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Rotational behavior of a nanoring protected by argon

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ABSTRACT

Using argon to protect the rotary nanoring made from curved carbon nanotube, we discover that the gas can act as an on–off and/or a speed controller of the rotary nanoring. The mechanism is that the argon cluster formed at lower temperature provides friction on the nanoring, which may stop rotating due to the friction. Molecular dynamics simulation results demonstrate that the nanoring cannot rotate at 100 K, but rotates at 300 K, or it rotates faster at higher temperature. Periodic fluctuation of the rotational frequency of the ring happens when the argon cluster is formed periodically. Using the nanoring as an engine of a nanomachine, the speed of the machine can be adjusted by changing the ambient temperature. Hence, the argon on–off provides potential application in nanodevices.

1. Introduction

Low dimensional carbon materials, such as carbon nanotube (CNT) [1] and graphene [2], has two excellent mechanical properties. One is the extremely high modulus and strength [3,4], and the other is extremely low friction between neighbour layers [5,6]. The two properties are significant for the reliability of such nanodevices as oscillator [7–9], nanobearing [10–14], nanomotor [15–20], etc. Due to extremely low friction, the relative motion between neighbor components in one of the devices can be easily maintained. And the high strength of the carbon materials guarantees the stability of the carbon components working at gigahertz. According to the characteristics of motion, the nanodevices can be separated into two groups. One is the rotary nanodevices, e.g., rotary nanomotor/nanobearing. The other is linear nanomotor/nanobearing, and oscillator. Compared to the linear nanodevices, the rotary nanodevices are relatively difficult to manufacture and control with consideration of miniaturization. For example, in the CNT-linear bearing proposed by Cumings and Zettl [5], the size of the system along the motion direction can be higher than 1 μm. However, in the rotary CNT-actuator presented by Fennimore et al. [15], the size of the blade, which is attached to the CNT-shaft for both loading and observation, is about half of a micrometer. In the rotary nanobearing fabricated by Bourlon et al. [10], the size of the blade is even smaller. However, for any one of above system, the size of the moving part is far greater than 100 nm, which is the reason why some persons call the device as microdevice rather than nanodevice. Hence, miniaturization of the rotary nanodevices is urgent for wider application of the devices.

Considering application of above nanodevices, motion control of the moving components is more important. Up to now, most of previous studies focus on numerical prediction of models. For instance, Kang and Hwang [16] proposed a model for a nanoscale engine, in which the CNT actuator drives CNT motor to rotate via the motion of the nanofluid. The rotation of the nanomotor depends on the actuator's oscillation. Tu and Hu [17] suggested an external varying electric field to control the motion of a short outer CNT on a long inner tube. Wang et al. [18] adopted the electron tunneling effect to control the rotation of the blades via periodic charging and discharging. Recently, Cai et al. [19–22] discovered that the inner CNT in a fixed outer tube has a stable unidirectional rotation in an uniform temperature field. This is different from the thermal-gradient model proposed by Santamaria-Holek et al. [20].

In above models, the carbon nanosystem works in vaccum. Actually, people prefer the nanodevices if they can work in air or protecting gas. Besides, the rotation of the motor should be easily controlled. Argon, a type of inert gas, is usually adopted to be protecting gas in experiments [23,24]. In this study, a nanoring is proposed by bending a CNT and covalently bonding it edges. The nanoring from CNT has been studied in the work by Neto and Nero [25], In their model, the nanoring was

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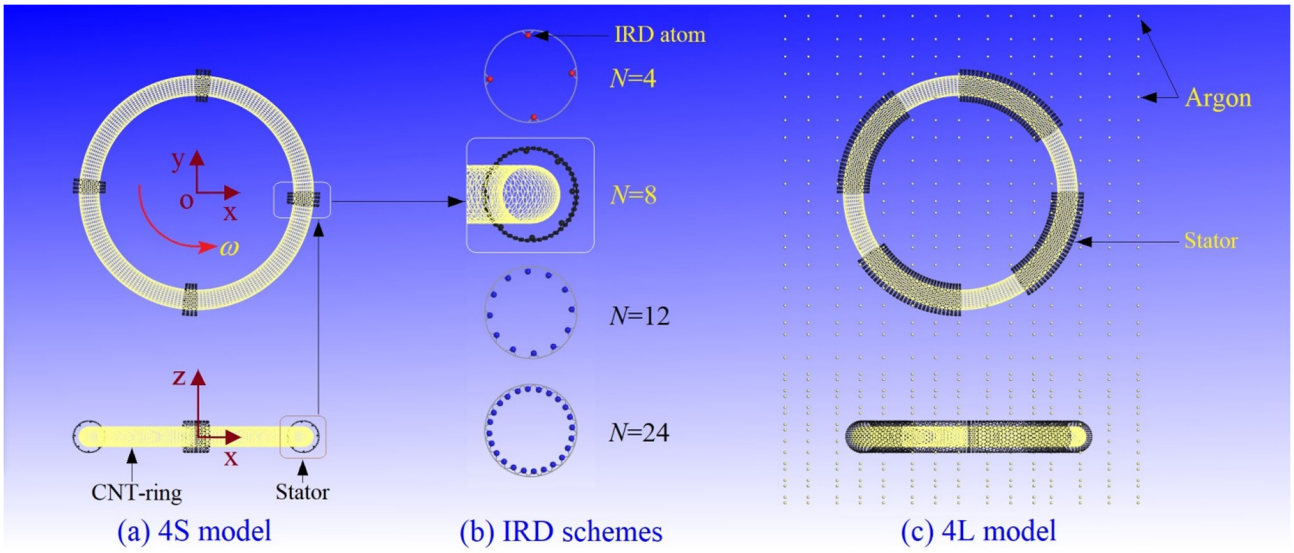

Fig. 1. Initial CNT-ring models in argon environment. (a) 4S model, which contains a CNT-ring constrained by 4 short stators from the same CNT. (b) IRD schemes. At the oblique edge of a stator, there are N carbon atoms have the same inwardly radial deviation (IRD) [26]. N = 4, 8, 12 or 24 is involved in tests. (c) 4L model in argon environment, which has a CNT-ring constrained by four long stators. ω is the rotational frequency of the ring along the z-axis. Negative value of ω means clockwise rotation, positive means anti-clockwise rotation.

fixed and a small capsule moved in the nanoring. In our study, the nanoring is constrained by four outer CNTs with some atoms having radial deviation. Using molecular dynamics simulation, we evaluate the rotational behavior of the nanoring protected by argon, and observe some interesting phenomena which can be helpful for design of a nanomotor with controllable rotation.

2. Models and methodology

2.1. Models of rotary nanoring

Fig. 1 illustrates two models of nanorings constrained by four stators. Each stator has two edges, i.e., one is aligned with x-/y-axis, the other is oblique. All of the components are made from uniformly curved CNTs. In the 4L model, the stators are longer than those in the 4S model. Both models have the same ring, which is obtained by bonding both edges of a curved CNT with specified length. The detailed parameters of the CNTs are listed in Table 1. In Fig. 1c, the argon atoms are put in the simulation box with density of $\rho = 0$, 40 kg/m^3 (2127 argon atoms), or 80 km/m^3 (4254 argon atoms). The simulation box with periodic boundaries along three dimensions has sizes of 21 nm × 8 nm × 21 nm. To create the asymmetry of geometry of the stators, some of the carbon atoms at the oblique edge of each stator are pushed inwardly along the radial direction within the local cross section of the stator, and the atoms are called IRD atoms. In this work, all the IRD atoms have the same radial deviation of ~0.0568 nm.

Table 1
Parameters of each component in different nanoring models. Dimension unit: nm.

Component	Chiral index	Tube radius	Tube length	Curvature (/nm)	Num. of atoms	Model
Ring	(15, 0)	0.5872	40.044	1/6.37	5640	Both models
Short stator	(24, 0)	0.9395	0.710	1/6.37	192	4S model
Long stator	(24, 0)	0.9395	6.428	1/6.37	1440	4L model

2.2. Methodology

Molecular dynamics (MD) simulation approach is adopted to reveal the dynamic behavior of the CNT-ring in different conditions. The MD simulations are fulfilled in the open code LAMMPS [27]. The flowchart of each simulation contains following major steps, i.e.,

Step 1. Choose a double walled CNTs with chiral index (15, 0)/(24, 0), and tailor the CNTs with one inner tube and four outer tubes, their lengths are shown in Table 1;
Step 2. Curve the CNTs with the same curvature, covalently bond both edges of the inner tube into the CNT-ring;
Step 3. Reshape the structure using minimization of the potential energy of the system, and initiate the velocities of the atoms at given temperature, the distribution of the velocities satisfies Gaussian distribution;
Step 4. Fix all of the degrees of freedom of the atoms in the four stators, and put the rotor and argon atoms (if has) in the NVT ensemble with specified temperature. Temperature involved in simulations would be 50 K, 100 K, 200 K, or 300 K;
Step 5. Put the system in the Nose-Hoover thermostat [28,29], and record the data of ring and argon atoms.
Step 6. Stop for post processing.

In time integration, the timestep is set to be 0.001 ps. The interaction among carbon atoms is evaluated by the AIREBO potential [30], which contains the REBO item for bonding interaction, torsion item for the local deformation of neighbor atoms, and Lennard-Jones item for non-bonding interaction [31].

3. Results and discussion

3.1. Rotation of ring in vacuum

Before studying the dyanmic behavior of the nanoring in argon environment, we calculate the rotational speed of the nanoring in vaccum. Fig. 2 shows the history of the rotational frequency of the nanoring constrained by four short CNT-stators. When the system is in vacuum, the stable value of ω depends on the number of IRD atoms on each stator. For example, the nanoring rotate clockwisely with the rotational frequency of ~3.16 GHz when each stator has 4 IRD atoms,