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Gap effect on stable rotation of a carbon nanotube nearby diamond needles

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ABSTRACT

A rotary nanomotor from carbon nanotube (CNT) and diamond is conceptually proposed, and the condition for stable rotation of the rotor is investigated. By putting several diamond needles (DNs) nearby a CNT, the tube can be driven to rotate at finite temperature. At finite temperature, thermal vibration of atoms in the CNT rotor and DNs leads to collision when their distance, i.e., Gap, is close to 0.34 nm, which is the equilibrium stance between neighbor sp^2 carbon nanostructures, e.g., graphene or CNT. The fixed DNs provide the rotor repulsion via their tip atoms during collision. If the repulsion can generate a torque moment with unchanged direction, the rotor will be accelerated to rotate. After a period of acceleration, the stable rotational frequency (SRF) of the rotor can be obtained when Gap is no more than 0.34 nm. Numerical results demonstrate that the rotational direction depends on the value of Gap when each DN has only one pair of tip atoms; the temperature has a significant effect on the value of SRF but little effect on the rotational direction; and the rotation of the rotor becomes unstable due to breakage of DNs when Gap is higher than 0.34 nm.

1. Introduction

Among allotropes of carbon [1–7], carbon nanotubes (CNT) and diamond belong to different types of carbon materials in terms of bond topologies. For example, a CNT is formed by sp^2-sp^2 covalently bonded carbon atoms, whilst, diamond has sp^3-sp^3 bonds. This is the reason for their significant differences in physical properties, e.g., optical and electronic properties [8–11]. Due to high strength of both sp^2-sp^2 and sp^3-sp^3 bonds, they exhibit extremely high modulus and strength [12,13]. The excellent mechanical properties bring them into wide applications in either micro- and macro-scales. For instance, diamond is used as anvil to provide extremely high pressure in experiments [6], acts as a cutter in practice.

However, for a CNT, it has a mechanical property which is much different from that of diamond. The property is superlubrication [14–16], i.e., between two neighbor concentric CNTs, their inter-shell friction is extremely low. This characteristic is caused by a fact that each carbon atom in CNTs has an anti-bonding delocalized electron. Hence, CNTs have both extremely high strength and extremely low friction, which are the reason why they are popular in the design of nanodevices, e.g., nano-oscillator [17–20], nano-transmission system [21,22], nanomotor [23–26].

Among the CNT-based nanomotor models, the rotors can be driven to rotate by different approaches. For example, Tu and Hu [23] presented an electrical motor at nanoscale. In their model, the short outer tube can move on a longer outer tube on the condition that the two CNTs have different chirality and the inner tube has varying electrical voltage between two ends. Differently, Wang et al. [24] proposed a nanomotor driven by external electric field. In their model, CNTs are adopted as blades and periodic charging and recharging happens during rotation. Barreiro et al. [25] discovered that a short outer tube can move along a long inner tube with thermal gradient between two ends. Both translation and rotation appear in their model. However, Cai and his colleagues [26–32] discovered that even without thermal gradient, the long inner CNT can also have a gigahertz rotation in a fixed outer tube.

In the present study, we propose a model of rotary carbon nanomotor based on Smoluchowski-Feynman ratchet effect, which implies that a component in the system has a uni-directional motion when the system in non-equilibrium state has lost symmetry in geometry. In the model, firstly a CNT is constrained by outer tubes, with the long CNT acting as rotor and the short CNTs as stators. Secondly, four diamond wedges are made by cutting along five crystal planes, i.e., (1 0 0), (0 1 0), (0 0 1) and two parallel (1 1 0) planes. Here, we call the wedges diamond needles (DNs). Thirdly, the four DNs are put beside the CNT rotor as drivers. To drive the rotor to rotate, the DNs should be put in chiral (see Fig. 1b). Finally, the system is put in a NVT ensemble, which has energy transformation for providing rotational kinetic energy to the

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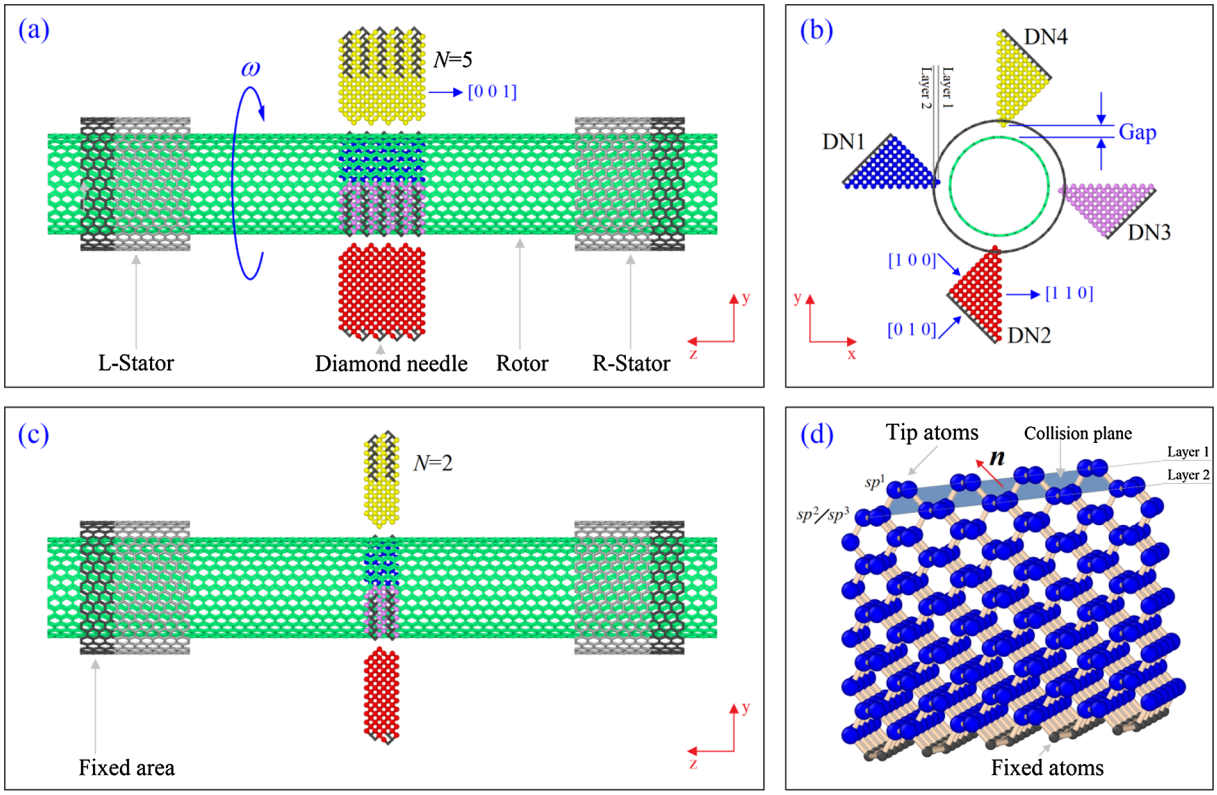

Fig. 1. Models of rotary nanomotor from carbon nanotubes (CNTs) and 4 diamond needles (DNs). (a) y-z view of motor with $N = 5$, i.e., five layers of atoms along z-direction in each DN. ω is the output rotation of the rotor. (b) x-y view of motor. Gap is the distance between tip of a DN and rotor. (c) y-z view of motor with $N = 2$. (d) Atoms in DN1. All atoms in Layer 1 are sp^1 atoms. Layer 2 contains both sp^2 and sp^3 atoms bonded relatively stable. Layers 1 and 2 form into a collision plane with the normal of $\boldsymbol{n}$.

rotor. If the DNs can actuate the rotor to move, their distance, i.e., Gap in Fig. 1b, should be less than 1 ns, which is the cutoff of non-bonding interaction in this study. In this study, we mainly focus on the stability of rotation of the rotor. The effects of gap, temperature, and thickness of DNs on the stability are discussed.

2. Models and methodology

The models of rotary nanomotor shown in Fig. 1a, c are made from (15,15)/(20,20) double-walled CNTs and four diamond needles. Both outer tubes are partly fixed, and act as stators. The distance between the two stators is 8 nm. The inner tube, which acts as rotor, can move freely in the two outer tubes. The four DNs are set with needle tips pointing toward the outer surface of the inner tube. As shown in Fig. 1b, the (1 1 0) crystal plane of each DN is vertical to the surface of the inner tube at start. Detailed parameters are listed in Table 1.

At finite temperature, the free atoms in each component of the nanomotor have thermal vibration, and the amplitude of thermal vibration increases with temperature. During thermal vibration, some of the atoms in the rotor collide with the tip atoms in DNs, and some collide with the atoms in stators. In particular, the colliding with the tip atoms in a DN results in repulsion in the rotor from the DN. During the collision, the (1 0 0) face of DN provides a tangential component of repulsion to the rotor. The component generates a torque moment which can cause an acceleration of rotation of the rotor. If the total torque from all of the DNs is higher than the resistant torque from the two stators, the rotor's rotational frequency, i.e., ω, can be controlled by the following equation:

$$\omega(t) = \int_{s=0}^{t} \frac{1}{J_{\text{axis}}}(M_{\text{DN}} - M_{\text{St}})\,\mathrm{d}s \tag{1}$$

where J_{axis} is the mass inertial of momentum of the rotor about its axis. At finite temperature, the value of J_{axis} can be considered as a constant. M_{DN} is the moment produced by DNs, and M_{St} is the resistant moment induced by friction from the two stators. Both moments are greater at higher temperature. Hence, one can improve the absolute value of ω by considering three factors: the number of tip atoms in DNs, the distance between DN tips and the rotor, i.e., Gap, and temperature. In this study, we choose two models of motor with different DNs, i.e., $N = 2$, or 5, respectively. The value of Gap varies from 0.25 nm to 5.0 nm. The system will work at 100 K or 300 K to show the effect of temperature on ω.

Molecular dynamics simulation approach is adopted to reveal the dynamic response of the rotor under different conditions. Each simulation contains four major steps, i.e., (1) create the model of nanomotor; (2) reshape the boundaries of components in the system by minimization of potential energy of system; (3) relax the system at a NVT ensemble with specified temperature; and (4) Record data for post-processing. The open source code LAMMPS [33] is used to conduct the computational simulations. The interaction among carbon atoms is described by AIREBO potential [34], which can reflect both bonding and nonbonding interaction, simultaneously. For the time integration, time step is set to 0.001 ps. No less than 20,000 ps of response will be simulated.

Table 1
Parameters of carbon components in the nanomotor models in Fig. 1.

Component	Rotor	L-Stator	R-Stator	DNs with N = 2	DNs with N = 5
Length/nm	13.773	2.214	2.214	0.622 of thickness	1.689
Diameter/nm	2.034	2.712	2.712	1.956 of (0 1 1) plane	1.956
Free atoms	3390	520	520	147 × 4	378 × 4
Fixed atoms	0	240	240	23 × 4	59 × 4