Molecular motor constructed from a double-walled carbon nanotube driven by axially varying voltage

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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 an inner tube and those in an outer one. Within the framework of the 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 of manufacturing this electrical motor from DWNT is discussed under the current conditions of the experimental technique.

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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.[1] This system is now called the Smoluchowski-Feynman ratchet because it was described by Smoluchowski in 1912.[2] One can observe the ratchet effect, where the ratchet rotates unidirectionally if two conditions are satisfied:[3] (i) the breaking of spatial inversion symmetry and (ii) the breaking of thermal equilibrium. Based on the Smoluchowski-Feynman ratchet, many statistical models are put forward, such as on-off ratchets,[4,5] fluctuating potential ratchets,[6] fluctuating force ratchets,[7,8] temperature ratchets,[9–11] 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.[12–14] 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 humans would manufacture devices even at the molecular levels in the future.[15] His prediction is being realized with the development of nanotechnology.[16] Especially, after the discovery of carbon nanotubes,[17] researchers designed many nanodevices, such as nanotube gears,[18,19] nanotube oscillators,[20–23] nanotube drills,[24,25] and so on. Tuzun predicted a doped nanotube motor driven by laser,[26] 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.[27] Kang *et al.* confirmed these predictions by molecular dynamics simulations and then put forward nanotube motors driven by fluid.[28] Viewed from statistical mechanics, the DWNT motor in Ref. 27 is a kind of temperature ratchet[9–11] 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 Brief Report, we show it is possible to construct a DWNT motor driven by the electrical field from a 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 an inner tube and those in an outer one. Within the framework of the 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 of manufacturing this electrical motor under the current conditions of the 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) single-walled carbon nanotubes (SWNTs), and put two-unit cells for the outer tube. The SWNTs have the same axis. One end of the inner tube is fixed while another is simply sustained. We put the DWNT in between a pair of parallel electrodes, without contacting either electrode, on which we apply a voltage varying with time. The axis of the 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[29] and the stereo effect of carbon nanotubes, the collisions of helium atoms at low temperature, e.g., $T=50$ K almost have no effect on the shape of carbon nanotubes as well as the coaxiality of two nanotubes. Two

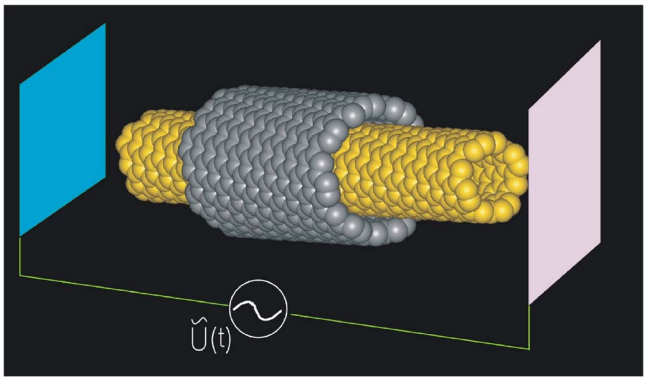

FIG. 1. (Color online) Schematic diagram of the DWNT motor driven by varying electrical field. The DWNT consists of a long inner tube and a short outer tube. It is put between a pair of electrodes with a varying voltage $\tilde{U}(t)$ applied on.

degrees of freedom will be excited by the collisions: the rotation of the outer tube around the inner one and the slide of the outer tube along the axis. In the following discussions, we assume that some device can fix the sliding degree of freedom of the outer tube. The interactions between atoms in the outer tube and those in the 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 the ratchet effect as discussed below. Recently Guo *et al.* found a large axial electrostrictive deformation of SWNTs in the presence of an axially electrical field by using numerical Hartree-Fock and density functional calculations[30] although SWNTs are usually regarded as nonpiezoelectric 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.[30] Although their calculations are concerned with the electrostatic field, it is easy to see that their results are also available for the varying electrical field with a period on the order of nanoseconds because the response time of an electron to the electrical field is usually about several femtoseconds. Thus, bond elongations are synchronous with the variation of the 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 the ratchet effect from the viewpoint of statistical physics.

To clarify 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[31] of SWNT, and the x axis passes through one carbon atom in the inner tube. The angle rotated by the outer tube around the inner tube is denoted by θ. All coordinates of atoms are also calculated by the method in Ref. 31. For theoretical simplicity, the interaction between any atom i in the outer tube and atom j in the inner tube is taken as the Lennard-Jones potential[32] $u(r_{ij})=4\epsilon[(\sigma/r_{ij})^{12}-(\sigma/r_{ij})^{6}]$, where r_{ij} is the distance between atoms i and j, $\epsilon=28$ K, and $\sigma=3.4$ Å.[33] The inner tube is long enough to be thought of as an infinite one. The total interaction, $V(\theta,a_{cc})=\Sigma_{ij}u(r_{ij})$, between the outer tube and the inner tube can be calculated by the method in Ref. 31, where a_{cc} is the length of the carbon-carbon bond whose value is 1.42 Å for zero voltage. Obviously, the potential can be expanded by the Taylor series $V(\theta,a_{cc})\simeq V_0(\theta)[1+\alpha(\theta)\varepsilon]$ for small elongations of bond length, where $V_0(\theta)=V(\theta,1.42\ \text{Å})$, $\alpha(\theta)$ is a function of θ, and ε is the bond elongation ratio. In Fig. 2, we show numerical results of the interaction between the outer tube and the inner tube for different bond lengths. Here the potentials $V(0,a_{cc})$ are put to zero by subtracting some constants that have no effect on our final results. We find that the potentials are functions with period $\pi/2$ and that $\alpha(\theta)$ is so weakly dependent on θ 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

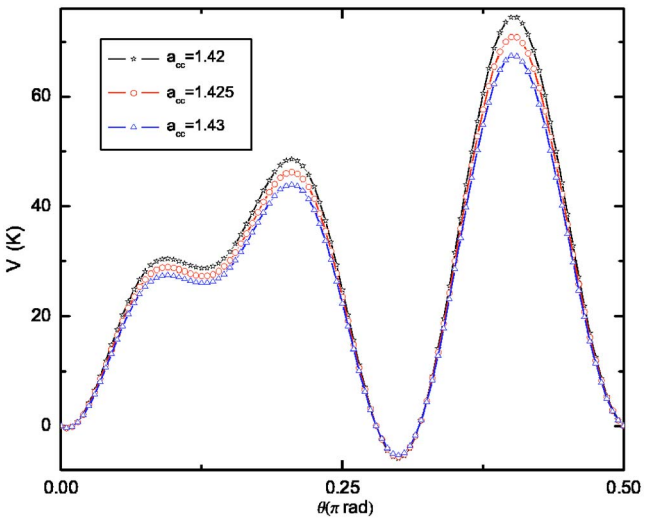

FIG. 2. (Color online) Interactions between the outer tube and the inner tube with different lengths of carbon-carbon bonds. Here the potentials $V(0,a_{cc})$ are set to zero by subtracting some constants.

dependence on the magnitude of the electrical field with the slope $\beta=0.25$ Å/V, provided that the applied voltage field is not too high. Moreover, the field dependence of the bond elongation ratio is insensitive to the diameters and chiral angles of SWNTs. Therefore, we obtain a shaking interaction, $V(\theta,t)=V_0(\theta)\{1+\mu[1+\cos(2\pi t/\mathcal{T})]\}$, between the outer tube and the inner tube under a varying voltage $\tilde{U}(t)=U_0[1+\cos(2\pi t/\mathcal{T})]$ between two electrodes, where U_0, $\mathcal{T}$, and $\mu=\alpha\beta U_0/l$ are constant quantities. Here l is the distance between two electrodes and $\mathcal{T}$ is assumed greater than 0.1 ns.

Next we will discuss the motion of the outer tube in helium gas. Because the mass of the outer tube is much larger than that of the 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 the outer tube containing 496 carbon atoms, and $R=7.75$ Å is the radius of the outer tube. η is the rotating viscosity coefficient, and the dot and the prime indicate, respectively, are differentiations with respect to time t and angle θ. $\xi(t)$ 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 $\ddot{\theta}\sim\dot{\theta}/\mathcal{T}$ and $\mathcal{T}>0.1$ ns. Thus it is reasonable to neglect the inertial term $mR^2\ddot{\theta}$. In this case, the Fokker-Planck equation corresponding to the Langevin equation is expressed as[3]

$$\frac{\partial P(\theta,t)}{\partial t}=\frac{\partial}{\partial\theta}\left[\frac{V'(\theta,t)}{\eta}P(\theta,t)\right]+\frac{T}{\eta}\frac{\partial^2 P(\theta,t)}{\partial\theta^2}, \qquad (1)$$

where $P(\theta,t)$ represents the probability of finding the outer tube at angle θ 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 the outer tube in the long-time limit[3] is

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

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

$$\frac{\partial P(\theta,\tau)}{\partial \tau} = \frac{\partial}{\partial \theta}\left\{ \left[1+\mu\left(1+\cos\frac{2\pi\tau}{\mathcal{J}} \right) \right] u'(\theta) P(\theta,\tau) \right\} + \frac{\partial^2 P(\theta,\tau)}{\partial \theta^2}, \quad (3)$$

$$\left\langle \frac{d\theta}{d\tau} \right\rangle = -\lim_{\tau\to\infty} \frac{1}{\mathcal{J}} \int_\tau^{\tau+\mathcal{J}} d\tau \times \int_0^{\pi/2} d\theta \left[1+\mu\left(1+\cos\frac{2\pi\tau}{\mathcal{J}} \right) \right] u'(\theta) P(\theta,\tau). \quad (4)$$

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 $u'(\theta)=V_0'(\theta)/T=\Sigma_{k=1}^{3}(v_k e^{4ik\theta}+v_k^* e^{-4ik\theta})$ with $v_1=-0.179-0.007i$, $v_2=-1.562-1.291i$, and $v_3=1.382-1.504i$. In the the long-time limit, $P(\theta,\tau)$ can be expanded by Fourier series $P(\theta,\tau)=\Sigma_{n,m=-\infty}^{\infty} p_{nm}\exp i[(2n\pi\tau/\mathcal{J})+4m\theta]$. Substituting them into (3), we arrive at a recursion equation

$$p_{nm} = \frac{2im\mathcal{R}_{nm}}{8m^2 + i(n\pi\tau/\mathcal{J})}, \quad (5)$$

with

$$\mathcal{R}_{nm} = \sum_{k=1}^{3} \{ (1+\mu)(v_k p_{n,m-k} + v_k^* p_{n,m+k}) + (\mu/2) \times [v_k(p_{n-1,m-k}+p_{n+1,m-k}) + v_k^*(p_{n-1,m+k}+p_{n+1,m+k})] \}.$$

Similarly, (4) is transformed into

$$\left\langle \frac{d\theta}{d\tau} \right\rangle = -(\pi/2)\mathcal{R}_{00}. \quad (6)$$

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 $\langle d\theta/d\tau\rangle$ by (6). The dimensionless period dependence of the average angular velocity of the outer tube rotating around the inner tube is shown in Fig. 3, from which we find the following: (i) $\langle d\theta/d\tau\rangle \to 0$ if $\mathcal{J}\to\infty$ which is equivalent to the case of an electrostatic voltage; (ii) $\langle d\theta/d\tau\rangle=0$ if $\mathcal{J}=0$ which corresponds to the case that the voltage varies so quickly that the outer tube cannot respond to it in time; (iii) the outer tube rotates counterclockwise around the tube axis for some $\mathcal{J}$, which corresponds to the positive value of $\langle d\theta/d\tau\rangle$, and clockwise for other $\mathcal{J}$, which corresponds to the minus value of $\langle d\theta/d\tau\rangle$; (iv) $\langle d\theta/d\tau\rangle$ has a significant value −347 nrad when $\mathcal{J}_c=0.15$.

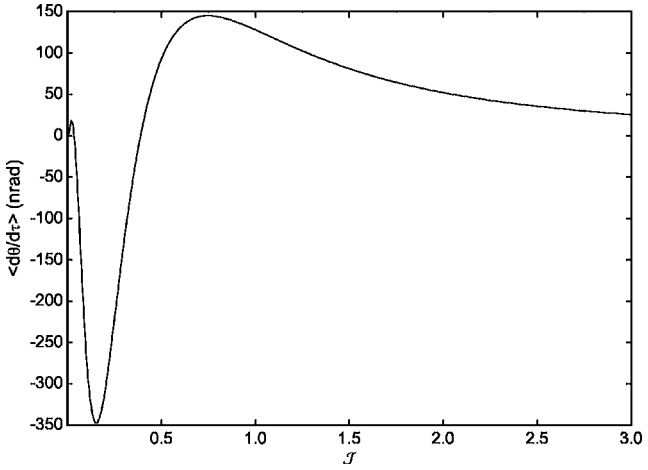

FIG. 3. Average dimensionless angular velocity $\langle d\theta/d\tau\rangle$ of the outer tube rotating around the inner one in isothermal bath when the varying axial voltage with dimensionless period $\mathcal{J}$ is applied. A negative number means clockwise rotation around the z axis while a positive number represents counterclockwise rotation.

For helium at $T=50$ K, we can calculate $\eta=1722$ K ns from its value at 273 K.[35] It is necessary to emphasize that η is the rotating viscosity coefficient, which is different from the viscosity coefficient of gas η_c in the common sense. The simple relationship between them is $\eta=2\pi R^2 L\eta_c$ for cylinders, where $L=27.39$ Å is the length of the outer tube. Therefore we obtain $\langle\dot{\theta}\rangle=-10.08$ nrad/ns (i.e., about one and a half rounds per second) when the period $\mathcal{T}_c=5.17$ ns. Here we obtain these values in disregard of the friction 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 as follows: (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 the 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 the 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, a different voltage dependence of bond elongation might exist for different chirality. Even if were the case, it does not hinder voltage from inducing the shaking of the potential. In short, a different DWNT and a different voltage dependence of bond elongation do not change the qualitative conclusion of this paper but merely modify the quantitive 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 a DWNT based on the synthesis technique in Ref. 37. The second difficulty is the varying voltage. Our device requires voltage ($U_0\sim 3$ V for

$l \sim 0.1$ μm) with a high frequency of gigahertz. The third one is the method to restrict the sliding degree of freedom of the 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 an "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.[38] Scientists have long had a dream of making 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.

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