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Concurrence of oscillatory and rotation of the rotors in a thermal nanotube motor

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ABSTRACT

In studying dynamic response of a nanomotor made from triple-walled carbon nanotubes (TWCNTs), we find the concurrence of oscillation and rotation of the rotors in the fixed outer tubes (i.e., stators) when the system is in a canonical NVT ensemble with temperature higher than 100 K. In the system, the mid tube, called mid-rotor, is driven to rotate by the collision between the end carbon atoms on mid-rotor and the inward radial deviated (IRD) atom(s) on stator(s). The collision depends on three factors, e.g., the inward radial deviation of end atom(s) on stator(s), the number of IRD atoms and temperature of environment. In present research, fixing the first factor with a constant, the acceleration of the mid-rotor needs lower time to approach the maximal rotational frequency when the stators have more IRD atoms. And the maximal rotational frequency of mid-rotor is greater at higher temperature. Due to intertube friction, the inner tube, called inner-rotor, is driven to rotate by the mid-rotor. The system is stable when the inner-rotor has a stable rotational frequency which can be different from that of mid-rotor. During rotating, the inner-rotor may have large-amplitude oscillation. Hence, the simple but interesting model suggests a potential application in a nano-electro-mechanical system (NEMS).

1. Introduction

Since the work by Cumings and Zettl [1], people have taken much effort on developing nanomotor made from carbon nanotubes (CNT) [2–14]. According to the motion types of the movers in motors, the motors can be classified into two types. One is the linear motor with translational motion along the axis of the stator (fixed tube(s)) and the other is the rotary motor with rotating along the axis of the stator.

Considering ultralow friction between adjacent walls [1,16], Zheng and Jiang [17] proposed a CNT-oscillator model to predict the oscillation response of the free inner tubes in outer tube. Commonly, such oscillator is also considered as a linear motor [7,18–26]. As a matter of fact, the rotary nanomotor is popular, too. For example, in experiments, Fennimore et al. [2] and Bourlon et al. [3] fabricated a rotary nanomotor in which the multi-walled carbon nanotubes (MWCNTs) acting as a bearing. Using simulation method, Tu and Hu [5] designed a rotary motor from DWCNTs, in which a short outer tube driven was actuated by varying electrical voltage along axis to rotate on a fixed long inner tube. Hamdi et al. [10] found that the charged inner tube in an opposing chirality outer tube can also be actuated to rotate in a static electronic field. In 2014, Cai et al. [14] found that the inner CNT in a fixed outer CNT would rotate at an NVT ensemble with constant temperature and the final stable rotational frequency of rotor was over 100 GHz. Due to only two tube, i.e., one is fixed and the other is free, in the system in a thermostat, it suggested the most simple rotary nanomotor model. Recently, Cai et al. [15] gave an accurate model on carbon nanotube based nanomotor driven by thermal vibration of atoms on motor.

In general, the movers may contain both of linear motion and rotation in a stator [24,25,27]. For either linear motion or rotation, the energy transfer/dissipation [24,26,28–30] of the rotor leads to the damped motion of the motor with time. How to control a system with simple model but stable rotation and large-amplitude oscillation is a challenge for its applications in a nano-electro-mechanical system (NEMS). For instance, Rivera et al. [18] measured the sliding resistance of the damped oscillation of a DWCNTs-based linear motor. Zhao et al. [19] studied the mechanism of energy transfer during oscillation and stated that the friction force per atoms was in 10^{-17}–10^{-14} N. Legoas et al. [21],

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suggested to providing magnetic force to obtain a stable oscillation of the movable core. To maintain stable oscillation, Neild et al. [22] suggested to providing periodically varying external force on the core along axis. Ershova et al. [23] gave a systematic study on the way to provide external force to drive the stable oscillation.

As one can see, the system mentioned above is small but very complicated, e.g., requiring Gega Hertz or even Tera Hertz external force field. Hence, in the present work, we build a new model shown in Fig. 1 inspired by the temperature nanomotor model proposed by Cai et al. [14,15]. In the triple-walled carbon nanotubes (TWCNTs), the outer tube is separated into to short parts which are fixed as stators. Both ends of the mid tube are almost aligned with the outer ends of stators. The mid tube will rotate if the outer end(s) of the stators have no geometric symmetry. Due to intertube friction, the rotational frequency of mid tube will have a maximal value, and the inner tube will also be actuated to rotate. We prepare a series of schemes on the stators and the temperature of environment to find the stable large-amplitude oscillation of the inner tube.

2. Models and methods

The system shown in Fig. 1a is made from TWCNTs, in which the outer tube is separated into two parts named left stator (L-stator) and right stator (R-stator), the mid tube and the inner tube are rotors and called mid-rotor and inner-rotor, respectively. Each stator has 210 atoms, the mid tube and the inner tube have 460 and 500 atoms, respectively. To describe the interaction among atoms in the system, the Adaptive Intermolecular Reactive Empirical Bond Order (AIREBO) Potential proposed by Stuart et al. [31] is adopted in simulation which is carried out in the open sources molecular dynamic package of LAMMPS [32]. The time step for integration is 0.001 ps. After energy minimization on the initial model, the atoms (including IRD atoms) on the two stators are fixed. The two rotors are set at canonical NVT (*N*: the number of atoms in system; *V*: volume of system; *T*: temperature of system) ensemble. The simulation duration of dynamic response of the system is 8000 ps. For calculating the rotational frequency of inner-rotor, we use syntax “variable omg_in equal omega(inner, *z*) $*$ 500/3.14159265357”, in which “inner” means inner-rotor, *z* is the axial direction of inner-rotor (from left to right in the present simulation). The unit of omg_in will be GHz. For obtaining the oscillation of inner-rotor, we adopt syntax “variable disin equal xcm(inner, *z*)/10”, and the unit of “disin” is nm.

3. Results and discussions

3.1. Dynamics response of the model with different IRD schemes

Mechanism of rotation of both rotors is as following. The mid-rotor is driven to rotate by the thermal vibration of the end atoms on the rotor and the IRD atoms on the stators. The reason for that is the thermal vibration of end atoms on rotor results in collision between the end atoms and the IRD atoms on the stator(s) [15]. The collision produces circular and axial velocity of the rotor. The circular velocity results in rotation of rotor and the axial velocity raises oscillation. The rotor rotates in acceleration until the friction between the rotor and stator(s) is in balance with the impact force in collision. Hence, IRD schemes and temperature determines the dynamic behavior of the rotor. The rotation of inner-rotor is actuated by the friction between the two rotors. The oscillation of inner-rotor can happen due to serious end interaction with the mid-rotor.

Fig. 2a shows that the rotational acceleration process of mid-rotor is different at 400 K when the stators have different number of IRD atoms. The final stable rotational frequency of mid-rotor has small differences among the schemes, e.g., nearby 133 GHz. As one can see, the mid-rotor driven by the stators with more IRD atoms has shorter time of rotational acceleration. Except driven by the stators in the IRD schemes of 2L and 2LR, the difference of the

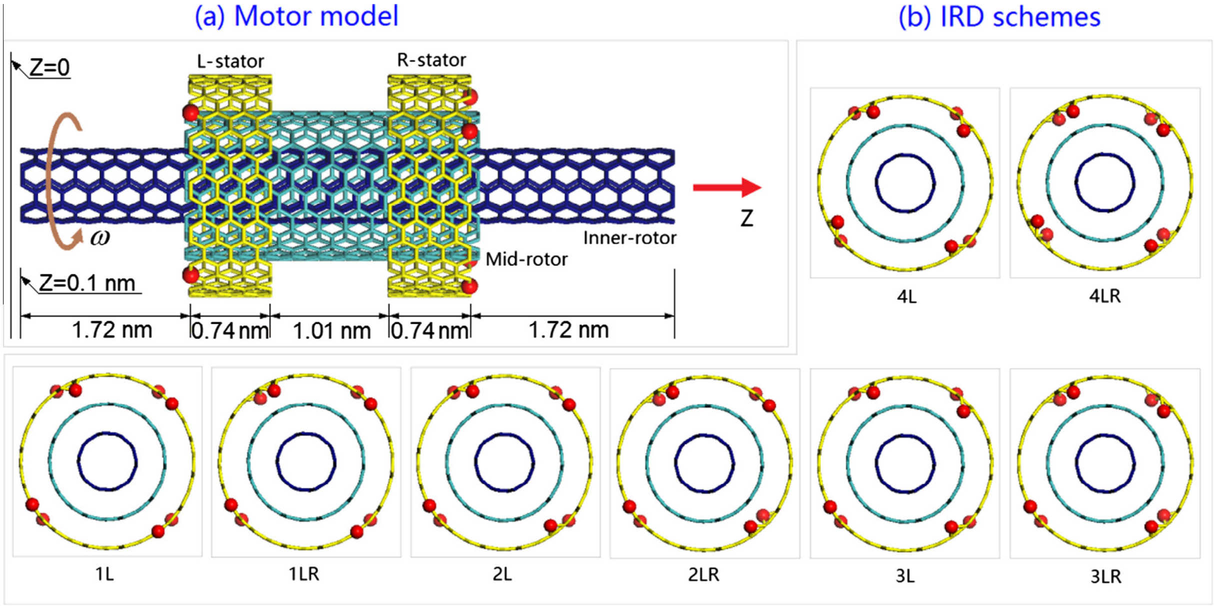

Fig. 1. (a) A model of nanomotor made from triple-walled carbon nanotubes, in which the two (15, 15) outer CNTs are fixed as stators, e.g., left stator (L-stator) and right stator (R-stator), the (10, 10) CNT acts as a rotor (mid-rotor), which is driven to rotate at NVT ensemble by the stator(s). The (5, 5) inner CNT acts as both o f a rotor and an oscillator when the mid tube is rotating along *z*-axis. (b) Schematics of 8 schemes of the layout of the inward radial deviated (IRD) atoms (red balls) on the outer ends of stator (s) to represent the geometrical asymmetry of ends. 1L means there is only one IRD atom on the left end of the L-stator, similarly, the number of IRD atoms can also be 2, 3 or 4, with respect to 2L, 3L or 4L scheme. 1LR indicates that on both outer ends of the stators there is an IRD atom, similarly, the number of IRD atoms can be 2, 3 or 4, with respect to 2LR, 3LR or 4LR scheme. The inward radial deviations of the IRD atoms are the same, i.e., 0.4 times of the sp^2 carbon-carbon bond length (0.142 nm). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)