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Contact resistance between carbon nanotubes

Alper Buldum and Jian Ping Lu
Department of Physics and Astronomy, The University of North Carolina at Chapel Hill, Chapel Hill, North Carolina 27599
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Fascinating properties of nanotubes arise when they form intermolecular junctions. In this rapid communication, we demonstrate that such nanotube junctions have atomic scale characteristics and the contact resistance between the tubes depends strongly on atomic structure in the contact region. Our calculations show that the optimal electronic transport between nanotubes occurs when the tubes are in atomic scale registry. The contact resistance can vary several orders of magnitude with atomic scale movements. Phenomena such as the negative differential resistance and nonlinear variation of resistance are found. These properties may lead to new device applications.

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Individual carbon nanotubes are perfect molecular wires with well-known structural, electronic, and transport properties.[1–8] Nanoscale contacts can be formed with two or more nanotubes. In this rapid communication, we present fascinating properties of nanotubes when intermolecular nanotube junctions are formed. It is demonstrated here that these nanotube junctions have atomic scale characteristics and the contact resistance depends strongly on the atomic structure in the contact region. The optimal electronic transport between the nanotubes occurs when the tubes are in the atomic scale registry. It is also found that the contact resistance can vary several orders of magnitude with atomic scale movement. In some configurations the intermolecular conductance is comparable to that of perfect nanotubes. Phenomena such as the negative differential resistance and nonlinear variation of resistance with the contact area are found. The large variation of transport properties found here is similar to the sensitive dependence of mechanical-frictional properties on atomic scale registry.[9,10] These unusual properties may lead to new nanoelectronic device applications.

Several techniques have been used to calculate the quantum conductance of carbon nanotubes.[8,12–15] Among these the Green's-function technique is effective and efficient when localized orbital basis sets are used.[8,14,15] In our calculations, the Landauer-Büttiker formalism is employed to calculate the conductance and the I-V characteristics with the surface Green's-function matching method.[15,16] In this formalism the current on terminal i can be written as[17]

$$I_i=\frac{2e}{h}\int_{-\infty}^{\infty}\overline{T}_{ij}(E,V)[f_i(E)-f_j(E)]dE, \qquad (1)$$

where $\overline{T}_{ij}(E,V)$ is the transmission coefficient from terminal i to j and $f_i(E)$ is the Fermi function for terminal i. In the presence of an applied bias, the energy levels are shifted and $\overline{T}_{ij}(E,V)$ is modified. The electronic structure and interactions between nanotubes are modeled using the π-orbital tight-binding Hamiltonian.[18,19] Our conductance calculations are based on single-particle linear-response theory. Thus, electron-electron interactions are not included. As nanotubes are perfect one dimensional quantum wires, the e-e interaction effects may be important. For nanotubes, these were shown to be low energy effects (<1 meV).[20,21] Further investigations may be required for these low energy regimes.

Intermolecular nanotube junctions can be formed in many geometrical forms. For example, two tubes can be connected in parallel, perpendicular, or two tubes ends can be brought together. We have studied the quantum conductance and current-voltage characteristics of these junctions for different nanotube positions, orientations and chiralities. The simplest two-terminal nanotube junction is constructed by bringing two tubes' ends together [see Fig. 1(a)]. This junction consists of two semi-infinite tubes in parallel and pointing to opposite directions. The equilibrium positions of these two nanotubes are found using molecular dynamics.[9] In equilibrium positions the tubes are in atomic scale registry and the contact region structure is like the A-B stacking of graphite. As the contact (or interaction) region is finite this junction shows quantum-interference effects. The interference of waves transmitted and reflected from the ends of the tubes yields resonances in electron transport as shown in Fig. 1(b). The number of resonances increases with increasing contact length, l. This quantum-interference effect introduces the negative differential resistance (NDR) in the current-voltage characteristics [shown in Fig. 1(c)]. NDR has many applications including high-speed switching, memory, and amplification.[22]

An interesting feature of this junction is the sensitive dependence of conductance on the contact length, l. Figure 2 shows the conductance values for armchair-armchair and

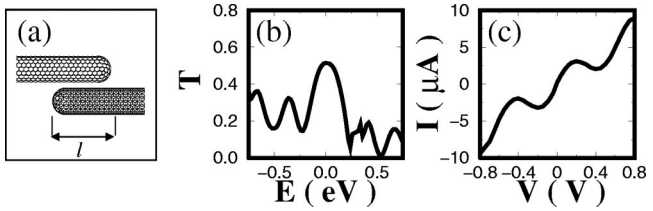

FIG. 1. (a) A two-terminal nanotube junction can be formed by bringing two tubes' ends together in parallel and pointing opposite directions (l is the contact length). (b) The transmission coefficient T of the two armchair tube [(10,10)-(10,10)] junction as a function of energy E for $l=64$ Å. Interference of electron waves yields resonances in transport. (c) Current-voltage characteristics of the (10,10)-(10,10) junction for $l=46$ Å.

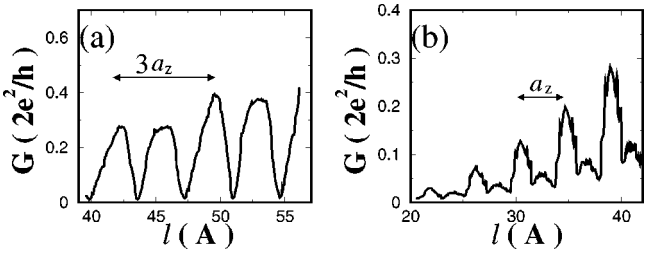

FIG. 2. (a) The variation of conductance at the Fermi energy as a function of contact length, l for the (10,10)-(10,10) junction. Each pair of peaks form a period with length $3a_z$ ($a_z=2.46$ Å unit-cell length of armchair tubes). (b) Variation of conductance with l for the (18,0)-(18,0) junction. The period is the unit-cell length ($a_z=4.26$ Å) for zigzag tubes.

zigzag-zigzag tube junctions. In both cases the dependence of conductance on l is nonlinear and quasiperiodic but the periods are different. In the armchair tubes' case [Fig. 2(a)] the period is $3a_z$ ($a_z=2.46$ Å, unit cell length of armchair tubes), which is the Fermi wavelength for armchair tubes. The same periodicity was found in earlier experiments and theoretical calculations on the scanning tunneling microscopy images of finite nanotubes.[23] In zigzag tubes' case, however, the period is found to be the unit cell length ($a_z=4.26$ Å). As the Fermi wavelength for zigzag tubes is infinite, only atomic corrugation is responsible for the variation of conductance.

It is also interesting to note that the conductance values are high and comparable to ideal tubes when the tubes are in-registry. Therefore, this simple end-end contact geometry is an ideal way of connecting multiple tubes in device applications. On the other hand, small displacements of tubes from the in-registry configurations lead to dramatic reduction in the intertube conductance. Thus, rapid switching between high and low conductance states can be achieved and fast atomic scale switches can be constructed by using these end-end junctions. We also have investigated a mixed junction of an armchair (10,10) and a zigzag (18,0) tube. In this case, the conductance values are an order of magnitude smaller with no apparent periodic variations.

A four-terminal junction can be formed by placing one nanotube perpendicular to another as shown in Fig. 3(a). Multiprobe measurements can be performed on this junction[11] with current passing two terminals and voltage measured using the other two. We find that the conductance between the tubes depends strongly on the atomic structure in the contact region. The conductance is high when two tubes are in-registry where atoms from one tube are placed on top of another like A-B stacking of graphite. Thus, an armchair tube crossing a zigzag tube forms an in-registry junction and the conductance is high. In contrast two perpendicular armchair tubes forms an out-of-registry junction, the conductance between the tubes is low.

In general, different transport properties can be achieved by manipulating these junctions such as rotating or translating one of the tubes with respect to the other. In Figs. 3(b) and 3(c) the variations of contact resistance with respect to rotation angle Θ between the tubes is presented. A large variation of resistance is observed. Lower resistance values

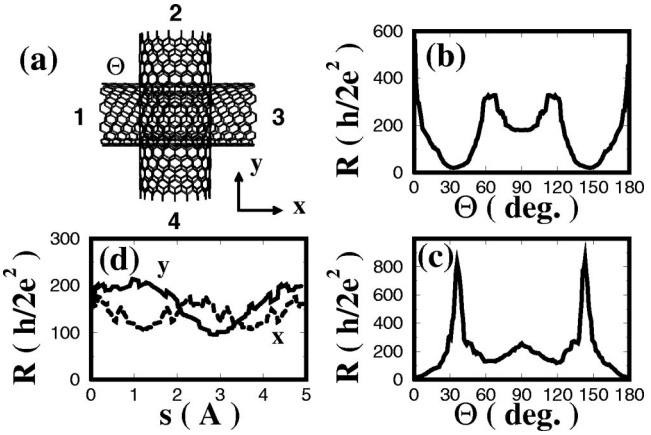

FIG. 3. (a) A model of four-terminal junction formed by crossing two nanotubes. The terminal labels, rotation angle, Θ and the translation directions are shown. The tubes are considered to be rigid. The current is passing between 1 and 4 and voltage is measured between 2 and 3. (b) Contact resistance of the (18,0)-(10,10) junction as a function of rotation angle Θ. The tubes are in-registry at $\Theta=30,90,150°$. (c) Resistance of the (10,10)-(10,10) junction. The tubes are in-registry at $\Theta=0,60,120,180°$. (d) Resistance of the (18,0)-(10,10) junction as functions of translation of one tube relative to the other in the x and y directions.

are found when the junction is in-registry configurations. In the case of the (18,0)-(10,10) junction the tubes are in-registry at $\Theta=30,90,150°$. In the (10,10)-(10,10) junction the tubes are in-registry at $\Theta=0,60,120,180°$. Even when the tubes are in-registry the contact resistance can be different at different Θ due to change in the contact area. For example, in the (18,0)-(10,10) junction, the resistance is lower at $\Theta=30°$ than at $\Theta=90°$ as the contact area at $\Theta=30°$ is larger. In Fig. 3(d), the variation of resistance with the translation of upper tube is shown for the (18,0)-(10,10) junction. The variation is small in comparison to the case of rotating the tubes. The lowest resistance is achieved when the contact structure is like A-A stacking of graphite.

When the junctions are placed on a substrate, electronic contact can be significantly enhanced by the structural relaxation of the tubes and adhesion between tubes and the substrate. We investigate the effect of relaxation by performing molecular dynamics simulations using empirical potentials.[24] The cross junction is relaxed on a rigid surface[25] and constant forces (3.0 nN) are applied to the ends of the upper tube (of length 127 Å) to simulate the effect of substrate adhesion. An example of relaxed junction is shown in Fig. 4(a). Current-voltage characteristics of rigid and relaxed cross junctions are presented in Figs. 4(b) and 4(c) for two different nanotube junctions. We found that, when tubes are in-registry, the resistance drops dramatically with relaxation and/or applying forces. In contrast, when the tubes are out of registry, the change in resistance with relaxation and/or applying forces is small. For example, in the case of the (18,0)-(10,10) (in-registry) junction [Fig. 4(b)] the resistance is 2.05 MΩ for rigid tubes but reduced to 682 KΩ after relaxation. When forces are applied the resistance drops to 121 KΩ. On the other hand, two perpendicular (10,10) tubes are out of registry [Fig. 4(c)], the resistance between

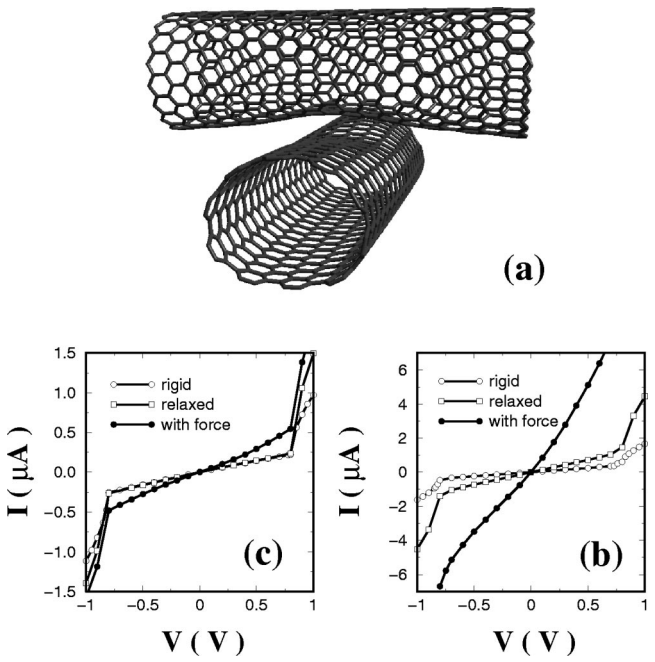

FIG. 4. (a) An example of the relaxed cross junction with applied forces. Deformation in the contact region can be clearly seen. The tubes are 127 Å long and only the central part of the junction is shown here. (b) *I-V* characteristics of a (18,0)-(10,10) (in-registry) cross junction. The resistance value for the rigid case is 2.05 MΩ, but decreases to 682 KΩ with relaxation and to 121 KΩ with force. (c) *I-V* characteristics of a (10,10)-(10,10) (out-of-registry) cross junction. The resistance values are 3.36, 3.21, and 1.66 MΩ for a rigid, relaxed without force and relaxed with force cases.

tubes is 3.36 MΩ for the rigid junction and decreases to 3.21 MΩ when the junction is relaxed. Applying forces reduces the resistance to 1.66 MΩ.

The contact resistance we have calculated is in good agreement with recent experiment[11] which found 90–360 KΩ resistances for metal-metal cross junctions on a surface. Our results suggest that modest pressure and/or force can dramatically enhance the intertube transport if the tubes are in-registry.

The low contact resistance in the case of in-registry configurations can be understood considering the coupling of electronic states between the tubes. Strong coupling occurs when the tubes are in-registry. Although the magnitudes of individual hopping integrals between the atoms on different tubes are similar for in-registry and out-of-registry junctions, phase coherence is achieved in the in-registry junction which enhances the coupling of the electronic states between the tubes.

We have also investigated the dependence of the contact resistance on nanotube size and found that the resistance increase with tube diameter. This effect is due to the fact that the two conducting channels of the nanotube are extended states around the whole circumference. Increasing the tube size, though increasing the geometrical contact area, in fact reduces the relative weight of conducting channel wave function around the contact. However, we found the effect of relaxation and forces are more dramatic for larger tubes as they are more susceptible to deformation.

In conclusion, quantum transport properties of intermolecular nanotube junctions are investigated. We find that nanotube junctions have atomic scale characteristics in their transport properties and the contact resistance strongly depends on the atomic structure in the contact region. The optimal electronic transport between nanotubes occurs when the tubes are in atomic scale registry. The contact resistance can vary several orders of magnitude with atomic scale manipulations. The negative differential resistance is found in nanotube end-end contacts. Similar properties may be found in the contacts of other nanoscale wires and structures. These unusual properties may lead to new atomic scale switches, resistors, amplifiers, and memory devices.

Note added: Recent experiments[26] performed at UNC-Chapel Hill found that the contact resistance between nanotube and graphite varied more than an order of magnitude by changing the angular alignment between tube and graphite lattice, similar to the effects predicted in this article.

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