancies (a) and (b), and versus thread angle (c) and (d). (a) and (c) correspond to double-walled nanotubes with vacancies in the inner wall, (b) and (d) correspond to the double-walled nanotubes with vacancies in the outer wall. Fill squares, circles and triangles correspond to the double-walled nanotubes from the \((4k, k)@(4(k + 2), k + 2), (2k, k)@(2(k + 4), k + 4)\) and \((3k, 2k)@(3(k + 2), 2(k + 2))\) families, respectively. Open circles correspond to the double-walled nanotubes from the families with only one the first member considered.

\[
\begin{align*}
    &+ \frac{E_1}{2} \left( 1 - \cos \left[ \frac{2\pi}{a_1 b_2 - a_2 b_1} (-a_2 R_p \varphi - \varphi_{\min}) + a_1 [z - z_{\min}] \right] \right) \\
    &+ \frac{E_2}{2} \left( 1 - \cos \left[ \frac{2\pi}{\sqrt{3}a_0^2} (b_2 R_p \varphi - \varphi_{\min}) - b_1 [z - z_{\min}] \right] \right)
\end{align*}
\]  

(5)

where \(a = (a_1, a_2)\) and \(b = (b_1, b_2)\) are the lattice vectors of the lattice formed by the minima of the potential surface (see Fig. 1); \(\varphi_{\min}\) and \(z_{\min}\) are coordinates of arbitrary minimum of the potential surface. The potential surface described by the expression (5) presents a superposition of two plane waves. The wave-vectors of these plane waves which form the potential surface are the lattice vectors of the reciprocal lattice of the lattice formed by the minima.

For all DWNTs with a single defect per elementary cell considered here one have \(|a| = |b| = a_0\) and \(\angle (a, b) = 60^\circ\). In this case the expression (5) takes the form

\[
\begin{align*}
    &\frac{E_1}{2} \left( 1 - \cos \left[ \frac{2\pi}{a_1 b_2 - a_2 b_1} (-a_2 R_p \varphi - \varphi_{\min}) + a_1 [z - z_{\min}] \right] \right) \\
    &+ \frac{E_2}{2} \left( 1 - \cos \left[ \frac{4\pi}{\sqrt{3}a_0^2} (-a_2 R_p \varphi_{\min}) + a_1 [z - z_{\min}] \right] \right)
\end{align*}
\]  

(6)

Let us introduce the ratio \(Q\) between the root-mean-square deviation of the calculated potential surface from the interpolated surface described by Eq. (6) and the root-mean-square deviation of the calculated potential surfaces from its minimum. This ratio characterizes the accuracy of the interpolation of the potential surface by Eq. (6).

Fig. 4. Barriers \(E_1\) and \(E_2\) to the relative motion of the walls along the thread line and twist-off, respectively, vs. radius of the wall without vacancies for the \((4k, k)@(4(k + 2), k + 2)\) family of the double-walled nanotubes. Circles and squares correspond to the barriers \(E_1\) and \(E_2\) to the relative motion of the walls along the thread line and twist-off, respectively. (a) and (b) correspond to the vacancies in the inner and outer walls, respectively.
In the case of the DWNTs with vacancies in the inner wall the ratio $Q$ has tendency to rise with the increase of the DWNT radius. The smallest values of the ratio $Q$ is equal to 0.5, 1 and 1.5% for the (4, 2)$@$(12, 6), (4, 1)$@$(12, 3) and (3, 2)$@$(9, 6) DWNTs, respectively, which have the smallest radii, and is within 10% for the majority of the considered DWNTs with vacancies in the inner wall except for the (12, 3)$@$(20, 5), (16, 4)$@$(24, 8) and (20, 5)$@$(28, 7) DWNTs which have the greatest radiuses. For all considered DWNTs with vacancies in the outer wall the ratio $Q$ is between 10 and 30% (see Table II).

It is worth noting that the revealed possibility to approximate the potential surface of the interwall interaction energy by the simple expression is the common property for relative motion of graphene-like layers. For example, both ab initio and empirical calculations show that the first Fourier components are sufficient to approximate such potential surfaces for the relative motion of the walls of the DWNTs with perfect achiral walls and layers of bilayer graphene. The mentioned approximation of the potential surface for bilayer graphene was used for the interpretation of the results obtained for the motion of the graphene flake on a graphite surface with the help of friction force microscopy. Thus the approximation (6) can be useful for interpretation of motion of the short outer wall relative the inner walls of the nanotube studied using a friction force microscope.

Let us consider the forces which are necessary for nanotube-based bolt/nut pair operation. The calculated threshold forces $F_1$ and $F_2$ for the relative motion of walls along the thread line and across it, respectively, are presented in Table II. Note that these forces correspond to the range which is typical for atomic force microscopy, thus nanotube-based bolt/nut pairs are suitable for application in NEMS. It was shown that both threshold forces $F_1$ and $F_2$ can be calculated as the angles of the maximal slope for dependencies of the interwall interaction energy $U$ on the coordinate $l$ which characterizes the relative wall position along the corresponding path between the minima of the potential surface in the coordinate system $(L, z)$.

It is evident from Eq. (5) that dependencies $U(l)$ are very close to cosines. Then these forces can be estimated as

$$F_1 = \frac{\pi E_1}{a_0}, \quad F_2 = \frac{\pi E_2}{a_0}$$

(7)

The ratios between the calculated forces and their estimations using Eq. (7) are listed in Table II. It is found that differences between the calculated forces and their estimations are less than 0.6% These differences decreases with the increase of the nanotube radius. Thus, values of the threshold forces if they are measured experimentally can be used for estimation of the barriers $E_1$ and $E_2$, which are essential in consideration of the wall relative diffusion and drift along the thread line, and therefore for operation of the nanotube-based nanomotor driven by a thermal gradient.

4. SUMMARY

In the present paper we have calculated the potential surfaces of interwall interaction energy is calculated for 15 DWNTs with chiral commensurate walls and atomic scale defects of structure. The simple expression which approximately describes the calculated potential surfaces for all considered DWNTs is introduced. This expression can be useful for interpretation the relative motion of the nanotube walls studied using a friction force microscope.

On the base of the calculated surfaces the characteristics of DWNTs as bolt/nut pairs are studied. Namely the thread angle, the pitch of thread, the barriers and the threshold forces for relative motion of walls along the thread line and for the twist-off are calculated. The quality characteristic of thread, the relative thread depth, equal to ratio of barriers to the relative motion of the walls along the thread line for and the twist-off is also determined. We have found that the relative thread depth strongly increases with the decrease of the DWNT radius, only slightly depends on the chirality angles of the walls and does not correlate with the interwall distance. Thus only DWNTs with the smallest radiuses can be used as bolt/nut pairs. Namely the (4, 1)$@$(12, 3) and (3, 2)$@$(9, 6) DWNT have the best quality of the thread for the cases of the vacancy in the inner and outer walls respectively, therefore these DWNTs are perspective for use as bolt/nut pairs.

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References

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