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Dynamic response of a carbon nanotube-based rotary nano device with different carbon-hydrogen bonding layout

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ABSTRACT

In a nano rotational transmission system (RTS) which consists of a single walled carbon nanotube (SWCNT) as the motor and a coaxially arranged double walled carbon nanotube (DWCNT) as a bearing, the interaction between the motor and the rotor in bearing, which has great effects on the response of the RTS, is determined by their adjacent edges. Using molecular dynamics (MD) simulation, the interaction is analyzed when the adjacent edges have different carbon-hydrogen (C—H) bonding layouts. In the computational models, the rotor in bearing and the motor with a specific input rotational speed are made from the same armchair SWCNT. Simulation results demonstrate that a perfect rotational transmission could happen when the motor and rotor have the same C—H bonding layout on their adjacent ends. If only half or less of the carbon atoms on the adjacent ends are bonded with hydrogen atoms, the strong attraction between the lower speed (100 GHz) motor and rotor leads to a synchronous rotational transmission. If only the motor or the rotor has C—H bonds on their adjacent ends, no rotational transmission happens due to weak interaction between the bonded hydrogen atoms on one end with the sp^1 bonded carbon atoms on the other end.

1. Introduction

Many efforts have been made to study the ultralow friction feature since it was found in the relative motion between multi-walled carbon nanotubes (MWCNTs) [1,2]. This feature has potential applications in the design of nano electro mechanical systems (NEMS) such as gigahertz oscillators [3,4], bearings [5,6], nanopump [7,8] and motors [9–12]. To actuate the relative rotation in a MWCNT, Fennimore et al. [13] and Bourlon et al. [14] experimentally made the rotational system using MWCNTs with metal plates attached to the outer or inner shells, and three-stator electrodes acting as the driver. Barreiro et al. [15] observed the relative rotation between the tubes in MWCNTs with the temperature gradient along the axial axis from both experiments and numerical simulations. In the above reports, however, the rotational frequency of motor was low. To obtain a high speed rotary motor, Kang and Hwang [9] simulated the rotation of the motor driven by fluidic gas and their motor had a super-high rotational frequency of over 200 GHz. Tu and Hu [10] conceptually designed a rotary motor with axially varying voltage. Wang et al. [12] simulated a rotary motor driven by an external electric field that periodically charged and discharged the blades on the axial axis. Vacek and Michl [11] suggested an alternative way, i.e., light absorption, to drive the rotation of a nano motor.

Recently, a rotational transmission system (RTS) was proposed [16,17] based on a SWCNT as high speed rotation motor and a coaxially arranged DWCNT as rotor and stator. In the system, both synchronous and asynchronous transmission results can be obtained under specific conditions, i.e. tube chirality, input rotational frequency, tube end configuration and operation temperature. From the previous study, the interaction between the adjacent edges of the motor and the rotor in the bearing plays an important role in the rotational transmission. Meanwhile, as a component in a NEMS, it should have such excellent properties as stability and easy operation. Hence, one can adjust the interaction between the motor and the rotor by covalently bonding the sp^1 carbon atoms with hydrogen atoms (Lebedeva et al. [18] and Popov et al. [19]) on their adjacent edges. To explore the edge effect of C—H bonds on the rotational transmission behavior, we employ several types of C—H bonding layouts in molecular dynamics (MD) simulation. In addition, we also investigate the coupling effect between the C—H bonding and the relative motion between the motor and rotor on the rotational transmission behavior.

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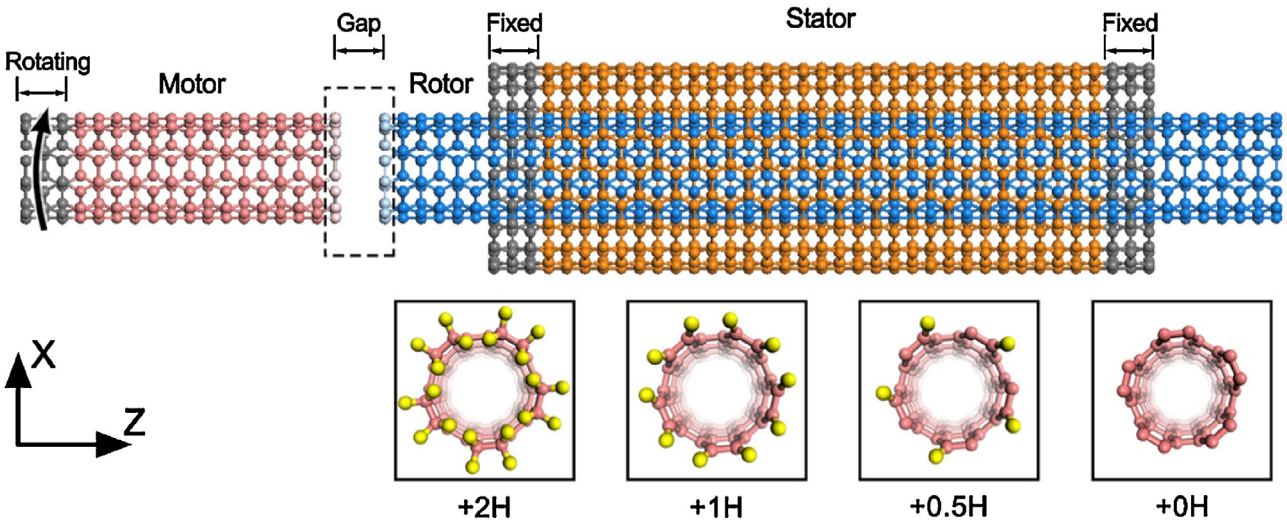

Fig. 1. The proposed rotational transmission system consisting of a (5, 5) SWCNT-based motor and (5, 5)/(10, 10) DWCNT-based bearing. The atoms in dashed box are end carbon atoms on the motor and rotor. The motor rotates with a specific input rotational frequency and the rotor is driven to produce an output rotational speed. Four C—H bonding layout schemes, i.e., (+2H), (+1H), (+0.5H) and (+0H), are considered. In each insert map, the yellow atoms are hydrogen atoms, the rest are carbon atoms. The gap between the motor and the rotor is the distance between their adjacent carbon atom ends. The initial gap between the motor and rotor is around 0.34 nm. If the value of gap is larger, the rotational transmission needs more time to start or even fails. It has slight influence on the other dynamics response of the system.

2. Methods

Fig. 1 shows the rotational transmission system which consists of a motor from a SWCNT of (5, 5) and a bearing from a DWCNT of (5, 5)/(10, 10). We call the carbon atoms on the adjacent ends of motor and rotor as end carbon atoms. To demonstrate the effect of C—H bonding layout on the rotational transmission response, the end carbon atoms are bonded with hydrogen atoms (within the dashed box) in different ways. Namely, (a) each end carbon atom is covalently bonded with two hydrogen atoms labeled as (+2H), (b) each end carbon atom is bonded with one hydrogen atom labeled as (+1H), (c) every other end carbon atom is bonded with one hydrogen atom labeled as (+0.5H), and (d) no hydrogen atom being bonded is labeled as (+0H). If the hydrogen atoms are both on the motor and rotor, the scheme is labeled as "B + xH" (x = 2, 1, 0.5 and 0), while "M + xH" or "R + xH" represents the case in which only the motor or only the rotor has hydrogen atoms on its end. In our MD simulation, the AIREBO potential [20–22] is chosen to describe the interaction between carbon/hydrogen and carbon/hydrogen atoms. To consider the non-bonding effect among tubes and saturated carbon atoms ("+2H" scheme), both of the L–J and torsion terms are turned on during simulation.

The lengths of tubes in the present study are similar to those in the previous rotational bearing simulation works [6,23,24]. According to the conclusion given by Zhu et al. [23], i.e., the energy dissipation rate is almost proportional to the contact area between adjacent tubes, one can also have different rotational transmission state by changing the lengths of tubes. Since the rotational transmission state depending on the attraction between the adjacent ends of the motor and rotor and the friction between the rotor and stator, changing one or both of the interaction, one will obtain different dynamic response. To show the effect of C—H bonding layout on the dynamic response, we choose the tubes with the fixed lengths for the convenience of comparison. As demonstrated in Fig. 1, the lengths of the rotor (blue) and outer tube (orange) are about 6.0 nm and 4.0 nm, respectively, while the left part (pink) is the driving motor with the length of 2.1 nm. The initial gap between motor and rotor is around 0.34 nm, and this value varies in simulation due to the edge interaction between the motor and rotor [16,17]. As the tube edge effect cannot be neglected in this case, the boundary of simulation box is set to be fixed in all dimensions. Before simulation, a Nosé-Hoover heat bath at 300 K is applied for achieving the entire system relaxation. After 100 ps of relaxation, a constant rotational speed is specified on the motor. Meanwhile, the axial translational motion of motor is constrained. The rotor can move freely in the stator. The whole system is under the canonical NVT ensemble at 300 K with damping time of 0.1 ps. The duration of each simulation is 5 ns and the time step is 0.001 ps in all simulations.

3. Results and discussion

In Figs. 2 and 3, the rotational frequencies of rotor are illustrated with different types of C—H bonding layout and with different rotational frequencies of the driving motor. Fig. 2 illustrates the rotational transmission responses of the system with no hydrogen atom, i.e., (+0H) scheme. It is found that the rotor is actuated immediately to rotate synchronously within a few time steps. The reason is that the original end carbon atoms on both the motor and rotor are sp^1 bonded atoms so that they become sp^2 bonded atoms quickly [17]. The strong bond interaction provides the powerful driving torque to overcome the intertube friction on the rotor.

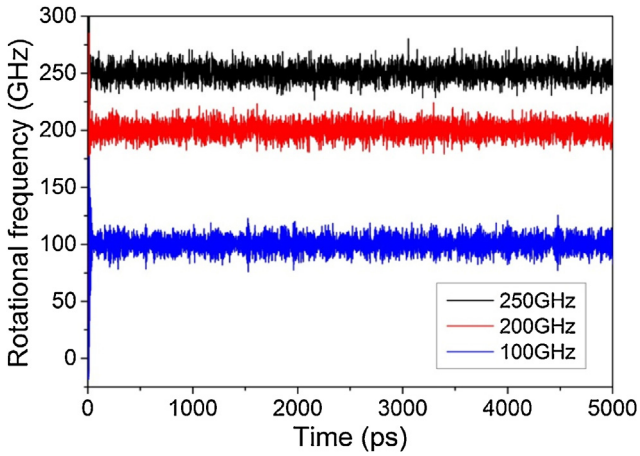

Fig. 2. Histories of the output rotational frequency of the rotor driven by the motor with different input rotational speeds for the B + 0H scheme.