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Effect of hydrogenation and curvature of rotor on the rotation transmission of a curved nanobearing

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A B S T R A C T

When fixing the outer tube of a double-wall carbon nanotube (DWCNT), the rotation and/or oscillation of the inner tube (rotor) can be actuated by a co-axial-layout nanotube-based motor. Both the motor and DWCNT-based bearing form a nanodevice called motion transmission system (MTS). Generally, the rotor and motor have differently dynamic responses. To obtain stable output signals from an MTS, we study the dynamic response of a curved rotor with hydrogenated ends. Both stability and efficiency of motion transmission depend on the interaction between the adjacent ends of motor and rotor. By analyzing the motion transmission state of rotor with some typical carbon-hydrogen (C—H) bonding layout schemes, we find that a stable output rotation of the curved rotor can be obtained if either the rotor or motor has C—H bonds at the adjacent end. If both the rotor and motor have the same C—H bonding layout at the adjacent ends, the output motion of rotor is very sensitive to both the input rotation and C—H bonding layout, which means that the dynamic response of the curved rotor becomes uncontrollable. The above phenomena are very different from those as observed for a straight rotor in the same system.

1. Introduction

Over recent two decades, much research has been performed on the development of nanoscale machines by mimicking the macroscopic ones. Nanomotors, which are a kind of nanodevices that convert input into motion or force, are the essential component in practical nanomachines. Designing and fabricating new nanomotors and developing propulsion methods are still the most exciting challenges in current nanotechnology. The motion of a nanomotor can be either chemically self-propelled or propelled by external energy, including thermal vibration [1–4], magnetic or electrical fields [5–8], nanoflow [9,10] and light [11].

When using the motion of a nanomotor as a signal, the stability of either input or output signal should be controllable. At nanoscale, due to strong surface energy and finite particles in the system, the stability of motion is sensitive to the configuration of the nanodevice and its environment. To maintain the stability, the nanodevice should have a stable structure during motion. Besides, the damping effect on the motion direction should be small in order to keep the sensitivity of the output signals to the input signals. Considering the structural stability, researchers suggest the use of carbon nanostructures to form the component due to the strong in-plane C—C bonds and superlubrication between graphene sheets [12,13] or between two carbon nanotubes [14–16]. Hence, many efforts have been made on the design of such nanodevices as nanomotor and nanobearing based on carbon nanotubes. For example, by experiments, Fennimore et al. [5] and Bourlon et al. [6] investigated the motion of metal plates-attached outer CNT on an inner tube. In their experiments, the motion of outer tube was driven by electric current. Barreiro et al. [1] observed the rotation of the outer tube on the fixed inner tube which has temperature gradient along the axis. By simulation approaches, Kang and Hwang [9] suggested to drive the rotation of the CNT-based nanomotor using fluidic gas. Wang et al. [8] adopted an external electric field to actuate the rotation of a rotary motor. In 2014, Cai and his colleagues [2] found that the inner tube can be driven to rotate by the fixed outer tube at certain high temperature when the outer tube loses symmetry on its cross section. And recently, they [3] provided an accurate model of thermal-driven rotary nanomotor from double-walled carbon nanotubes. In addition to rotation, linear motion of MWCNTs has also been attractive since

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Zheng and Jiang [17] and Legoas et al. [18] proposed a giga-hertz nano oscillator model from the MWCNTs, respectively.

In some cases, the motions of the rotors/oscillators in the above nanomotors must be adjusted to be specified motions as output signals. To obtain the required motions, Cai and his colleagues [19] proposed a rotation transmission system from carbon nanotubes. In the system, the input rotation of a CNT-based nanomotor will be changed into other motions (rotation or oscillation) of the rotor in the DWCNTs-based nanobearing. Recently, Yin et al. [20] investigated the influence of carbon-hydrogen (C—H) bonding [21] at the adjacent ends of motor and rotor on the output signals. And they found that the motion transmission may fail if only motor or rotor is hydrogenated at the adjacent end. To have a stable motion transmission system with such kind of adjacent ends, we investigate the effects of both hydrogenation and curvature on the output signals of nanobearing in present work.

2. Models and methods

To reveal the influence of hydrogenated adjacent ends on the output motions of rotor, six schemes as shown below are considered in present study.

(1) Scheme 1: “M+1H”&“R+0H” (there is no C—H bond on the left end of rotor);
(2) Scheme 2: “M+0.5H”&“R+0H”;
(3) Scheme 3: “M+0H”&“R+1H” (there is no C—H bond on the right end of motor);
(4) Scheme 4: “M+0H”&“R+0.5H”;
(5) Scheme 5: “M+1H”&“R+1H”;
(6) Scheme 6: “M+0.5H”&“R+0.5H”.

Molecular dynamics simulation for present study is carried out using the open source code LAMMPS [22]. The interaction among the carbon and/or hydrogen atoms in the system is described by AIREBO potential [23]. The simulation steps are as following:

Step 1: Build the motion transmission system using standard bond lengths and bond angles (Table 1);
Step 2: Reshape the components in the system using potential minimization with steepest descending algorithm;
Step 3: Map the straight bearing into a curved bearing with specified value of θ;
Step 4: Fix all the atoms on the two stators, 4 layers of carbon atoms on the right end of rotor and 4 layers of carbon atoms on the left end of motor before relaxation;
Step 5: Put the system in a canonical NVT ensemble with T = 300 K (controlled with Nosé–Hoover bath). The three directions of simulation box are set to be free boundaries;
Step 6: After 400 ps of relaxation, release motor and rotor and apply input rotational frequency on the left end of motor;
Step 7: Record the calculation results in the next 5 ns for analysis.

The time step for integration is 0.001 ps. The input rotational frequency of motor are set to be 50, 100, 200, 250 and 300 GHz, respectively on the motor in the above six schemes. For finding more information on dynamic response of the rotor in Schemes 5

Table 1
Chirality and number of atoms on each component of the transmission system shown in Fig. 1.

	Motor	Rotor	Stator 1	Stator 2
Chirality of CNT	(9, 9)	(5, 5)	(10, 10)	(10, 10)
Number of atoms	324C+(0, 9 or 18)H	920C+(0, 5 or 10)H	240C	240C

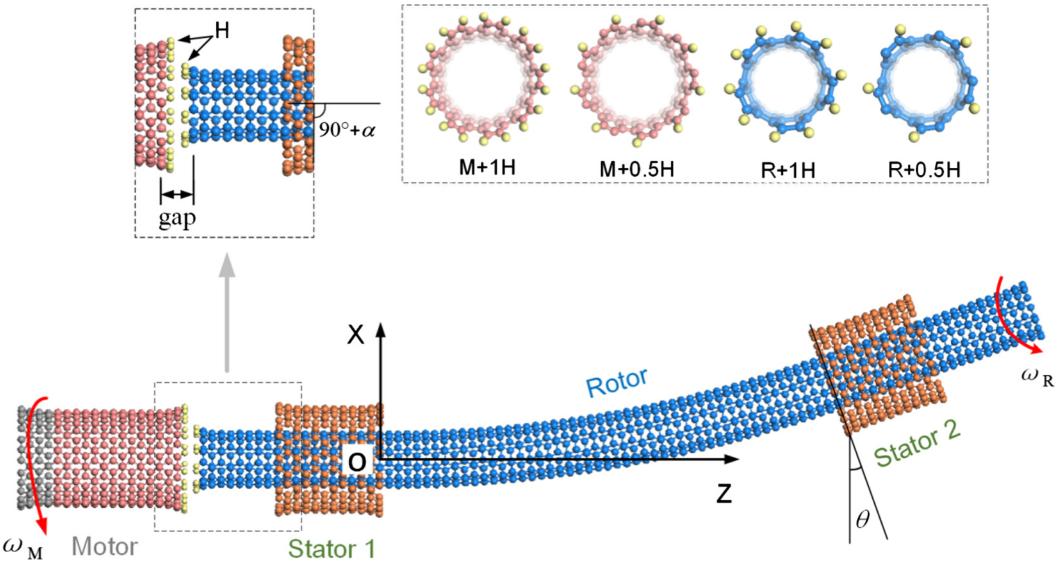

Fig. 1. A nano motion transmission system formed with a CNT motor and a CNT universal joint (curved rotor in two stators). ω_M is the input rotational frequency of motor. ω_R is the output rotational frequency of rotor. θ is the intersection angle between the two axes of stators, and $\theta = 20°$ in present model. The magnitude of “gap” between motor and rotor represents the axial oscillation of rotor. The initial distance between motor and stator 1 along z-axis is 1.332 nm. α is the intersection angle between the axis of rotor at the left end and Z-axis. α is small but not equal to zero. For the carbon atoms on the adjacent ends of motor and rotor, they may wholly or partly be bonded with hydrogen (H) atoms. For example, “**M+1H**” represents each carbon atom on the right end of motor is bonded with one H atom. “**R+0.5H**” means that every second carbon atom on the left end of rotor is bonded with one H atom. Detailed hydrogenation schemes are given above.