A Molecular Motor Constructed from a Double-Walled Carbon Nanotube Driven by Axially Varying Voltage

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Abstract

A new molecular motor is conceptually constructed from a double-walled carbon nanotube (DWNT) consisting of a long inner single-walled carbon nanotube (SWNT) and a short outer SWNT with different chirality. The interaction between inner and outer tubes is the sum of the Lennard-Jones potentials between carbon atoms in inner tube and those in outer one. Within the framework of Smoluchowski-Feynman ratchet, it is theoretically shown that this system in an isothermal bath will exhibit a unidirectional rotation in the presence of a varying axial electrical voltage. Moreover, the possibility to manufacture this electrical motor from DWNT is discussed under the current conditions of experimental technique.

PACS numbers: 61.46.+w, 85.35.Kt
In order to illustrate that the second law of thermodynamics cannot be violated, Feynman introduced an imaginary ratchet-and-paw system in his famous lectures. This system is now called Smoluchowski-Feynman ratchet because it was first described by Smoluchowski in 1912. One can observe the ratchet effect that the ratchet rotates unidirectionally if two conditions are satisfied: (i) breaking of spatial inversion symmetry and (ii) breaking of thermal equilibrium. Based on Smoluchowski-Feynman ratchet, many statistical models are put forward, such as on-off ratchets, fluctuating potential ratchets, fluctuating force ratchets, temperature ratchets, and so on. These models can explain the directional matter transport at the molecular levels in biological systems with the aid of the special protein systems. Now the small devices or systems at molecular levels are called molecular motors if they can transform chemical, electrical or other forms of energy into mechanical energy.

In another classic talk given by Feynman at the annual meeting of the American Physical Society in 1959, he predicted that Human would manufacture devices even at the molecular levels in the future. His prediction are being realized with the development of nanotechnology. Especially, after the discovery of carbon nanotubes, researchers designed many nanodevices, such as nanotube gears, nanotube oscillators, nanotube drills and so on. Tuzun predicted a doped nanotube motor driven by laser, and one of the present authors and Ou-Yang proposed a molecular motor constructed from a double-walled carbon nanotube (DWNT) driven by temperature variation. Kang et al. confirmed these predictions by molecular dynamics simulations and then put forward nanotube motors driven by fluid. Viewed from statistical mechanics, the DWNT motor in Ref. is a kind of temperature ratchets in essence. But it is not easy to control the variation of temperature. Thus we may ask: can we design a more convenient way, for example using the electrical field, to drive this motor?

In this report, we show it is possible to construct a DWNT motor driven by electrical field in physical point of view. The motor consists of a long inner tube and a short outer tube. For simplicity, the interaction between inner and outer tubes is taken as the sum of the Lennard-Jones potentials between carbon atoms in inner tube and those in outer one. Within the framework of Smoluchowski-Feynman ratchet, we theoretically reveal that this system in an isothermal bath will exhibit a unidirectional rotation in the presence of a varying axial voltage. Moreover, we also discuss the possibility to manufacture this electrical
motor under the current conditions of experimental technique.

As illustrated in Fig. 1, the DWNT consists of a long inner tube and a short outer tube with different chirality. Without losing generality, we take (8, 4) and (14, 8) SWNTs, and put two-unit cells for outer tube. The SWNTs have the same axis. One end of inner tube is fixed while another is simply sustained. We put the DWNT in between, without contacting to, a pair of parallel electrodes on which we apply a voltage varying with time. The axis of DWNT is perpendicular to the electrodes. The whole system is put in a thermal bath, e.g., helium gas. Because of the extremely high Young’s modulus and stereo effect of carbon nanotubes, the collisions of helium atoms at low temperature, e.g., \( T = 50 \) K almost have not effect on the shape of carbon nanotubes as well as the coaxiality of two nanotubes. Two degrees of freedom will be excited by the collisions: the rotation of outer tube around the inner one and the slide of outer tube along the axis. In following contents, we assume that some device can fix the sliding degree of freedom of outer tube. The interactions between atoms in outer tube and those in inner tube provide potentials asymmetric with respect to the relative rotation of the two nanotubes because of the difference in chirality. This property breaks the spatial inversion symmetry and naturally makes our device satisfy the first condition to exhibit the ratchet effect.

The applied varying electrical voltage will achieve the second condition of ratchet effect as discussed below. Recently Guo et al. found a large axial electrostrictive deformation of SWNTs in the presence of axially electrical field by using numerical Hartree-Fock and density functional calculations although SWNTs are usually regarded as non-piezoelectric materials. According to these authors, the electrical field changes the electronic structures of SWNTs and induces elongations of carbon-carbon bonds without changing bond angles. Although their calculations are concerned to the electrostatic field, it is easy to see that their results are also available to the varying electrical field with period in the order of nanoseconds because the response time of electron to electrical field is usually about several femtoseconds. Thus, bond elongations are synchronous with the variation of electrical field, which induces the shaking interaction between outer and inner tubes. Consequently, we obtain a fluctuating potential which, according to Ref. 6, is sufficient to clear the second condition for ratchet effect in the statistical point of view.

To specify the above idea, we select an orthogonal coordinate system \( Oxyz \) by adopting the convention in Ref. 31 whose \( z \)-axis is the tube axis parallel to the translation vector of
SWNT, and $x$-axis passes through some carbon atom in inner tube. The angle rotated by outer tube around inner tube is denoted by $\theta$. All coordinates of atoms are also calculated by the method in Ref. [31]. For theoretical simplicity, the interaction between any atom $i$ in outer tube and atom $j$ in inner tube is taken as Lennard-Jones potential $^{32}$

$$u(r_{ij}) = 4\epsilon\left[\frac{(\sigma/r_{ij})^12}{(\sigma/r_{ij})^6}\right],$$

where $r_{ij}$ is the distance between atoms $i$ and $j$, $\epsilon = 28$ K, and $\sigma = 3.4\text{\AA}.^{33}$

The inner tube is long enough to be thought of as an infinite one. The total interaction, $V(\theta, a_{cc}) = \sum_{ij} u(r_{ij})$, between outer tube and inner tube can be calculated by the method in Ref. [31], where $a_{cc}$ is the length of carbon-carbon bond whose value is $1.42\text{\AA}$ for zero voltage. Obviously, the potential can be expanded by Taylor series $V(\theta, a_{cc}) \simeq V_0(\theta)[1 + \alpha(\theta)\varepsilon]$ for small elongations of bond-length, where $V_0(\theta) = V(\theta, 1.42\text{\AA})$, $\alpha(\theta)$ is a function of $\theta$ and $\varepsilon$ the bond elongation ratio. In Fig. 2, we show numerical results of the interaction between outer tube and inner tube for different bond-lengths. Here the potentials $V(0, a_{cc})$ are put to zero by subtracting some constants which have no effect to our final results. We find that the potentials are functions with period $\pi/2$ and that $\alpha(\theta)$ is so weakly dependent on $\theta$ that we can fit it by $\alpha(\theta) = -14.2$ from Fig. 2. On the other hand, from Fig. 2 in the work of Guo et al., we know the bond elongation ratio shows approximately a linear dependence on the magnitude of electrical field with the slope $\beta = 0.25\text{\AA}/V$ provided that the applied voltage field is not too high. Moreover, the field dependence of bond elongation ratio is insensitive to the diameters and chiral angles of SWNTs. Therefore, we obtain a shaking interaction,

$$V(\theta, t) = V_0(\theta)\{1 + \mu[1 + \cos(2\pi t/T)]\},$$

between outer tube and inner tube under a varying voltage $\dot{U}(t) = U_0[1 + \cos(2\pi t/T)]$ between two electrodes, where $U_0$, $T$ and $\mu = \alpha\beta U_0/l$ are constant quantities. Here $l$ is the distance between two electrodes and $T$ is assumed greater than 0.1 ns.

Next we will discuss the motion of outer tube in helium gas. Because the mass of outer tube is much larger than that of helium atom, its motion can be described by the Langevin equation $mR^2\ddot{\theta} = -V'(\theta, t) - \eta\dot{\theta} + \xi(t)^{34}$ where $m \sim 10^{-23}$ Kg, the mass of outer tube containing 496 carbon atoms, and $R = 7.75\text{\AA}$ is the radius of outer tube. $\eta$ is the rotating viscosity coefficient, and the dot and the prime indicate, respectively, differentiations with respect to time $t$ and angle $\theta$. $\xi(t)$ is thermal noise which satisfies $\langle \xi(t) \rangle = 0$ and the fluctuation-dissipation relation $\langle \xi(t)\xi(0) \rangle = 2\eta T\delta(t)^{34}$ where $T = 50$ K and the Boltzmann factor is set to 1. We estimate $mR^2\ddot{\theta}/(\eta\dot{\theta}) < 10^{-3}$ by taking $\dot{\theta} \sim \dot{\theta}/T$ and $T > 0.1$ ns. Thus it is reasonable to neglect the inertial term $mR^2\ddot{\theta}$. In this case, the Fokker-Planck equation

$$mR^2\ddot{\theta}/(\eta\dot{\theta}) < 10^{-3}$$

is valid.
corresponding to the Langevin equation is expressed as

$$\frac{\partial P(\theta, t)}{\partial t} = \frac{\partial}{\partial \theta} \left[ \frac{V'(\theta, t)}{\eta} P(\theta, t) \right] + \frac{T}{\eta} \frac{\partial^2 P(\theta, t)}{\partial \theta^2},$$

(1)

where $P(\theta, t)$ represents the probability of finding the outer tube at angle $\theta$ and time $t$ which satisfies $P(\theta + \pi/2, t) = P(\theta, t)$ and $\int_0^{\pi/2} P(\theta, t) d\theta = 1$. It follows that the average angular velocity of outer tube in the long-time limit

$$\langle \dot{\theta} \rangle = \lim_{t \to \infty} \frac{1}{T} \int_t^{t+T} dt \int_0^{\pi/2} d\theta \left[ -\frac{V'(\theta, t) P(\theta, t)}{\eta} \right].$$

(2)

Let $D = \frac{T}{\eta}$, $t = D^{-1} \tau$, $T = D^{-1} \mathcal{J}$, $V_0(\theta) = u(\theta)T$, we obtain the dimensionless forms of (1) and (2):

$$\frac{\partial P(\theta, \tau)}{\partial \tau} = \frac{\partial}{\partial \theta} \left\{ 1 + \mu \left[ 1 + \cos \frac{2\pi \tau}{\mathcal{J}} \right] \right\} u'(\theta)P(\theta, \tau) + \frac{\partial^2 P(\theta, \tau)}{\partial \theta^2},$$

(3)

$$\left\langle \frac{d\theta}{d\tau} \right\rangle = -\lim_{\tau \to \infty} \frac{1}{\mathcal{J}} \int_\tau^{\tau+\mathcal{J}} d\tau \int_0^{\pi/2} d\theta \left[ 1 + \mu \left[ 1 + \cos \frac{2\pi \tau}{\mathcal{J}} \right] \right] u'(\theta)P(\theta, \tau).$$

(4)

Because $V_0(\theta)$ is a periodic function, we can expand it by Fourier series and find that it is well fit by $V_0(\theta) = 29.12 - 0.18 \cos 4\theta - 16.14 \cos 8\theta - 12.53 \cos 12\theta - 4.48 \sin 4\theta - 19.52 \sin 8\theta + 11.52 \sin 12\theta$ (K), where high-order terms are neglected because their coefficients are very small. Thus $u'(\theta) = V_0'(\theta)/T = \sum_{k=1}^3 (v_k e^{4ik\theta} + v_k e^{-4ik\theta})$ with $v_1 = -0.179 - 0.007i$, $v_2 = -1.562 - 1.291i$ and $v_3 = 1.382 - 1.504i$. In the long-time limit, $P(\theta, \tau)$ can be expanded by Fourier series $P(\theta, \tau) = \sum_{n,m=-\infty}^{\infty} p_{nm} \exp i[(2n\pi \tau/\mathcal{J}) + 4m\theta]$. Substituting them into (3), we arrive at a recursion equation

$$p_{nm} = \frac{2im \mathcal{R}_{nm}}{8m^2 + i(n\pi \tau/\mathcal{J})},$$

(5)

with $\mathcal{R}_{nm} = \sum_{k=1}^3 \{ (1 + \mu)(v_k p_{n,m-k} + v_k e^{-4ik\theta}) + (\mu/2)[v_k (p_{n-1,m-k} + p_{n+1,m-k}) + v_k (p_{n-1,m+k} + p_{n+1,m+k})] \}$. Similarly, (1) is transformed into

$$\left\langle \frac{d\theta}{d\tau} \right\rangle = -(\pi/2) \mathcal{R}_{00}.$$

(6)

Considering the constraint $p_{n0} = (2/\pi) \delta_{n0}$ coming from $\int_0^{\pi/2} P(\theta, t) d\theta = 1$, we solve the recursion equation (5) with $\mu = -0.01$ for different dimensionless period $\mathcal{J}$, and then calculate the dimensionless average angular velocity $\langle \frac{d\theta}{d\tau} \rangle$ by (6). The dimensionless period dependence of average angular velocity of outer tube rotating around inner tube is shown
in Fig. 3 from which we find that: (i) \( \langle \frac{d\theta}{d\tau} \rangle \to 0 \) if \( J \to \infty \) which is equivalent to the case of an electrostatic voltage; (ii) \( \langle \frac{d\theta}{d\tau} \rangle = 0 \) if \( J = 0 \) which corresponds to the case that the voltage varies so quickly that outer tube can not respond to it in time; (iii) Outer tube rotates counterclockwise around the tube axis for some \( J \), which corresponds to the positive value of \( \langle \frac{d\theta}{d\tau} \rangle \), and clockwise for other \( J \), which corresponds to the minus value of \( \langle \frac{d\theta}{d\tau} \rangle \); (iv) \( \langle \frac{d\theta}{d\tau} \rangle \) has a significant value \(-347 \text{ nrad}\) when \( J_c = 0.15 \).

For helium at \( T = 50 \text{ K}\), we can calculate \( \eta = 1722 \text{ K-ns} \) from its value at \( 273 \text{ K} \).\(^{35}\) It is necessary to emphasize that \( \eta \) is the rotating viscosity coefficient which is different from the viscosity coefficient of gas \( \eta_c \) in the common sense. The simple relationship between them is \( \eta = 2\pi R^2 L \eta_c \) for cylinders, where \( L = 27.39 \text{ Å} \) is the length of outer tube. Therefore we obtain \( \langle \dot{\theta} \rangle = -10.08 \text{ nrad/ns} \) (i.e., about one and a half rounds per second) when the period \( T_c = 5.17 \text{ ns} \). Here we obtain these values in disregard of the fiction between nanotubes because it is very small.\(^{36}\)

The above discussions demonstrate that we can construct an electrical motor from DWNT in principle. Two key points are: (i) DWNT with different outer and inner chirality induces a potential that breaks spatial inversion symmetry; (ii) Some mechanism (varying voltage in this paper) induces the shaking of the potential that breaks thermal equilibrium. Therefore, similar results are available in any DWNT with different outer and inner chirality although our discussions are focused on \((8,4)@(14,8)\) tube. Additionally, we use the results obtained from density functional theory in Ref. \(^{30}\) that shows large axial electrostrictive deformation for armchair and zigzag tubes with different diameters. These investigated cases reveal that the electrostrictive deformation is insensitive to the diameters and chiral angles of SWNTs. Generally speaking, different voltage dependence of bond-elongation might exist for different chirality. Even if were the case, it does not hinder from inducing the shaking of the potential. In short, different DWNT and different voltage dependence of bond-elongation do not change the qualitative conclusion of this paper but merely modify the quantitative value of the average angular velocity.

Can this device be made in reality? There are several technological difficulties. The first one is to make the DWNT with different chirality of outer and inner tubes. Experimentalists can overcome it by producing DWNT based on the synthesis technique in Ref. \(^{37}\). The second difficulty is the varying voltage. Our device requires voltage \( (U_0 \sim 3 \text{ V for } l \sim 0.1 \mu\text{m}) \) with high frequency of gigahertz. The third one is the method to restrict the sliding
degree of freedom of outer tube. It is possible to manufacture the DWNT motor driven by varying electrical voltage provided that researchers overcome the above difficulties.

In summary, we conceptually design a new molecular motor from DWNT driven by varying electrical voltage. In this sense, it can be called “electrical motor” in nanometer scale. Similarly, we may design another molecular motor if we replace carbon nanotubes with boron nitride nanotubes because the latter is a piezoelectric material. People have a long dream to make machines in nanoscales. The key component to these machines is the power device. Our motor is expected to be the power device if it is manufactured in the future with the development of nanotechnology.

We are grateful to Dr. Q. X. Li and B. Y. Zhu for their technical helps.

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FIG. 1: Schematic diagram of the DWNT motor driven by varying electrical field. The DWNT consists of a long inner tube and a short outer tube. It is put between a pair of electrodes with a varying voltage $\tilde{U}(t)$ applied on.
FIG. 2: Interactions between outer tube and inner tube with different lengths of carbon-carbon bonds. Here the potentials $V(0, a_{cc})$ are put to zero by subtracting some constants.
FIG. 3: Average dimensionless angular velocity $\langle d\theta/d\tau \rangle$ of outer tube rotating around inner one in isothermal bath when varying axial voltage with dimensionless period $J$ is applied. The minus sign means the clockwise rotation around $z$-axis while the positive represents counterclockwise rotation.