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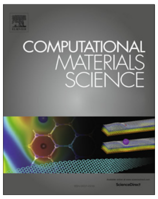

A nano converter from carbon nanotubes with multiple output signals

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ABSTRACT

To obtain a multi-signal nano device in a nano-electromechanical system (NEMS), a new converter is designed with a single-walled carbon nanotube (SWCNT) acting as a rotary motor, and multiple-walled (such as the triple-walled used in the present study) carbon nanotubes (MWCNTs/TWCNTs) acting as a converter. The dynamic response of the system is investigated using molecular dynamics (MD) simulation. In the system, the rotary motor has a specified rotational speed as an input signal. The outer tube in the bearing is fixed as a stator and the inner tubes' responses are used as output signals. When using hydrogen atoms to modify the tube ends, the differences among the rotational frequencies of the motor and the inner tubes are very large. The inner tubes act as oscillators or rotors or both of them depending on the difference among their radii.

1. Introduction

Carbon nanotubes (CNTs) have been proved to have an extraordinary interlayer lubricating feature and other excellent mechanical properties at nanoscale [1,2]. It has inspired a lot of application studies for fabricating an NEMS from CNTs over the past decade, such as gigahertz oscillators [3–9], switch [10], bearings [11,12], nanopump [13,14] and motors [15–20]. For the interlayer motion of multi-walled carbon nanotubes (MWCNTs), both of the rotational and translational motions may exist, which suggests signal transmission with a nano device. For example, Legoas et al. [4,5] first chose MD simulation to study the oscillatory behavior of MWCNTs, in which the inner tubes have translational motion. Based on their prediction, the frequency of oscillator reached to as large as 87 GHz. Rivera et al. [6,7] presented the simulation under constant temperature. In their models, the lengths of the incommensurate DWCNTs' are between 12.21 and 98.24 nm. Their results implied that the inner tube had damping oscillation at gigahertz frequencies and the amplitude of oscillation showed proportional to the tube length. To investigate the interlayer rotational motions in MWCNTs, Fennimore et al. [21] first designed a rotational system using MWCNTs. In the system, a metal plate is glued on the outer tube and driven to rotate by electricity. Considering the characteristics of the potential barrier of DWCNT [22], Barreiro et al. [23] observed the relative motion of the outer tube on the long inner tube when the thermal gradient exists along the tube axis. Hamdi et al. [24] proposed a rotary nano motor made from two axially aligned, opposing chirality MWCNTs. And they simulated the motions of the inner tubes when the two segments of system had different charges. The motion can vary from a pure translational motion to pure rotation based on the combination of the chiralities of tubes. The motions as observed in above devices are very slow, e.g., only a few GHz predicted by MD simulation of rotation. On the other hand, the high-frequency rotation, which is difficult to observe directly, of the nano motor made from CNTs has also been studied using MD simulation. For example, Kang and Hwang [15] built a fluidic gas driven rotary motor with its rotational frequency being over 200 GHz according to their simulation results. We recently studied the gradientless temperature driven motor made from DWCNTs [19,25], and obtained the super high speed of rotation of nano motor, too. Up to now, such high speed rotation motor cannot be achieved and observed by the present state-of-the-art experiments.

However, the nano motors as mentioned above, which are made from pure carbon nanotubes, are difficult to fabricate using the best available techniques [21]. To perform a qualitative investigation on the prototypes of such nano devices, MD simulation approaches are usually adopted. In NEMS, either translational or rotational motion of CNT can be considered as a signal/state of system. A design of transmission system [26–28] can achieve the signal transmission with different output level. To design a controllable device with multiple signal outputs [29], we propose in this study the concept of a new rotational transmission system with a rotary motor made from a SWCNT and a coaxially bearing from TWCNTs. The inner

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tube and mid tube in the system will move when driven by the rotary motor, and their motions are used as output signals.

2. Model and method

Fig. 1 demonstrates the proposed armchair transmission system made from an SWCNT (5,5) and a TWCNTs bearing (5,5)/(10,10)/(15,15) as a converter. In the system of (5,5)@(5,5)/(10,10)/(15,15), the tube lengths are 1.96 nm@6.19 nm/4.47 nm/2.95 nm, respectively. There are 160@500/720/720 atoms in each tube. The initial value of gap 1 is 0.335 nm, and gap 2 is 1.11 nm since the lengths of the two rotors are not equal. The system is relaxed under a canonical NVT ensemble with $T = 300$ K. After 100 ps of relaxation, the dynamic response of the system is simulated within 5 ns under the same NVT ensemble. The time step is 1 fs. The AIREBO potential [30] is adopted to descript the force field among the atoms in the system.

In this study, three cases are under consideration. First, the transmission behavior of the two rotors is investigated when there is no hydrogen atom in the system. In this case, we mainly discuss the effects of both motor type and motor speed on the output motions of rotors. Second, the high potential of end (sp^1) carbon atoms is reduced by introducing structural modification [31], e.g., using hydrogen atoms bonded with the end carbon atoms. The output motion of the rotors, driven by the same chirality CNT motor, is studied when the length of the rotor 2 (mid tube) is equal or not equal to that of the rotor 1(inner tube). Finally, the output motion of the equal-length rotors in the system with C–H bonds is demonstrated when driven by (9,9) motor.

3. Results and discussion

3.1. Dynamic response of rotors in the system with only carbon atoms

From Fig. 2(a), (c) and (e) (or Table 1), we find that the rotor 1 ((5,5) inner tube) always rotates synchronously with the (5,5) motor when the motor has any rotational frequency. From Fig. 2(b), (d), and (f), we find that the value of gap 1 changes slightly around 0.132 nm. Hence, we conclude that the motor and rotor 1 are connected with new covalent bonds between their end carbon atoms. The strong attraction between the motor and rotor 1 leads to the synchronous rotation of rotor 1. The rotational frequency of rotor 2 is far less than that of rotor 1. For example, 80 GHz of rotor 2 vs. 250 GHz of rotor 1 in Fig. 2(a); 63 GHz vs. 200 GHz in Fig. 2(c); 23 GHz vs. 100 GHz in Fig. 2(e). The reason is that the intertube friction between rotor 1 and rotor 2, which provides the angular acceleration of rotor 2, increases with the increase of the rotational speed of rotor 1. However, the stator provides the resistance to the rotor 2 to reduce the speed of rotor 2 at the same time. As a result, the resultant force leads to the lower speed of rotor 2 when comparing with rotor 1. Actually, the rotor 2 may also be attracted by the stator to stop rotating [25].

When driven by the 250 GHz (9,9) motor, the rotor 1 has lower rotational frequency than that of the motor. As the rotational speed of motor is 200 or 100 GHz, the rotor 1 rotates synchronously with the motor because the new covalent bonds are generated between the end atoms on the motor and rotor 1 (see the red lines in Fig. 2 (c) and (e)).

Driven by either (5,5) or (9,9) motor, the rotor 2 has obvious oscillation (see Fig. 2(b), (d) and (f)). Except for the time during (0,2000) ps driven by the 250 GHz (5,5) motor, the oscillation of rotor 2 is disordered. Therefore, the results in Fig. 2(a) and (b) may suggest a potential application of "rotor + oscillator" system [9], i.e., the mid tube (rotor 2) acts as both a rotor and an oscillator in the system simultaneously.

3.2. Dynamic response of transmission system with C–H bonding ends

With the existence of hydrogen atoms, no new C–C bonds appear between motor and rotor. The effect of length difference (EQ and NE) of two rotors on transmission needs to be demonstrated in detail. Fig. 3 demonstrates the rotational speeds and oscillations of the two rotors when driven by the (5,5) motor. In this model, each end carbon atom in the whole system, including the motor, stator and two rotors, is bonded with a hydrogen atom. The rotor 1 rotates faster than the rotor 2 with either "EQ" or "NE" length, and the fluctuation of the rotational frequency of rotor 1 is far greater than that of rotor 2. However, the rotor 1 is not always rotating synchronously with the motor except for the case where the rotational frequency of the motor is low, e.g., 100 GHz (Fig. 3 (e)). For instance, the rotational speed of rotor 1 is ~94 ("EQ") or ~115 GHz ("NE") when it is driven by 250 GHz (5,5) motor. The rotational frequency of rotor 1 is ~80 ("EQ") or ~83.4 GHz driven by 200 GHz motor. The reason is that the interaction between the two C–H ends of motor and rotor 1 is not strong enough to drive the rotor 1 rotating synchronously with the motor. When the two rotors have equal length ("EQ"), the attraction of motor on the rotor 1 is higher than on the rotor 2. And the attraction of the motor and rotor 1 on the rotor 2 is also stronger than the friction between the motor and the rotor 2. That is why the two rotors rotate synchronously before 3500 ps (black and grey lines in Fig. 3

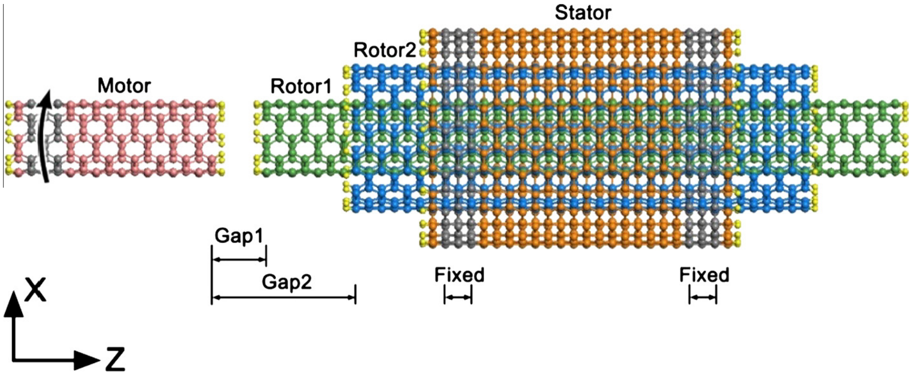

Fig. 1. Proposed (armchair) transmission system (labeled with (m,m)@(r1,r1)/(r2,r2)/(s,s)) made from an SWCNT (5,5) motor and a TWCNTs bearing of (5,5)/(10,10)/(15,15), in which "m, r1, r2 and s" represent chirality components of the motor, rotor 1 (inner tube), rotor 2 (mid tube) and stator (outer tube), respectively. The outer tube in bearing acts as a stator. Gap 1 is the axial distance between the motor and rotor 1. Gap 2 is the axial distance between the motor and rotor 2. Each carbon atom on the ends of tubes, i.e., an end carbon atom, is bonded with a hydrogen atom (green atom) when the system has carbon–hydrogen (C–H) covalent bonds. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)