Bolt-and-Nut Pairs Made from Carbon Nanotubes with Artificial Defects

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Abstract: Structures of double-wall carbon nanotubes (DWNTs) with atomic scale defects that can operate as bolt-and-nut pair are analyzed. The relative thread depth for such bolt-and-nut pair is calculated for various types of defects in inner and outer walls of (4,6)@(12,8) and (8,2)@(16,4) DWNTs. It is found that a type of defect determines only the absolute thread depth but weakly influences on the relative thread depth. Possibility of producing of the DWNT (which can operate as bolt-and-nut pair) by self-organization is proposed.

Keywords: Carbon nanotubes, interwall interaction, electromechanical nanodevices, bolt-and-nut pair

The search of possible movable parts of nanomachines is one of main challenges for development of nanomechanics. The recent observation of relative motion of carbon nanotube walls (1) allows to consider them as promising candidates for NEMS. Since the nanotube wall has a helical symmetry it was recently proposed that a double-wall nanotube (DWNT) can be bolt-and-nut pair (2). Such bolt-and-nut pair can operate, for example, as an auger of a perforating nanodrill or a nanodevice in which the force directed along the nanotube axis is transformed into rotational motion of the walls (3).

However until now, the thread-like potential relief of the interwall interaction energy was found only for DWNTs with the incommensurate walls. 
In this case the thread depth is small, and considerably fluctuate the with change of the nanotube lengths (3). As for the DWNTs with commensurate walls their potential relief can not be thread-like or is extremely smooth due to the incompatibility of walls symmetries (4, 5). Recently we proposed to overcome these difficulties by the creation of artificial defects at an identical position for a lot of nanotube unit cells (4, 6). In this case, a thread depth is proportional to the number of unit cells with identical positions of defects.

To study the relative motion of the nanotube walls, the dependence of the interwall interaction energy $U$ of two neighboring nanotube walls on their relative position needs to be calculated. It is convenient to visualize the potential relief of the interwall interaction energy $U(z, \phi)$ as a map plotted on a cylindrical surface, where $z$ is the length of the wall relative displacement along the nanotube axis and $\phi$ is the angle of the wall relative rotation. The DWNT can operate as the bolt-and-nut pair if the potential relief have valleys directed along the helical line. 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 potential barriers but also by the ratio of the relative thread depth $\beta = E_2/E_1$ (3).

Here we study the thread-like potential relief for $(4,6)@$(12,8) and $(8,2)@$(16,4) DWNTs with commensurate walls including one vacancy or substituted atom per unit cell (one-atomic defects). As substituted atom we consider an atom of other element or a carbon atom with the modified electronic structure due to chemical adsorption of atoms and molecules. The interwall interaction for carbon atoms is described by 6-12 Lennard-Jones potential with the parameters $\sigma_0 = 2.968$ nm and $\varepsilon_0 = 3.407$ Å. This parameters $\sigma_1$ and $\varepsilon_1$ for interaction with substituted atom differ from those of carbon atoms interaction, as follows: $\sigma_1 = a\sigma_0$ and $\varepsilon_1 = g\varepsilon_0$.

In the case of one-atomic defects, barriers to any relative motion of the walls are proportional to $a^{-1}$, and therefore the relative thread depth $\beta$ does not depend on $a$ and the thread-like potential relief depends on parameter $g$ only. The relative thread depth $\beta$ also depends slightly on $g$ (as shown in Figure 1). The value of the relative thread depth $\beta$ for the substituted atom is also close to the value of $\beta$ for the case of vacancy.

We consider also the case where the substituted atom is displaced in radial direction from the position of carbon atom in the same site of wall network. The dependencies of the relative thread depth $\beta$ as the function of the radial displacement $d$ of the substituted atom from the cylindrical surface of the wall are presented in Figure 2. At the present time carbon nanotubes doped by boron and nitrogen (7) were produced. According to calculations the radial displacement of substituted atom is 0.02 Å for nitrogen and 0.11 Å for boron (8). Therefore Figure 2 shows that the relative thread depth $\beta$ changes slightly for possible values of displacement $d$. 
The results obtained show that one-atomic defect determine the quantitative energetic characteristics of the potential relief, such as the values of the barriers and the threshold forces for any kind of the relative motion of the walls. However, for any given DWNT with a given wall with defects, the qualitative energetic characteristic of the potential relief, such as the relative thread depth is nearly the same for the different types of defects. Thus we demonstrate that in the case of one-atomic defects the relative thread depth is determined mainly by the structure of the wall without defects. Therefore DWNTs with the best characteristics of the thread, that are the most perspective candidates for the bolt-and-nut pairs, can be selected with the use of the proposed model for subsequent precise ab initio study.

The present theoretical study brings up the question: can DWNTs with periodically positioned defects that operate as the bolt-and-nut pair be produced. The modern nanotechnology does not allow to made periodically positioned vacancies of one atom and the Stone–Wales defects or to substitute carbon atom by atom of another element. As for the adsorption of particles on the wall surface the transfer of a single atom adsorbed on the surface is possible in principle using STM or AFM tip. Of course such technique allows only limited production of the DWNTs which can operate as the bolt-and-nut pairs for laboratory examinations. However the adsorption of particles at the periodically positioned sites of the wall surface can correspond
to the calculated ground state of the system (9). Therefore we propose that the DWNTs that can operate as the bolt-and-nut pair can be obtained as a result of adsorbed particles self-organization. In this case the technique for industry production of such bolt-and-nut pair for mechanical nanodevices can be elaborated.

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REFERENCES


