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Rotary Nanomotors Based on Head-to-head Nanotube Shuttles

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***Abstract*—A novel rotary nanomotor is described using two axially aligned, opposing chirality nanotube shuttles. Based on inter-shell screw-like motion of nanotubes, rotary motion is generated by electrostatically pulling the two cores together. Simulations using molecular dynamics show the generation of rotation from armchair nanotube pairs and their actuation properties. The simulation results, together with recently reported progress in realizing batch-fabricated ultra-high density nanotube shuttles, point towards the use of these motors as building blocks in nanoelectromechanical systems (NEMS) and nanorobotic systems for sensing, actuation, and computation applications.**

***Index Terms*—Rotary nanomotor, nanotube, NEMS, nanorobotic system, molecular dynamics simulation**

I. Introduction

Since the discovery of carbon nanotubes (CNTs) [1], researchers have identified a number of promising applications in nanoelectronics, nanoelectromechanical systems (NEMS), and nanorobotic systems [2] based on their unique electrical and mechanical properties. The atomic smooth surfaces and weak van der Waals interactions between nanotube shells allow them to readily slide and rotate relative to each other. Previous reports on the inter-shell interactions and electrostatic actuation of telescoping multiwalled carbon nanotubes (MWNTs) [3-5] have demonstrated the robustness of these nanostructures. In these structures, motion at the nanometer scale can be generated in the form of sliding, rotation or screw-like motion between nanotube walls. Devices that have been proposed based on these forms of motion include bearings [3, 6, 7], linear servomotors with integrated position sensing [4], resonators/oscillators [8, 9], encoders [7], and electrical switches [10]. Experimental [11, 12] and computational [13, 14] investigations have also been performed on the geometric and energetic parameters that characterize the relative position and motion of the neighboring walls of a nanotube for rotational nanoactuators. In experimentally demonstrated devices [11, 12], nanotubes served as bearings for a nanometallic rotor, which is electrostatically actuated using microfabricated stator electrodes [11].

The chiral structures of nanotube shells [14, 15] offer alternate possibilities for generating rotary motion between coaxial nanotube shells without involving extra rotors. In another effort, a rotary motor [16] was conceptually constructed from a double-walled carbon nanotube (DWNT) consisting of two single-walled carbon nanotubes (SWNTs) with different length and chirality within the framework of the Smoluchowski-Feynman ratchet. In that design, the axial sliding motion of the inner tube has been assumed to be constrained and unidirectional rotation has been shown in the presence of a varying axial electrical voltage. Here we propose an electrostatic rotary nanomotor based on two axially aligned nanotube shuttles, where the axial sliding motion can be constrained by the two nanotubes against each other. In addition, our recent success on the batch fabrication of shell engineered nanotubes has demonstrated the key processes required to construct such shuttles for the first time [6]. The goal of the present work is to theoretically demonstrate their working principle and characterize their actuation properties using molecular dynamics simulations (MDS) by considering the combination of chirality pairs and their mutual, non-bonded atomic interactions.

II. Design and Fabrication of Rotary Nanotube Motors

The rotary nanomotor is schematically illustrated in Fig. 1 (a) and (b). The motor consists of two MWNT segments with opposing chiralities. The outermost shells are fixed and the inner shells are freely suspended inside the outer ones. By applying a DC actuation voltage between the segments,

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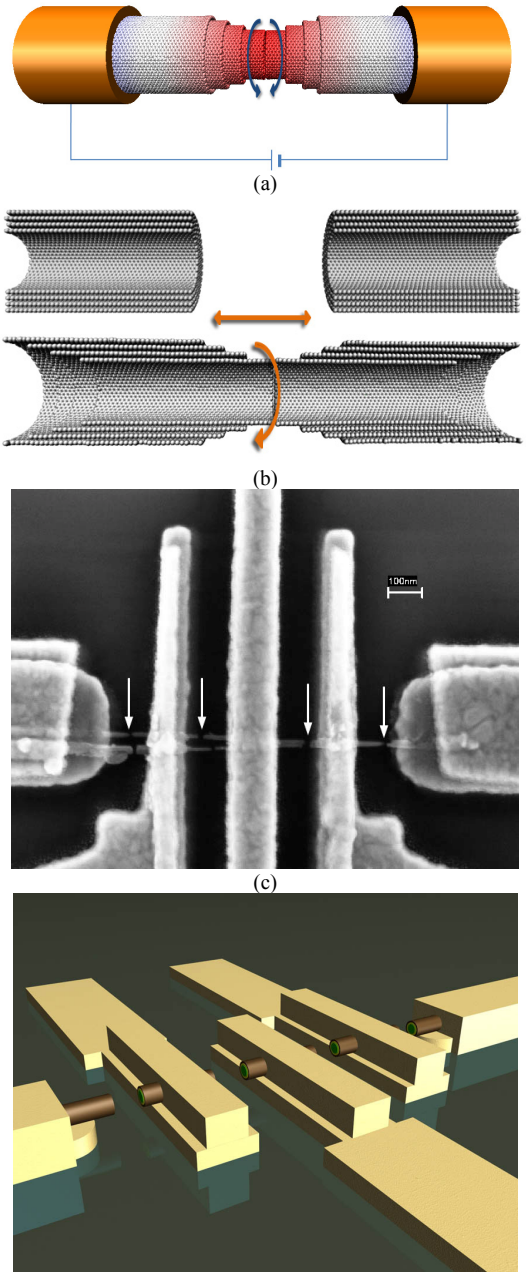


Fig. 1. (a) Schematic design of a rotary nanomotor based on axially aligned nanotube shuttles. (b) Cross-section view of the rotary nanomotor. (c) Shell engineered nanotube shuttles formed with a 220 nm pitch and separated by ~10 nm gaps. The arrows point to the inter-segment gaps in this image. (d) Schematic illustration of the core–shell mechanism with the inter-segment gaps exaggerated to reveal the shell structure.

the axially aligned inner tubes approach each other due to electrostatic forces. Due to their opposite chiralities, both sliding and rotation, i.e., a nanoscrew, will be generated simultaneously during this motion. After contact is made, the sliding motion will be constrained, whereas rotation will remain as the only possible degree-of-freedom for motion.

One possible route towards fabricating these nanostructures involves picking CNTs with opposing chiralities and placing them head-to-head using nanorobotic manipulation [2]. More recently, we have reported an alternate approach that realizes batch fabricated nanoshuttles using a combination of dielectrophoretic nanoassembly and high-yield, current-driven shell engineering processes [3, 6, 7]. In this approach, an individual MWNT is assembled onto multiple, electrically isolated electrodes. The NT segments between electrodes are then vaporized using the current-driven shell-etching technique (Fig. 1 (c) and (d)). Multiple, capless nanotube segments with a 220-nm pitch and 6 to 15nm spacing are created from a single nanotube using this method, which is outlined in detail in [3, 6, 7]. Since a single nanotube is broken into multiple, axially aligned segments with this approach, the requirement of creating nanoshuttles with opposing chiralities can be met only in the case of armchair nanotubes, where the helical angle can be regarded as either $\pi/6$ or $-\pi/6$. The rotational direction in the case of armchair nanotube pairs cannot be predetermined in theory, but the motor is expected to initiate rotation in one direction based on a random dynamic factor and further continue this unidirectional rotation. Thus, an important requirement for the use of this batch fabrication approach for realizing nanoshuttles outlined in this paper is that the nanotube sample, which is used for dielectrophoretic assembly, should contain only armchair nanotubes. While challenges remain in controlling the chirality of individual nanotubes, recent progress on this aspect of nanotube growth such as forming MWNTs with every shell having a zigzag helicity [17] and armchair SWNTs [18, 19] offer promising routes towards realizing all-armchair NTs as required for the batch fabrication approach.

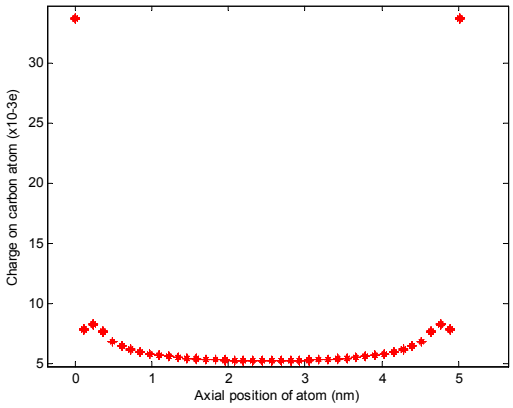
III. Molecular Dynamics Simulations on Rotary Motors

Since the nanotube wall has a helical symmetry, it was recently proposed that a DWNT can serve as a nanoscrew. Such nanoscrews can operate, for example, as an auger of a perforating nanodrill or a nanodevice in which a force or linear motion along the nanotube axis can be transformed into a torque or rotary motion of the core tube [16] . Previously, a classification scheme for non-chiral DWNTs has been developed [13], energetic barriers to the relative sliding and rotation of walls in DWNTs [14] and to the rotation of shells in double-shell nanoparticles[15, 16] have been calculated, and the theory for dynamics of the relative rotation, sliding and screw like motion of nanotube walls has been developed [14]. In this work, we show by molecular dynamics simulation that it is possible to construct a MWNT motor actuated by a DC voltage. Without losing generality, the molecular dynamics modeling and the working principle of the motor are investigated in this paper by taking a rotary motor consisting of two armchair nanotubes as an example. The motor consists of a shuttle structure as shown in Fig. 1 (a) and (b). Using classical molecular dynamics with empirical potentials, we show that the inner CNT can rotate.

A. Simulation method

In this work, we focus on simulating the nanotube rotary motor's performance using classical means. This approach

can consider structures that have dimensions comparable to the experimentally observed ones that have been highlighted in Fig. 1(c) and (d). Specifically, we have considered a 10-shell MWNT device with individual segments that are 200nm long and separated by a gap of 5nm. First, we apply an actuation bias and calculate the charge distribution along the carbon structure using the atomistic moment method. This atomic charge distribution and nanoshuttle structure serve as inputs to the molecular dynamics computations using an adaptive intermolecular REBO AIREBO potential [20] and electrostatic interactions. MD-based computations



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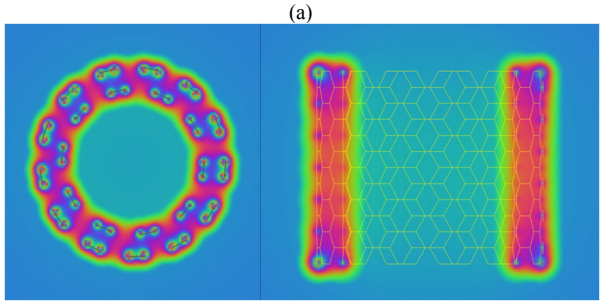

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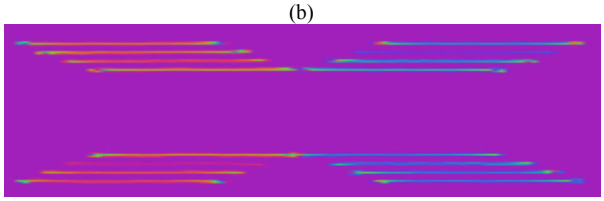

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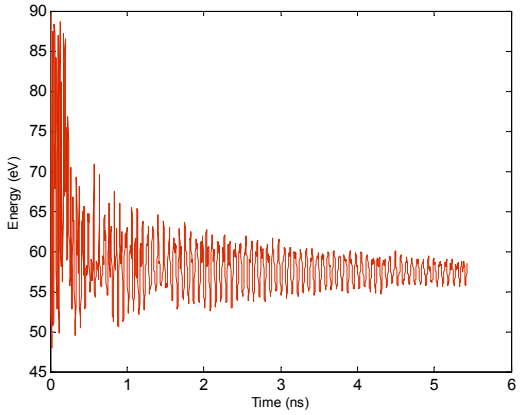

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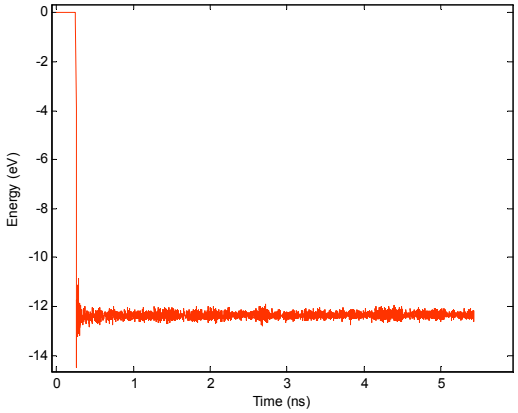


(e)

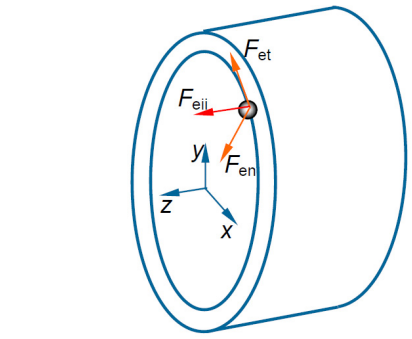
Fig. 2. (a) Charge distribution along the axial direction for an open ended nanotube (V=6V). (b) Electrostatic potential map along a DWNT structure. (c) Cross-sectional view showing the charge distribution during contact between neighboring segments. Negatively charged shells are located on the left, while the positively charged shells are located on the right. (d) Attractive electrostatic energy between two oppositely charged inner shells. (e) Repulsive electrostatic energy between the inner and outer shells. The sliding time of the system is 0.4ns.

are used to extract device performance characteristics like inter-shell and inter-segment interaction energies, rotation, friction and oscillation.

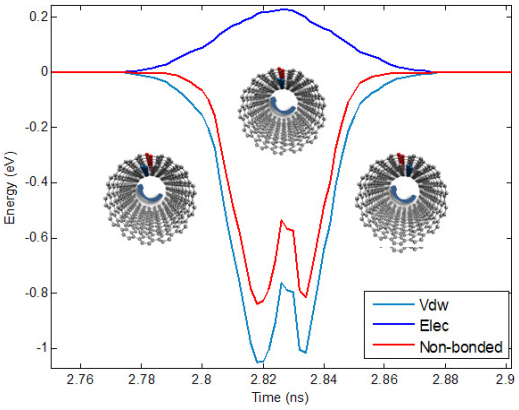
The total potential energy of system is given by $U^{tot} = U^{elec} + U^{P}$, where U^{elec} is the electrostatic energy due to extra charges on two carbon atoms and U^{P} is the AIREBO interatomic potential. AIREBO potential introduces non-bonded interactions through an adaptive treatment, which allows the reactivity of the REBO potential to be maintained. A possible problem due to the introduction of intermolecular interactions is that the repulsive barrier between non-bonded atoms may prevent chemical reactions from occurring. The AIREBO potential corrects this problem by modifying the strength of the intermolecular forces between pairs of atoms depending on their local environment. The AIREBO potential term [20] is given by:

$$U^{p} = \frac{1}{2}\sum_{i=1}^{N}\sum_{\substack{j=1 \\ j\neq i}}^{N}\left[\varphi^{R}\left(r_{i,j}\right) - b_{i,j}\varphi^{A}\left(r_{i,j}\right) + \varphi^{LJ}\left(r_{i,j}\right) + \sum_{\substack{k=1 \\ k\neq i,j}}^{N}\sum_{\substack{l=1 \\ l\neq i,j}}^{N}\varphi_{kijl}^{tor}\right] \quad (1)$$

where $\varphi^{R}\left(r_{i,j}\right)$ and $\varphi^{A}\left(r_{i,j}\right)$ are the interatomic repulsion and attraction terms, $\varphi^{LJ}\left(r_{i,j}\right)$ is the parameterized Lennard-Jones potential, $b_{i,j}$ is the bond order function, and φ_{kijl}^{tor} is the single bond torsional interaction. The electrostatic energy is calculated using



(a)



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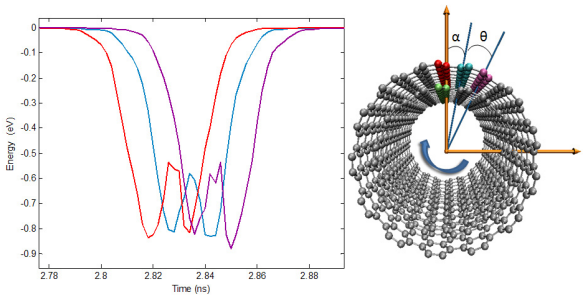


(c)

Fig. 3. (a) Forces acting on a terminus atom located within an inner shell. F_{eii} is the attractive electrostatic force between oppositely charged inner shells located within the neighboring segments. F_{et} and F_{en} are tangential and normal components, respectively, applied by the outer shell within the same nanotube segment. (b) Interaction energies between the two segments in inner and outer shells. Blue, cyan and red curves represent electrostatic, van der Waals and the total non-bonded energy components, respectively. (c) Total non-bonded energy attraction between a segment with green color in the inner nanotube and three successive segments in the outer nanotube.

Coulomb's law: $E_{ij}^{q} = \dfrac{q_i q_j}{4\pi\varepsilon R_{ij}}$, where q_i and q_j are extra charges on carbon atoms, R_{ij} is the interatomic distance, and ε is the permittivity.

B. Electrostatic charge distribution along the length of a carbon nanotube

Electron microscopy provides direct evidence for inter-shell displacements induced by electrostatic actuation [3, 4].

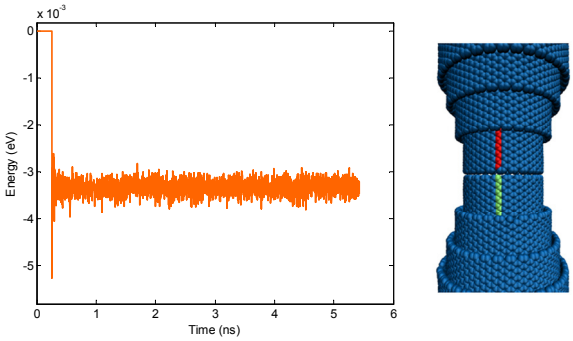


Fig. 4. Attractive electrostatic energy between the inner shells within two neighboring segments (red colored segment and green colored one). As shown by the curve, sliding occurs between 0 and 0.2ns, while at 0.2ns the inner shells establish contact. After 0.2ns, the energy is constant indicating that both inner shells rotate with the same velocity and in the same direction.

In our simulations, the charge distribution on the carbon nanotube is obtained by an atomistic moment method based on classical electrostatics theory [21]. We consider MWNTs with finite lengths. For simplicity, the nanotube is assumed to be situated in an idealized electric field, i.e., the voltage on the nanotube surface is V_0. For a nanotube with N atoms, the potential at an arbitrary atomic position [21] is given by :

$$V\left(r_i\right) = \sum_{j=1}^{N} \frac{q_j}{4\pi\varepsilon_0 \left| r_i - r_j \right|} \tag{2}$$

where V is the electric potential, q_j the point charge on atoms, r_i the location of the charged atom, and ε_0 the permittivity of vacuum. Because of the equipotential status of the nanotube surface, N equations can be written in a matrix form as follows:

$$[A]\{q\} = \{V\} \tag{3}$$

where $\{q\}$ and $\{V\}$ are the charge vector and the potential vector, respectively, and $[A]$ is an N×N matrix.

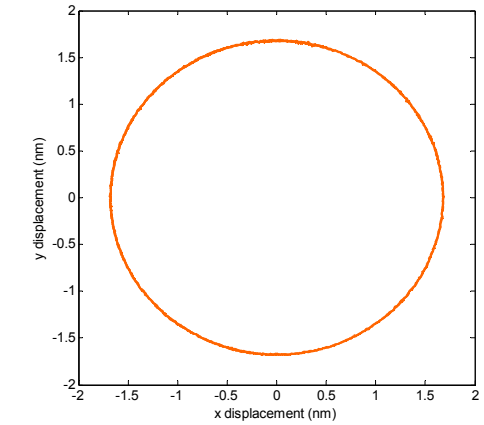
Using Density Function Theory (DFT) we calculated the charge redistribution along double walled nanotube [22 23]. We found that electrons are transferred from outer tube to the inner tube with charge transfer density of 0.002 e/Å.

IV. Results and Discussions

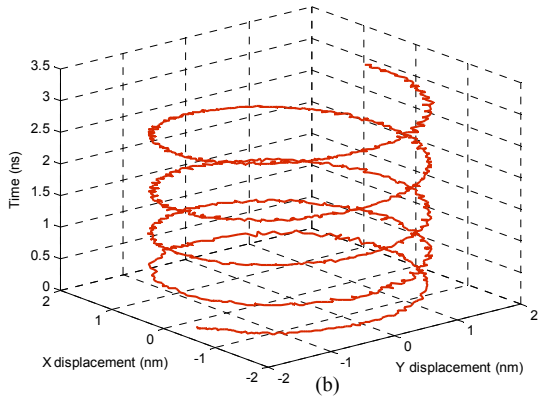
A. Nanomotor actuation

For structures with geometric parameters similar to those illustrated in Fig. 1(c) and (d), simulations establish that the MWNT shuttle-based devices can be actuated electrically, and the neighboring segments slide towards each other to come in contact at low voltages (~ 5V). In this effort, we have specifically investigated the rotation of inner shells in this contact state.

To explain the proprieties of nanomotor behavior, intershell electrostatic and van der Waals energies were investigated and inner CNT trajectories were studied using MDS. The charge distribution along the CNTs was



(a)



(b)

Fig. 5. Termini atom trajectory in an inner shell during rotation, (a) Rotating circular path of this terminus atom, (b) Terminus atom rotation as a function of time. This curve shows that the inner shell rotates with constant velocity.

calculated as described in section III. Fig. 2(a) shows the charge distribution on carbon atoms along the length of a 5 nm long SWNT when the electric potential on the surface is 6.0 V. The electric charge value is in the range of 5×10^{-3} to 34×10^{-3}e. It can be seen that the charges on atoms located at the central part of the tube do not vary significantly, whereas the charges on atoms at the two ends are much higher. The charge values reach up to 34×10^{-3} e for the open-ended nanotube. Fig. 2(b) shows the electrostatic potential along a DWNT. It can be seen that the tube ends carry significantly higher charges. In addition, the electrostatic potential is much higher at the outer nanotube as compared to the inner one[22].

When a potential difference is applied between the two MWNT segments, opposite charges are induced on these MWNT segments, as illustrated in Fig. 2(c). The electrostatic interactions due to these induced charges include attractive forces between oppositely charged neighboring MWNT segments and repulsive forces between the same-polarity shells within the individual MWNT segments. For a given bias, the attractive electrostatic energy between two oppositely charged inner nanotubes as a function of time is shown in Fig. 2(d). Fig. 2(e) depicts the repulsive electrostatic energy between the inner and the outer shells. The net effect of these electrostatic interactions due to an applied bias is an electrostatic force that tends to slide the inner shells within the two segments towards each other. When this applied excitation bias exceeds a characteristic threshold value, these electrostatic interactions become higher than the van der Waals forces that try to restrain the inner shells from extruding. This results in a closure of the inter-segment gap. For the system under consideration, the sliding time is 0-0.4 ns. This is comparable to device operation times estimated in [22].

B. Rotation of inner shells

1) Force analysis

At the closed state of the system, a terminus atom within the inner shell is subjected to van der Waals forces and three components of electrostatic forces. Fig. 3(a) shows a terminus carbon atom with these force components. F_{eii} is an attractive electrostatic force which is applied by the inner shell of the neighboring nanotube segment. F_{et} and F_{en} are the tangential and normal components, respectively, of the electrostatic repulsive force applied by the outer shell of the same nanotube segment (N.B. the van der Waals components are not shown in this figure).

In order to understand the origin of this inner shell rotation, we calculate the inter-layer interactions during rotation. We divide the nanotube into unit cells as illustrated in Fig. 3(b). This figure shows the two types of energies acting on an inner unit cell as it approaches an outer one. These two energies are added together to get the total non-bonded energy acting on the inner unit cell. The graph shows that from 2.780ns to 2.818ns, the total attractive non-bonded energy (red curve) increases, and from about 2.833 to 2.900 ns the total energy decreases when the two unit cells become close and separate. At 2.828ns, the non-bonded energy decreases to -0.55eV because of the repulsive van der Waals term when the atoms are very close. This clearly shows that the rotation of the inner nanotubes is mainly caused by the interlayer attractive non-bonded energy.

We characterized the interaction energy between a unit cell in the inner and three successive unit cells in the outer nanotube during a $\alpha+\beta$ rotation angle. Fig. 3(c) illustrates the interaction between these unit cells.

a) During the time interval between 2.780ns to 2.835ns, the total non-bonded energy between the inner segment (green colored) and the first outer segment (red) significantly increases. This means that the inner segment is strongly attracted by the first outer segment. At 2.828ns, the energy decreases to -0.55eV which is caused by the repulsive van der Waals energy when the neighboring segments become quite close.

b) During the time interval between 2.820ns to 2.848ns, the total non-bonded attractive energy between the inner segments (green) and the second outer segment (cyan) increases strongly. This means that the inner segment is strongly attracted by the first outer segment.

At 2.835ns, the energy decreases to -0.55eV which is caused by the repulsive van der Waals energy when the neighboring segments become very close.

c) During the time interval between 2.830 ns to 2.850 ns, the total non-bonded attractive energy between the inner segments (green) and the third outer segment (magenta) increases strongly. That means the inner segment is strongly attracted by the first outer segment. At 2.848ns, the energy decreases to -0.55eV which is caused by the repulsive van der Waals energy when the neighboring segments become close.

The calculations, using MD simulations coupled to electrostatic charge distribution calculations along the CNTs, show that electrostatic forces bring the two segments in contact (Fig. 3(b)). The calculations demonstrate that the interlayer van der Waals forces at the contact state can generate a torque and result in rotation (Fig. 3(c)). Van der Waals forces are stronger than the friction forces during rotation. The attractive electrostatic energy analysis between head to head CNTs shows that these CNTs rotate with the same velocity and in the same direction, as illustrated in Fig. 4. Based on the attractive electrostatic energy between the inner shells within two neighboring segments (Fig. 4, red colored segment and green colored one), sliding occurs between 0 and 0.2 ns, while at 0.2 ns the inner shells establish contact. After 0.2 ns, the energy is constant indicating that both inner shells rotate with the same velocity and in the same direction. The attractive electrostatic energy becomes stable after the neighboring segments come in contact with each other. The inner shell trajectory analysis shows rotation with constant velocity as illustrated in Fig. 5, where the termini atom trajectory in an inner shell during rotation is plotted including: Fig. 5 (a) shows the rotating circular path of this terminus atom and Fig. 5 (b) shows the terminus atom rotation as a function of time—the curve indicates that the inner shell rotates with constant velocity.

V. Conclusions

A rotary nanomotor has been designed using two axially aligned, opposing chirality nanotube shuttles. Based on inter-shell screw-like motion between nanotubes, rotary motion is generated by electrostatically pulling the inner shells together. Simulations using molecular dynamics were used to investigate how rotation from a pair of nested armchair nanotube pairs can be generated. The ultra-compact dimensions compared to previous designs and the progress on batch fabrication of similar nanostructures indicate that these motors are promising building blocks of NEMS and nanorobotic systems for sensing, actuation, and computation applications.

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