Carbon Nanotube Archimedes Screws

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ABSTRACT Recently, nanomechanical devices composed of a long stationary inner carbon nanotube and a shorter, slowly rotating outer tube have been fabricated. In this paper, we study the possibility of using such devices as nanoscale transducers of motion into electricity. When the outer tube is chiral, we show that such devices act like quantum Archimedes screws, which utilize mechanical energy to pump electrons between reservoirs. We calculate the pumped charge from one end of the inner tube to the other, driven by the rotation of a chiral outer nanotube. We show that the pumped charge can be greater than one electron per 360° rotation, and consequently, such a device operating with a rotational frequency of 10 MHz, for example, would deliver a current of $\approx$1 pAmp.

KEYWORDS: carbon nanotubes · multiwalled carbon nanotubes · NEMS · adiabatic quantum pumps · rotational actuators

Nanoscale energy harvesting is now recognized as a possible solution to the problem of powering future autonomous devices, with widespread applications to sensing, health, and environmental monitoring, processing, and communication.[1] To date, almost all harvesters are macroscopic, with sizes ranging from millimeters to tens or hundreds of micrometers. However, the current grand challenge is to harvest power for nanoelectromechanical systems (NEMS), which integrate nanoscale electrical functionality with mechanical devices such as actuators, pumps, or motors. Their high surface to volume ratios offer the potential for ultrasensitive physical, biological, and chemical sensing, while their low-power requirements make it feasible to power them *via* energy harvesting.

The aim of this paper is to introduce a new class of nanoscale, kinetic energy harvesters, capable of generating electrical energy from the environment. Kinetic energy harvesting requires a transduction mechanism to convert motion into electrical energy and a mechanical system that couples the transducer to environmental fluctuations. In MEMS devices, the latter typically involves an inertial mass with a coupling and frequency tuned to environmental vibrations. However, the downscaling of such an approach to the nanoscale is not straightforward because friction and other damping mechanisms begin to dominate. To overcome this problem, we propose a new class of devices shown in Figure 1, which are based on concentric shells of carbon nanotubes (CNTs), with different chiralities.

The mechanical coupling of the system of Figure 1 to environmental fluctuations has been demonstrated,[2] where it was shown that a thermal gradient can cause the outer shell to rotate (for an alternative rotation mechanism, see ref 3; for telescopic motion, see ref 4).

In this work, we demonstrate that such a device also possesses an intrinsic transduction mechanism, which is capable of efficient conversion of this rotation into electricity.

RESULTS AND DISCUSSION

In what follows, we demonstrate that the device of Figure 1 is in fact a NEMS analogue of a quantum Archimedes screw, in which rotation of the outer CNT shell pumps electrons from an electron reservoir on the left to another on the right, thus acting as a nanoscale transducer. This quantum pumping is the inverse of an effect reported recently,[5] in which a flow of electrons through a chiral CNT produces mechanical rotation.

The basic idea is that, if the two nanotubes have different chirality, the rotation of one of the tubes will produce a time-dependent potential that induces electron flow in the other. Such flow is clearly allowed by symmetry, but the question of whether or not the pumped charge is significant must be answered by quantitative

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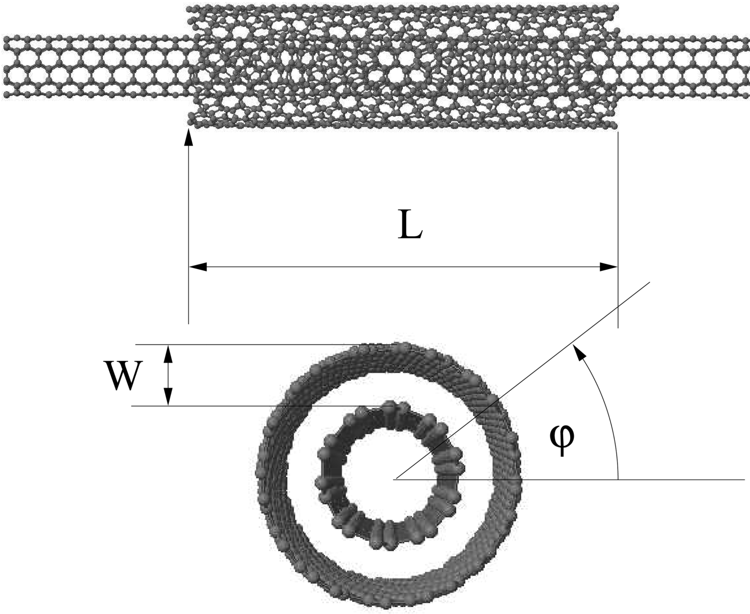

Figure 1. Device geometry used throughout our calculations. An outer nanotube of length *L* concentrically surrounds an inner tube, with an interlayer spacing *W* corresponding to the van der Waals distance ($L \approx 50$ Å, $W \approx 3.4$ Å). The inner wall remains fixed, while the outer tube is rotated about the tube axis.

calculations based on a realistic Hamiltonian. In what follows, the results of such a calculation are presented. As shown below, the proposed nanomechanical pump can operate at 30−40% of the theoretical upper limit, which makes it highly attractive as part of an energy scavenger.

Quantum pumps are time-dependent electron scatterers, which are able to transport electrons between two external reservoirs. They are adiabatic if the frequency of the pump cycle is smaller than the inverse of the characteristic time scale of the scatterer, namely, the Wigner delay time.[6] Experimental[7,8] and theoretical[9−15] studies of adiabatic quantum pumps have examined the conditions for optimal pumping and the effects of noise and dissipation. All of these devices are based on electrical pumping, whereas in this work, the proposed device is mechanically driven.

We calculate the pumped charge in the double-walled, carbon nanotube device shown in Figure 1, which mimics the experimental setup of ref 3. The inner tube is fixed, while the shorter outer tube slowly rotates. At low enough rotation frequencies, the adiabatically pumped charge is given by formulas derived by Büttiker, Thomas, and Pretre[16] and by Brouwer.[17] The details of our calculations can be found at the end of this paper and in the Supporting Information.

In the following, we present results for the pumped charge per 360° rotation for various inner and outer tubes with different chiral angles ϕ, chosen such that the interlayer distance roughly corresponds to the van der Waals distance. As an example, Figure 2 shows the pumped charge per 360° rotation for structures with the so-called (5,5) and (9,0) nanotubes as inner tubes, for a number of different Fermi energies and chiral angles of the outer tube (averaging is performed over relative positions of the two shells along the tube axis; see below). Results are plotted against the difference θ between the chiral angles of the inner and outer tubes. We find that the pumping is highest when θ is in the range of 18−20°. In carbon nanotube windmills, which are essentially the inverse of the devices studied here,[5] the anisotropy of the electronic structure (*i.e.*, the trigonal warping effect in single-walled carbon nanotubes) leads to there being a preferred angle difference between the chiral angles of the inner and outer tube. The

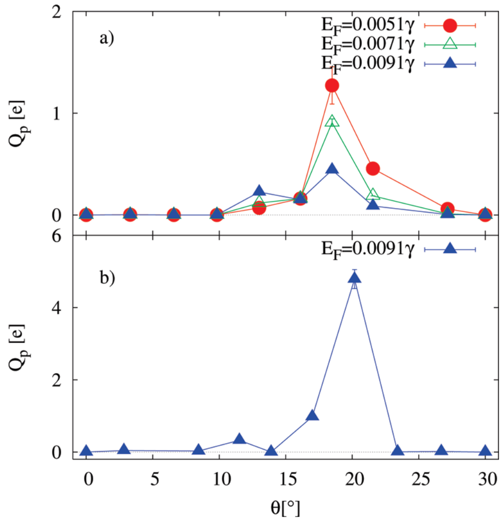

Figure 2. Average number of pumped electrons per 360° rotation with (a) (5,5) and (b) (9,0) inner CNT for different values of the chiral angle ϕ of the outer CNT. In the case of the (9,0) outer CNT, we define $\theta = \phi$. In the case of the (5,5), $\theta = 30° - \phi$. The averaging is performed over different relative positions along the tube axis. The outer CNTs used in these calculations are (10,10), (11,9), (12,8), (13,7), (14,6), (15,4), (15,5), (16,3), (17,1), and (18,0).

range of θ in the pump discussed above is close to the values which yield the largest transfer of angular momentum between tubes as electrons flow from one tube to the other in a windmill. Therefore, the most efficient windmills are also the most efficient pumps.

To check whether or not the position of the outer shell along the tube axis with respect to the inner tube has significant effect on the pumped charge, we calculated the pumped charge at 10 different nonequivalent positions. The pumped charges in Figure 2 are obtained from the average of these calculations, and the plotted error bar shows how much these values vary. This demonstrates that translating the outer tube relative to the inner tube produces only a small change in the pumped charge.

Figure 2 also reveals that the pumped charge per 360° rotation with a (9,0) inner CNT is significantly larger than that of the (5,5). This is because the (9,0) possesses a higher rotational symmetry than the (5,5). According to ref 11, the maximum pumped charge per parametric cycle of the underlying Hamiltonian is one electron per scattering channel. In our examples, a 360° rotation produces five parametric cycles in the case of (5,5) and nine cycles in the case of (9,0). This suggests that, from a practical point of view, the best inner shells for use in a carbon nanotube quantum pump are the ones with high rotational symmetry. The theoretical maximum for a 360° rotation of the (9,0) at low energies (where there are two open channels) is 18. The highest pumping found in our calculations is approximately one-third of this.

The reason why we do not get optimal pumping is very simple. The pumping effect is directly related to the intershell interaction in that pumping is driven directly by the interaction between the two shells. This means that intershell interaction works in favor of the pumping effect. However, once the pumped current starts flowing through the inner shell, reflection caused by the very same intershell interaction that generated the current will reduce the current. This is a kind of negative feedback that is inevitably present in the quantum pumps studied here. Due to this, the pumping can never be 100% efficient, and according to our results, the efficiency of nanotube-based quantum pumps caps at around 30−40% at optimal chiralities.

This, however, is an upper limit for the efficiency since it does not take into account the loss of energy invested into making the nanotube rotate. The magnitude of this loss will depend on the exact rotational mechanism. For example, rotation may be achieved by the method utilized in the work of Fennimore *et al.*,[3] in which a metal slab was attached to the outer shell and made to rotate by the use of an external field. Alternatively, the outer shell could be rotated mechanically by passing molecules, thus scavenging ambient mechanical energy. The latter method will likely have the smallest efficiency, yet it will be possibly the most desirable solution since it would be an energy scavenging tool that does not require a direct energy investment to function.

The loss of invested energy during rotation will be associated with two factors. One is the above-discussed coupling between the outer shell and whatever mechanism is used to make it rotate; the other is the friction between the inner and outer shell of the nanotube. This latter effect is known experimentally. According to ref 18, both the static and dynamic friction force is on the order of 10^{-14} N per atom. This friction is not very large and will not cause any significant losses during the operation of the pump; nevertheless, it must be taken into account when designing a particular setup for the nanotube-based quantum pump suggested in our work.

Another important question related to the efficiency is at what large frequencies one can operate the device. This is an important question because a faster operating frequency will yield a larger current. However, the frequency needs to be small enough to remain in the adiabatic limit. Our results are valid as long as the frequency of rotation is smaller than the inverse of the Wigner delay time,[6] which for the nanotubes we have studied is on the order of 10^{-11} s. This suggests that the Wigner delay does not raise any theoretical barriers before the application of the adiabatic approximation. Note, however, that electron−phonon coupling still limits the application of the adiabatic approximation, hence electron−phonon coupling will set an upper bound to the operating frequency.[21] This limit should be at very high frequencies, however (GHz−THz regime); therefore, the nanotube quantum pump should function fine at kHZ−MHz frequencies.

CONCLUSION

As detailed above, our calculations have shown that quantum pumping can be achieved by rotating the outer shell of a double-walled carbon nanotube around the inner shell. The effect is strongly chirality-dependent, and for well-chosen chiralities, the pumping effect can be a significant fraction of the theoretical upper limit. Note, however, that while our aim has been to provide a first demonstration of significant pumping in such devices and therefore we have focused on clean nanotubes in the adiabatic limit, one must address the question of technical feasibility when considering the actual construction of such a device.

A major question is whether the pumping effect is resilient to the presence of disorder. Impurities and other forms of disorder are always present in real nanotubes, and therefore, a nanotube quantum pump is only useful if disorder does not break down the pumping effect. It is known that, at least in one dimension, disorder which preserves the spatial symmetry of a lattice does not completely randomize the phase of scattering states,[19,20] and therefore, phase derivatives can be expected to retain a memory of the underlying chirality. Furthermore, in the absence of commensurability, translating the outer tube relative to the inner tube induces a range of different incommensurate scattering potentials, and as shown in Figure 2, this does not destroy charge pumping. We have performed calculations on a series of different types of defects to test the resilience to disorder (details of these calculations can be found in the Supporting Information). We have found that while on average the pumped charge is decreased by disorder, the decrease is typically less than an order of magnitude, which suggests that pumping is resilient to the presence of disorder.

Finally, let us address what is possibly the most important technical question regarding the application of nanotube-based quantum pumps as energy scavenging power sources, namely, the question of how much current can be produced by such a quantum pump. An estimate of the current I delivered by the pump is $I = enfN$ Amps, where n is the number of electrons pumped per rotation and f is the frequency of rotation. For $n = 1$ and $f = 10$ MHz, this means that the current delivered by a device is $I \approx 1$ pAmp. This current is more than sufficient to drive NEMS devices, thus carbon-nanotube-based quantum pumps are ideal candidates as nanoscale transducers of motion into electricity.

METHODS

During the calculation, we used the Landauer−Büttiker formalism to compute the transmission through the system. For the Hamiltonian H, we used a tight-binding type description of both the intramolecular and the intermolecular interaction (applying the so-called intermolecular Hückel model, as detailed in the Supporting Information). The pumping effect is obtained by first computing the Green's function $G = (E - H)^{-1}$ and the associated scattering matrix S[22,23] and then applying the formulas of Büttiker *et al.* and Brouwer,[16,17] which show that for a time-varying scatterer connected by scattering channels (labeled j) to external reservoirs, the charge Q_j pumped into the jth channel is given by $\dot{Q}_j \approx (e/h)\, E_{jj}$, where E_{jj} is the energy shift matrix as defined by $E(t,\mu) = i\hbar(\partial_t S(t, \mu))S^{\dagger}(t,\mu)$, where S is the scattering matrix and μ is the Fermi energy. The time-dependent $Q_j(t)$ carries all the information on the pumped charge; hence, once this quantity is obtained from the above equations, one can evaluate the pumping effect in detail. The explicit details of this method can be found in the Supporting Information.

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Supporting Information Available: Details on the Hamiltonian and the disorder calculations can be found in the Supporting Information, along with video files illustrating the pumping effect. This material is available free of charge *via* the Internet at http://pubs.acs.org.

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