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Configuration jumps of rotor in a nanomotor from carbon nanostructures

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ABSTRACT

Measuring the rotation of a rotor in a thermally driven motor made from double-wall carbon nanotubes (DWCNTs) involves challenges based in the small size of the nanotube (radius usually being less than or equal to 5 nm) and the high frequency of rotation (over 100 GHz). These features motivated us to study a rotor with variable configurations, in which the rotor is fabricated initially by bonding a graphene (GN) nanoribbon on a carbon nanotube (CNT). The width of the GN nanoribbon is far greater than the radius of the CNT. Using molecular dynamics simulation, we find that the "CNT + GN" rotor generally experiences three representative stages. In the first stage, the GN nanoribbon winds onto the CNT and the rotor becomes a carbon nanoscroll (CNS) within 100 ps (picoseconds). The second stage is acceleration of the rotor's rotation. The duration of that stage is controlled by the number of inward radial deviation (IRD) carbon atoms on the stator and the inertial moment of the rotor. When the rotational speed of the CNT reaches a critical value, the CNS unwinds within 80 ps into a nanoribbon, which can be considered as the third stage. When hydrogen atoms are initially added to the GN, more configuration variations of the rotor can be identified. The rotation of the "CNT + GN" rotor can be feasibly measured by observing the configuration variations of the rotor.

1. Introduction

Carbon nanostructures are commonly formed with sp^2 and/or sp^3 carbon atoms. According to their dimensions, nanostructures are classified as zero-dimensional, e.g., buckyball ([1]); one-dimensional, e.g., CNT ([2]), CNS ([3,4]); two-dimensional, e.g., graphene ([5,6]), or graphone ([7]); and naturally three-dimensional structures, e.g., diamond, and complex three-dimensional structures made from lower dimensional nanostructures ([8]). These nanostructures have attracted much attention in the last two decades due to the unique mechanical properties ([6,9]) within each individual nanostructure and the ultra-weak interaction between adjacent tubes and/or graphene (GN) nanoribbons ([10,11]). Consequently, carbon nanostructures have been considered important candidate components in next-generation nano/micro-electromechanical systems (NEMS/MEMS) ([12,13]) and nano devices, such as nanomotors ([14–16]), nano bearings ([17]), sensors ([18,19]) and so on.

Among nano devices, CNT-based nanomotors have attracted much attention in recent years. For example, Barreiro, Rurali et al. [14] confirmed the rotary and translational motions along the tube axis between the tubes in a multi-wall carbon nanotube (MWCNT) by experimentation. They demonstrated that the motion was actuated by the interaction among atoms on the tubes with a thermal gradient. More evidence can also be found in the work of [15] and of [16]. These experiments displayed the same 2 characteristics. First, the motions were of low velocity. Secondly, the size of the nano device was around a few hundred nanometers (nm). Even now, it is still difficult experimentally to investigate ([20]) the dynamic behaviors, namely rotation and oscillation, of a high-frequency (over 1 GHz) rotary nanomotor not more than 20 nm in size. To prove the theoretical investigation of small motors with over 1 GHz rotational frequency, molecular dynamics (MD) simulation seems to be the most favored method. Using simulation, many schemes, such as electric field ([21–23]), gas or liquid flow ([24,25]), and thermal vibration or light absorption, have been

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proposed to drive the rotation of a nanotube in a MWCNT-based bearing.

In particular, thermal vibration of atoms in MWCNTs with fixed outer shells can also result in the rotation of free inner shells. The first result was mentioned briefly in the work of ([26]), who investigated the large amplitude axial oscillation of the inner tube in a DWCNT at a finite environmental temperature. In 2014 ([27]), we gave a definite answer as to the existence of a rotary CNT-based nanomotor in a NVT ensemble with a constant temperature (rather than a varying temperature or a temperature with a gradient along the tube axis).

The finding of a uniform temperature driven CNT-based nanomotor inspired measurement of the rotational speed of the rotor for two major reasons. The first is that the rotational speed of the rotor is too high, that is, generally greater than 100 GHz. Common video devices cannot capture the real motion of such a rotor. The other reason is that the rotor has a very small radius, making it difficult to capture variations of its configuration. To overcome these difficulties, the radial size of the rotor needs to be enlarged, for example, by bonding a piece of GN nanoribbon on the inner tube. In that model, the nanomotor has a "CNT + GN" rotor. However, if the configuration of the "CNT + GN" rotor remains unchanged, it is still difficult to measure the rotor's rotational speed. Fortunately, GN bonded with an inner tube (CNT) has a variable configuration due to van der Waals interaction. Moreover, the GN nanoribbon wound on the CNT can also be unwound from the CNT when the rotational speed is sufficiently high ([28]). If the change in the configuration can be observed, the rotation of the rotor can also be found. In the present study, we use a MD simulation approach to verify the feasibility of measuring the rotation of the rotor in a DWCNT-based motor.

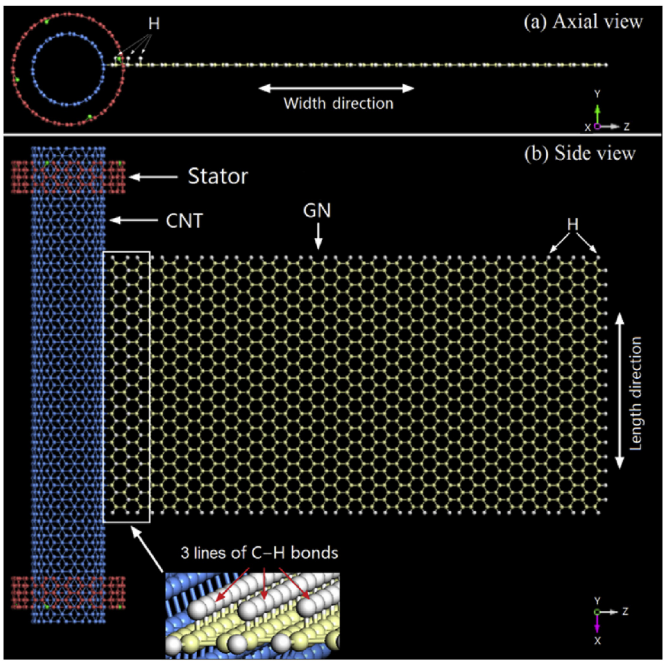

Fig. 2. Initial model of thermal motor with the CNT + GN rotor. (a) Axial view; (b) Side view. The tubes in the thermal motor are the same as those in Fig. 1 and a GN (light yellow atoms) 8.4 nm × 4.2 nm is symmetrically bonded on the inner tube (blue atoms/CNT). Each carbon atom on the three free sides of the GN is bonded with a hydrogen (white) atom. Near the contact side between the CNT and GN along the axial/x-direction, on the GN, q lines (parallel axis of inner tube) of carbon atoms are hydrogenated, so in the present model, $q = 3$. (A colour version of this figure can be viewed online.)

2. Models and methods

In the thermal motor model shown in Fig. 1, the inner tube ((9, 9) CNT) will be driven to rotate if the configuration of the stators ((14, 14) CNT) is not symmetric axially, where the outer tubes are fixed as stators. To express the non-symmetry of a stator, we measure the IRD value of an end atom on the stator and label it "Δr". Concretely, the atom has "Δr" of displacement along the dash line (See the four enlarged sub-figures below in Fig. 1 labeled with 1, 2, 3 and 4) from its initial position on the ideal circle. In the present study, we set Δr=0.4$l_{c\text{-}c}$ for all simulations, where $l_{c\text{-}c}$ = 0.142 nm, i.e., the bond length between two carbon atoms on the GN. If all the atoms on the stators have no IRD, the axial view of a stator is an ideal circle. Mathematically, the distance between the IRD atom and its neighbor carbon atom is $1+\alpha^2$ times of $l_{c\text{-}c}$, where α is the ratio of Δr over $l_{c\text{-}c}$. When α = 0.4, the bond length is 1.077 times of $l_{c\text{-}c}$. Suggestion is that α is less than 0.7.

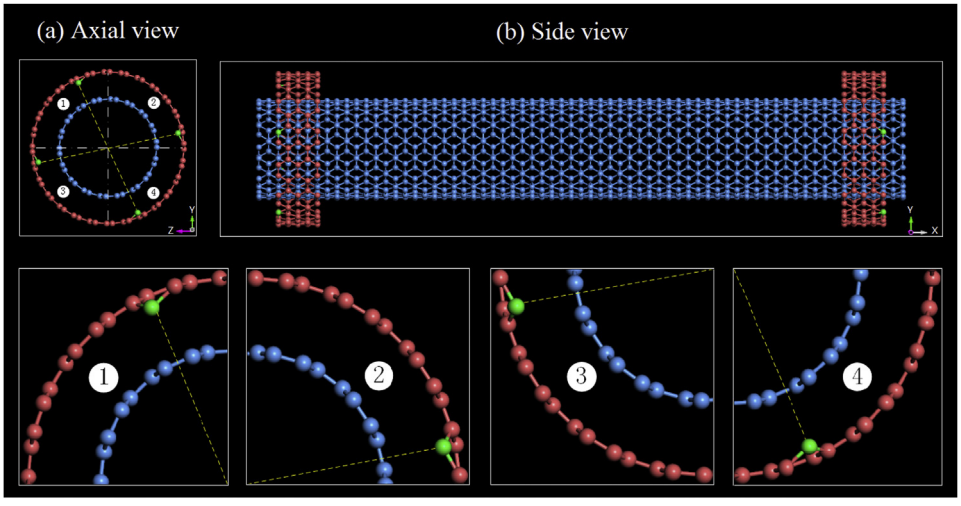

Fig. 1. A thermal nanomotor is made from a (9, 9)/(14, 14) DWCNT in which the inner tube (CNT rotor) is free and the two stators are fixed in simulation. The axial distance between two stators is 6.642 nm. The initial axial distance between the outer ends of the stator and the CNT rotor is 0.246 nm. (a) Axial view of motor. On each outer end of the stator are 4 atoms with IRD. Briefly, this stator is called a "4-IRD-atom" stator. (b) Side view of the motor. Below are four sub-figures for showing the IRD atoms clearly. (A colour version of this figure can be viewed online.)