Journal of
Computational and Theoretical Nanoscience
Vol. 4, 574–577, 2007

Carbon Nanotube Electronic Displacement Encoder with Sub-Nanometer Resolution

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Electric conductance of a telescope double-walled carbon nanotube oscillates as a function of telescoping distance. The period of such oscillation is one half of the lattice constant of graphene, $a/2 = 0.123$ nm, instead of the lattice constant a as expected. The halving of the period results from the combination of the periodic interlayer lattice alignment and the occurrence of antiresonance. When combined with the periodicity in the energy space at a fixed displacement, the telescopic displacement can be reliably and accurately determined to the sub-nanometer resolution. This effect can be used to design an electronic displacement encoder.

Keywords: Carbon Nanotube Encoder, Nanometrology, Interlayer Tunneling.

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1. INTRODUCTION

Ultrahigh precision metrology at the nanoscale, termed nanometrology, is increasingly important with the continuing development in the science and application of nanotechnology. One of the challenges facing nanometrology is the measurement of displacement or distance on the micro and nanoscale with high accuracy and high precision; another challenge is the miniaturization of the measurement devices to allow integration into practical systems. Over the years, methods and systems have been developed to achieve critical dimension measurement, such as laser interferometry, capacitive sensory, X-ray or electron diffraction, and scanning probe metrology. A promising and reliable approach is to develop a system that allows the measurement immediately traceable to accurately-defined physical constants, such as the lattice constant of crystalline material. Such a system can achieve simultaneously high measurement accuracy and precision. However, measurement systems developed based on this principle (e.g., systems based on scanning probe techniques or X-ray interferometry with graphite, mica or crystalline Si)[1–5] have so far relied on complex design and extensive engineering, and are often too large and expensive for economical industrial applications.

Recent progress in the synthesis and study of novel nanomaterials offers new opportunities and strategies in nanometrology. For example, carbon nanotubes (CNTs), with a highly graphitized nature and cylindrical structure, have been used to reveal many intriguing phenomena associated with their intrinsic lattice structure and underlying physics.[6] Scanning tunneling microscopy studies have revealed the tunable electrical contact resistance at the CNT-graphite tunneling junction by varying the lattice registry through the azimuthal rotation of CNT on graphite surface.[7] *In-situ* telescoping studies of CNTs in transmission electron microscopy[8] have observed monotonic change of resistance with telescope distance. These experimental studies were also complemented by recent theoretical works that attempt to reveal the fundamental nature of electronics states and quantum transport in double-walled carbon nanotubes (DWCNTs).[9–15] Inspired by these recent discoveries of the unique properties of DWCNTs, in this paper we describe and demonstrate an encoder nanodevice for nanometrology, that exploits the principle of interlayer tunneling physics to couple the displacement measurement with the lattice constant of graphite. Such a CNT encoder can be made small enough to fit into micro- and nanoelectromechanical systems.

2. COMPUTATIONAL SCHEME AND PHYSICAL ANALYSIS

Figure 1 illustrates the basic concept of the encoder nanodevice utilizing a DWCNT. When the DWCNT is

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1546-198X/2007/4/574/004 doi:10.1166/jctn.2007.018

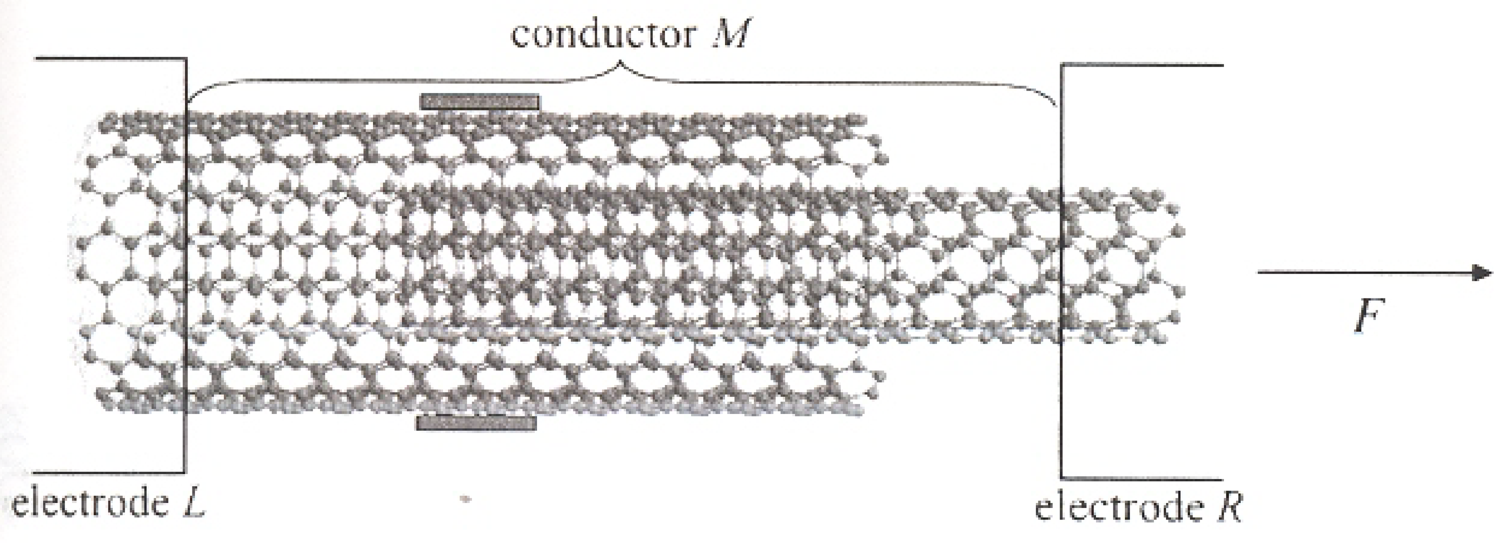

Fig. 1. The schematic diagram of an electronic displacement encoder based on telescope double-walled carbon nanotube (DWCNT). The outer wall is clamped in order to eliminate rigid-body motion; the inner wall is pulled out by imposing a uniform displacement parallel to the coaxial direction of the DWCNT at its right end. The two electrodes are connected to the outer wall and inner wall, respectively.

continuously telescoped, the lattice alignment between the layers in the double-walled segment (i.e., overlapped region in Fig. 1) is expected to vary periodically with the telescope displacement. Such a periodic variation should in principle give rise to a periodic change of the interlayer electrical conductance (G), governed by tunneling, and can be monitored and taken as the direct reading of the mechanical displacement. Surprisingly, the periodicity of conductance is one half of the lattice constant a of graphite, instead of a. We find out that the halving of the period results from the combination of the periodic interlayer lattice alignment and the antiresonance effect in the telescope DWCNT. We also find that this periodicity ($a/2$) is largely preserved even under a finite bias voltage. For the same antiresonance effect, at a fixed length of the double-walled segment, the electrical conductance changes periodically in the energy space.[15] We will exploit the periodicity in real space and energy space to design a mechanical displacement nano-encoder with sub-nanometer resolution. Besides the sub-nanometer resolution, this CNT encoder also possesses many unique features that distinguishes it from existing nanometrology systems. First, the CNT encoder is stand alone and miniaturized. Second, the conductance variation is large enough for the encoder to be functional using conventional electronics.[7,8] Finally, the double-walled structure of the CNT encoder itself provides a ready-made and friction-free mechanical guidance mechanism to ensure stable and reproducible operation.

The antiresonance[14,15] of the electron wave function in the double-walled segment will cause periodicity in real space and energy space. The effect is illustrated by a simple quantum model, as shown in Figure 2. A single transport channel (for example, the π channel in the outer wall) splits into two channels (in the double-walled segment) with wave vectors k_1 and k_2, and these two channels then recombine into a single channel (in the inner wall). In this model, due to the wave function interference, the transmission $T \propto \sin^2(\theta/2) = (1-\cos\theta)/2$.[14] The antiresonance in transmission occurs whenever

$$\theta = (k_1+k_2)L+\theta_0 = 2n\pi \tag{1}$$

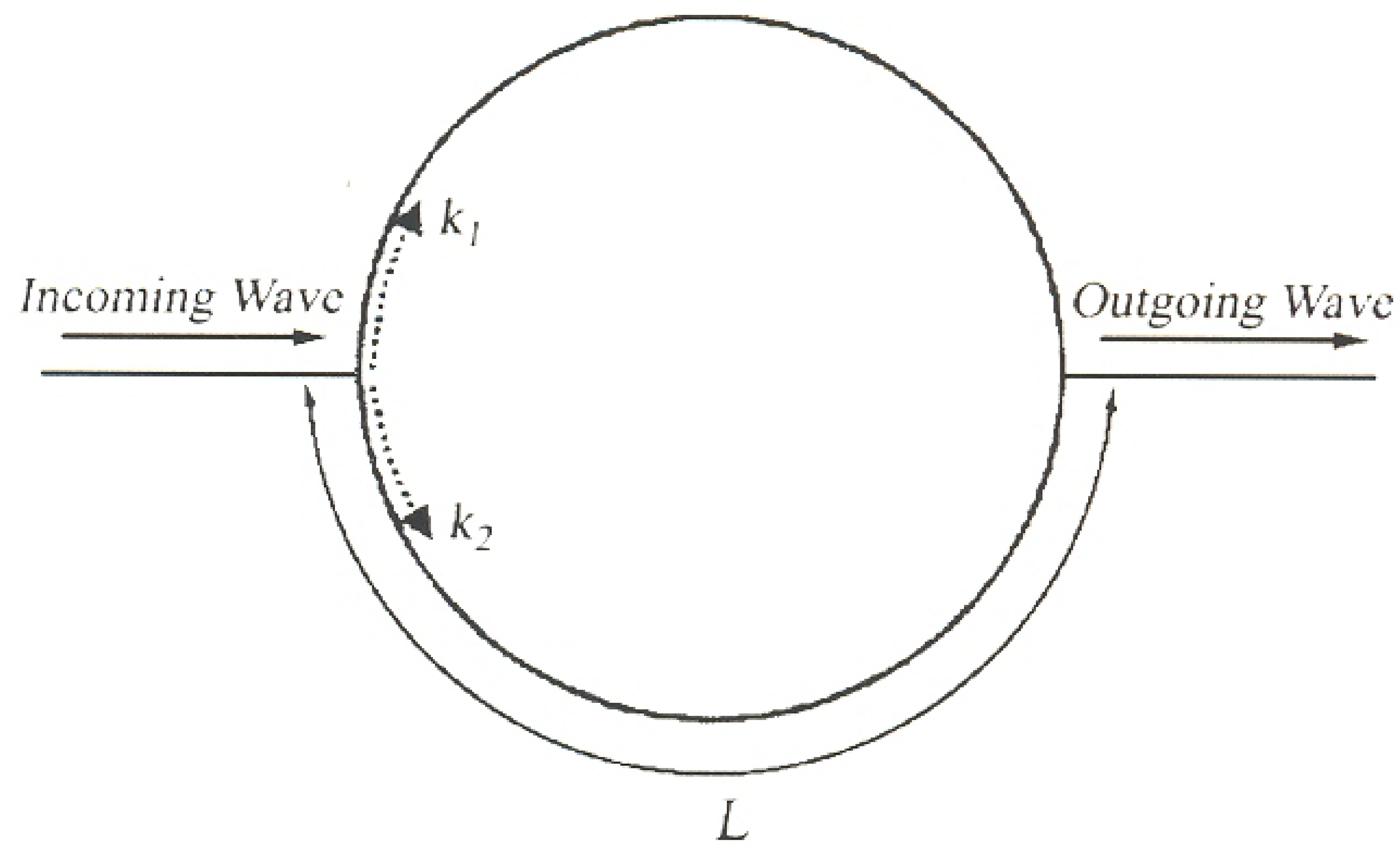

Fig. 2. A simple quantum model for the electronic transport in telescope double-walled carbon nanotube. In this model, a single incident channel splits into two channels with wave vector k_1 and k_2 in the ring and then recombine into a single channel.

where L is the length of the split channel as shown in Figure 2, θ_0 is the initial phase difference in wave functions, and n is an integer. Due to the occurrence of antiresonance, the total reflection of the incident wave leads to zero conductance across the system. The antiresonance condition, Eq. (1), also determines the formation of allowable quantum states inside the resonance region (the ring in Fig. 2), which form periodic peaks in the density of states (DOS) as we will show in our simulation results. Eq. (1) leads to conductance periodicity in real space L_p and in energy space E_p,

$$L_p = 2\pi/(k_1+k_2), \quad E_p = \frac{2\pi}{L}\frac{\partial E}{\partial(k_1+k_2)} \tag{2}$$

Periodicity in the real space in armchair/armchair telescope DWCNT—The energy dispersion relation around Fermi energy E_F for armchair CNT is characterized by two bands crossing at the Fermi wave vector $k_F(=2\pi/3a)$, $E = E_F \pm \gamma_0[1-2\cos(ka/2)]$,[20] where $\gamma_0(=2.9\ \text{eV})$ is the nearest-neighbor hopping integral for the tight-binding Hamiltonian of the CNT. In armchair/armchair telescope DWCNT, the conductance contains an antiresonance factor from Eq. (1), $G(E_F, L) = g(E_F, L)\{1-\cos[(k_1+k_2)L+\theta_0]\}$, where L is the length of double-walled segment, and k_1, k_2 can be reasonably assumed to very close to k_F. Approximately, $g(E, L)$ varies slowly with both E and L, so the periodicity of conductance is determined by $\cos[(k_1+k_2)L+\theta_0]$. This approximation is reasonable, as shown later by our simulation results. Thus, at the Fermi energy, the conductance periodicity in real space is $L_p = 2\pi/(k_1+k_2) \approx 3a/2$. Approximately, $G(E_F, L) = G(E_F, L+3a/2)$. In addition to this period, the translational symmetry along the telescoping direction provides another period a in the conductance, i.e., $G(E_F, L) = G(E_F, L+a)$. This combination of periods $3a/2$ and a for conductance leads to a new period of $a/2$, $G(E_F, L+a/2) = G(E_F, L+a/2+a) = G(E_F, L)$.

The period of $a/2$ is preserved under the effect of a small bias. Under a small bias, the current can be calculated

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from the energy integration of the conductance, $I(V,L) = (1/e)\int_{-eV/2}^{eV/2} G(E_F + E, L)\,dE = (1/e)\int_{-eV/2}^{eV/2} g(E_F + E, L)(1 - \cos\{2[k_F + \delta k(E)]L + \theta_0\})\,dE$. As $g(E,L)$ varies slowly with both E and L, $I(V,L) \approx I_0 - (\bar{g}/e)\int_{-eV/2}^{eV/2} \cos\{2[k_F + \delta k(E)]L + \theta_0\}\,dE$, where $I_0 = \bar{g}V$, and $\bar{g}$ is the average of $g(E,L)$ between $-eV/2$ and $eV/2$. From the energy dispersion relation of armchair CNT, $\delta k(E) = \frac{2}{\sqrt{3}\gamma_0 a}E$. Thus,

$$I(V,L) = I_0 - \frac{\sqrt{3}\gamma_0 a\bar{g}}{4eL}\sin\left(\frac{2eVL}{\sqrt{3}\gamma_0 a}\right)\cos(2k_F L + \theta_0)$$
$$= I_0 - I_m \cos(2k_F L + \theta_0) \qquad (3)$$

Here, I_m is a function of L with a period of $\sqrt{3}\pi\gamma_0 a/(eV)$. For $V \ll |2\pi\gamma_0/(\sqrt{3}e)| = 10.6$ V, the period of I_m is much larger than $a/2$. Thus, in the expression of $I(V,L)$, I_m is just an envelope function for the more rapidly oscillating $\cos(2k_F L + \theta_0)$ with period $3a/2$. For any value of L, one can always find a voltage V for which $I_m \neq 0$. Again, combining with the period a from the translational symmetry, the period of $a/2$ is preserved for I under a small bias voltage. On the other hand, at a fixed voltage, near the nodes of I_m at certain values of L, the $a/2$ periodicity of current I is destroyed. To avoid the nodes of I_m in measurements, one can select the bias voltage, guided by the conductance periodicity in the energy space.

Periodicity in the energy space in armchair/armchair telescope DWCNT—The second factor that we exploit is the periodicity of the conductance in the energy space. For a fixed length of the double-walled segment, the conductance changes periodically as a function of energy.[15] The two group velocities $\partial E/\partial k_1$ and $\partial E/\partial k_2$ in armchair/armchair DWCNT can be approximated by $\sqrt{3}/2\gamma_0 a$.[15] Based on the Eq. (2), we find the period of the conductance in the energy space to be $E_p = \sqrt{3}/2\pi\gamma_0 a/L$. Under a small bias, ($V \ll |\pi\gamma_0/(\sqrt{3}e)| = 5.3$ V), the differential conductance, which can be measured directly in experiments, is approximated by $G_d(V,L) = \partial I/\partial V = [G(E_F - eV/2, L) + G(E_F + eV/2, L)]/2$. Thus, the differential conductance oscillates periodically as a function of the bias voltage. From Eq. (3), the period of G_d is $V_p = (1/e)\sqrt{3}\pi\gamma_0 a/L$, which is exactly twice of E_p.

The periodicities analyzed above provide the basic principles of a displacement encoder based on the telescope DWCNT. In the following, we will illustrate these principles by telescoping a (6,6)/(11,11) DWCNT, as shown in Figure 1. The relaxed, equilibrium configuration of the telescope DWCNT is determined by molecular mechanics simulation.[16] The transport properties of the telescope DWCNT is then studied by using the tight binding[17] Green function method within the framework of the Landauer approach.[18,19]

Figure 3(a) shows the variation of the conductance G at the Fermi energy E_F in telescoping the (6,6)/(11,11) DWCNT. The conductance varies periodically between

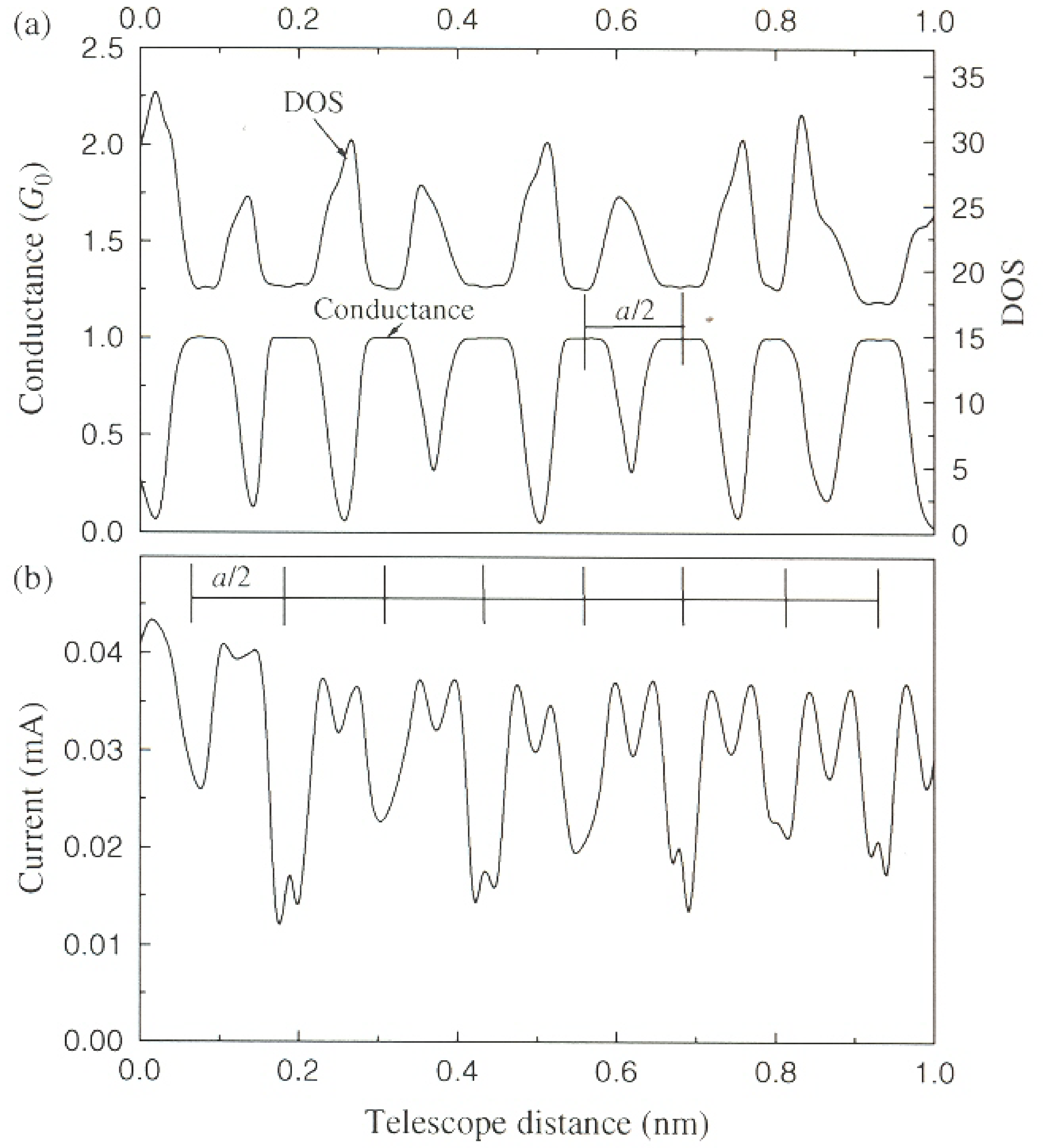

Fig. 3. Periodicity in the real space. (a) Periodic variations of electron conductance and density of states (DOS) with telescope distance for a (6,6)/(11,11) telescope double-walled carbon nanotube (DWCNT). $G_0 = 2e^2/h$. (b) Periodic variation of current for a (6,6)/(11,11) telescope DWCNT under an external bias of 0.5 V.

0 and 1, in unit of the quantum conductance $G_0(=2e^2/h)$, as the inner wall is pulled out continuously, showing an ON/OFF transport behavior. The variation has a stable period of 0.123 nm, corresponding to one half of the lattice constant a of graphite ($a = 0.246$ nm), as predicted by our theoretical analysis. The peak-valley correlation of the DOS and conductance in Figure 3(a) is the typical characteristics of the antiresonance effect. The robustness of the $a/2$ period is demonstrated in Figure 3(b), which shows that the current under a bias voltage of 0.5 volts exhibits the same period. This result implies that the CNT encoder is capable of achieving stable and reproducible measurements.

In Figure 4, we show the calculated period V_p for the differential conductance as a function of the length L of the double-walled segments. The fitting curve from the calculated results yields $V_p = 3.84$ V $\cdot$ nm$/L$, which is in excellent agreement with the prediction based on the earlier theoretical analyses, which yields $(1/e)\sqrt{3}\pi\gamma_0 a = 3.88$ V $\cdot$ nm. Thus, besides the voltage selection as mentioned above, the measurement of the period in the differential conductance dI/dV as a function of the voltage can be used to estimate the absolute value of the displacement L. This complements the measurement of the real space period which yields a relative displacement but with a higher accuracy. The combination of these two measurements together, provides an innovative application of the telescope DWCNT as a sub-nanometer resolution

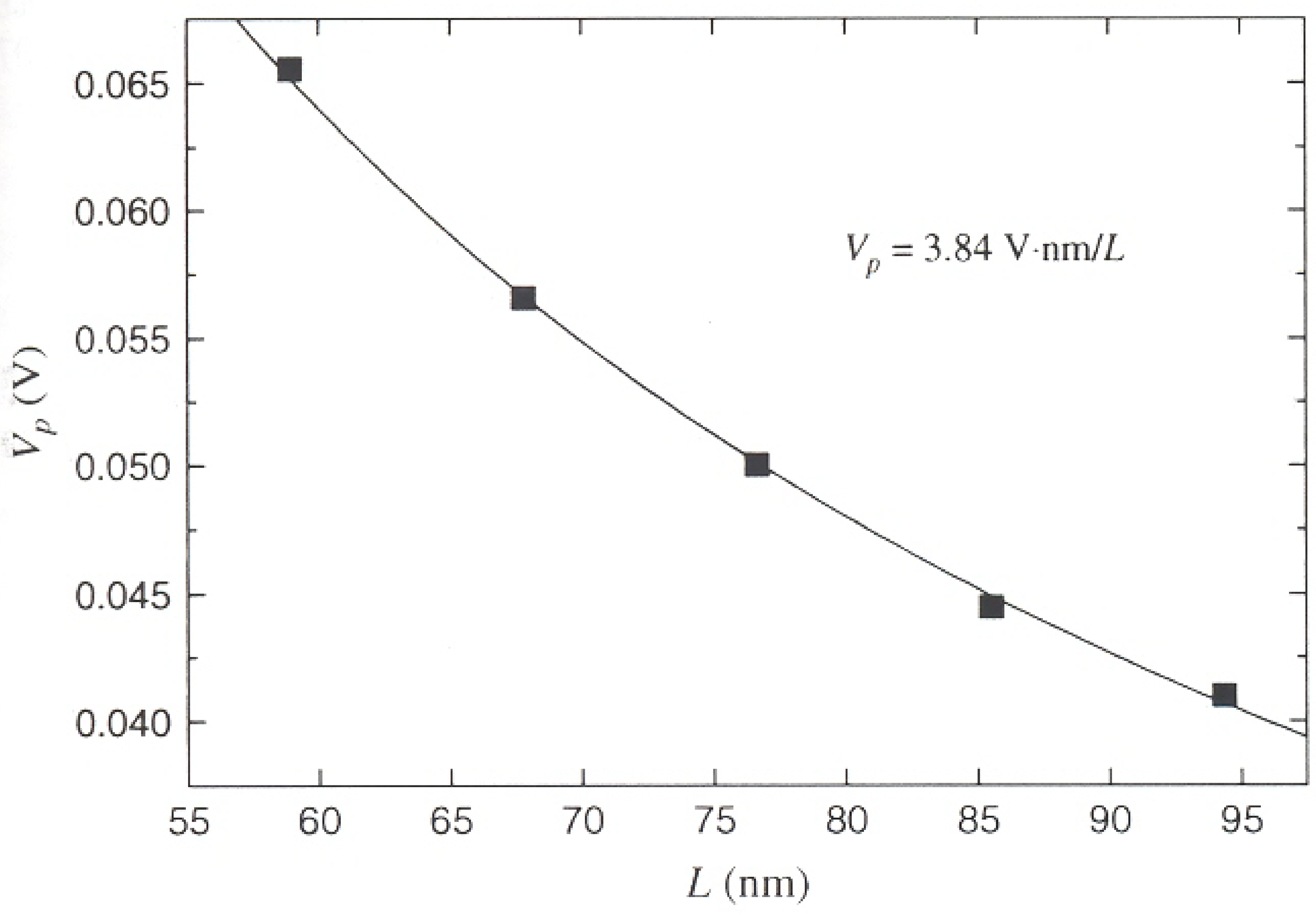

Fig. 4. Periodicity in the energy space. The differential conductance periodicity as function of length of double-walled segments for a (6,6)/(11,11) telescope double-wall carbon nanotube.

displacement encoder which produces absolute displacement measurements traceable to a physical constant.

3. CONCLUSION

In conclusion, the unique transport behaviors in telescope DWCNT revealed in this study, especially the $a/2$ period oscillation of current and the length dependent period oscillation of differential conductance, present fascinating opportunities for the engineering of a new class of nanometrology devices. Such devices, besides being physically small and mechanically robust, also possess intrinsic measurement traceability to a physical constant (the lattice constant of graphite), and thus represent the ultimate nanodevices for high precision nanometrology. Though the nanoencoder is modeled on a (6,6)/(11,11) telescope DWCNT, our reasoning is valid also for other armchair/armchair telescope DWCNTs, such as (5,5)/(10,10) telescope DWCNT. The recent experimental demonstration[8] of a variable resistance telescope DWCNT rheostat strongly indicates the promising realization of the nanoencoder. To date, fine-scale telescope distance adjustment (down to sub-nanometer) has not been performed, so the periodic conductance oscillation has yet to be observed experimentally.

Acknowledgments: Part of this research was conducted at the CNMS sponsored at ORNL by the Division of Scientific User Facilities and by the Division of Chemical Sciences, US DOE. H. J. acknowledges the financial support from the Fulton School of Engineering at ASU. M.-F. Y. acknowledges the supports from NSF NSEC Nano-CEMMS (DMI-0328162) and NSF CCF-0508416. Y. H. acknowledges the supports from the NSF through Nano-CEMMS (grant no. DMI 03-28162) at the University of Illinois and ONR Composites for Marine Structures Program (grant N00014-01-1-0205, Program Manager Dr. Y. D. S. Rajapakse).

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Received: 28 August 2006. Accepted: 10 September 2006.