# Coupling of carbon nanotubes to metallic contacts

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## Abstract

The modeling of carbon nanotube-metal contacts is important from both basic and applied view points. For many applications, it is important to design contacts such that the transmission is dictated by intrinsic properties of the nanotube rather than by details of the contact. In this paper, we calculate the electron transmission probability from a nanotube to a free electron metal, which is side-contacted. If the metal-nanotube interface is sufficiently ordered, we find that k-vector conservation plays an important role in determining the coupling, with the physics depending on the area of contact, tube diameter and chirality. The main results of this paper are: (i) conductance scales with contact length, a phenomena that has been observed in experiments and (ii) in the case of uniform coupling between metal and nanotube, the threshold value of the metal Fermi wave vector (below which coupling is insignificant) depends on chirality. Disorder and small phase coherence length relax the need for k-vector conservation, thereby making the coupling stronger.

**Introduction**: Carbon nanotubes represent an intriguing new material that has attracted much attention both from theorists and experimentalists since the early 1990s.[1] Particularly exciting is the possibility of one dimensional metallic conductors at room temperature that can be used as a probe in scanning probe microscopy or as a low resistance ballistic interconnect for electron devices.[2–4] From a more basic point of view, much can be learnt about the physics of conduction by studying the conductance of such a one dimensional conductor at low temperatures. To exploit these possibilities it is important to understand the physics of the nanotube-metal contacts and to experimentally demonstrate low resistance contacts in a reproducible manner. The contact between carbon nanotubes and metal can occur at the end of the tube (end-contact)[5,6] and along the circumference of the tube (side-contact)[2,7,8]. The low contact resistance in Refs. 5 and 6 are due to strong interaction between metal and carbon atoms at the end of the nanotube, or/and due to lack of tranlational symmetry.[9] From a more basic view point, transport through end-contacted nanotubes with caps show interesting effects due to localized states.[10] In comparison, the interaction between metal and carbon atoms in side-contaced nanotubes is weak. The metal can make contact to carbon atoms located either over a sector[2] or the entire circumference of the nanotube.[8]

Recently, Tersoff in a perceptive paper[9] qualitatively discussed the importance of k-vector conservation in nanotube transport experiments. For free electron like metal contacts, the important physical quantities are the diameter and chirality of the nanotube, Fermi wave vector of the metal, area of contact, and details of the metal-nanotube contact. In this paper, we study the physics of side-contacted nanotube-metal contacts relevant to these experiments[2,8] along the lines of Ref. 9 by addressing how these physical quantities affect the transmission of electrons from the nanotube to the metal contact. For small diameter nanotubes, our conclusions do not fully agree with Ref. 9. Our calculations also show that the condutance scales with contact length, a phenomena that has been observed experimentally in references 2 and 8. In the remainder of the paper, we first discuss the salient results using simple arguments. We then present results from numerical calculations to support these

arguments.

**Basic idea**: The first Brillouin zone of graphene touches the Fermi surface at six points. Of these only two points are inequivalent (that is, do not differ by a reciprocal lattice vector). The conduction properties of graphite at low bias are controlled by the nature of eigen states around these points. Consider a metal making uniform contact to graphene. The in-plane wave vector should be conserved when an electron tunnels from the metal to the nanotube. As a result, for good coupling between metal and graphene, the metal Fermi wave vector should be comparable to $4\pi/3a_0$, which corresponds to the Fermi wave vector of graphene. $a_0$ is the lattice vector length of graphene.

To discuss the case of nanotubes making contact to metal, we consider the scattering rate $(1/\tau_{c-m})$ from the metal to nanotube within the Born approximation,

$$1/\tau_{c-m} \propto < \Psi_c | H_{c-m} | \Psi_m > \ , \tag{1}$$

where, $\Psi_m$ ($\Psi_c$) is the metal (nanotube) wave function and $H_{c-m}$ represents the nanotube-metal coupling. The wave function of an (n,m) nanotube is, $\Psi_c = e^{ik_t pu}\phi_c$, where $k_t$ is the axial wave vector, $u$ is the 1D unit cell length, $p$ is an integer representing the various unit cells and $\phi_c$ is a vector representing the wave function of all atoms in a unit cell. It is assumed that the wave function of the metal is separable in the axial and radial directions of the nanotube, $|\Psi_m >= e^{ik_m pu}|\phi_m >$, where $k_m$ is the metal wave vector component along the nanotube axis. When the coupling between the nanotube and metal is uniform, the scattering rate is [Eq. (1)],

$$1/\tau_{c-m} \propto t_{c-m} < \phi_c | \phi_m > \sum_p e^{i(k_m - k_t)pu} \ , \tag{2}$$

where, the summation is performed over all unit cells making contact to metal and $t_{c-m}$ represents a uniform coupling constant between the metal and nanotube. It is clear from Eq. (2) that provided the metal and nanotube make contact over several unit cells, wave vector conservation along the axial direction is enforced as $\sum_p e^{i(k_m - k_t)pu} \sim \delta(k_m - k_t)$. The axial wave vector corresponding to $E = 0$ are $2\pi/3a_0$ and 0 for armchair and zigzag

tubes respectively, and the wave vector for other chiralities varies between these two limits. As a result, the threshold value of Fermi wave vector below which coupling between an armchair (zigzag) nanotube and metal is poor is $2\pi/3a_0$ (0). The threshold value of the metal Fermi wave vector for chiral tubes is in between that of zigzag and armchair tubes. As the diameter of the nanotube increases, wave vector conservation along the cirumference also becomes important, as the strip approaches a graphene sheet.

**Method**: The method used to calculate transmission is the same as that in reference 4, with the only addition being the connection of a metal contact.[11] The metal contact has a rectangular cross section and is infinite in the third dimension [Fig. 1]. Such a geometry is similar to the experimental set up in reference 2. A perfectly cylindrical nanotube would touch the metal surface only along a line. To simplify modeling this interface, we stretch the entire circumference of the nanotube over the metal surface. The surface Green's function of the metal is calculated within the free electron approximation using standard procedures and the strength of the nanotube-metal coupling used are given in Table 1. The transmission and local density of states are calculated in a structure that can be conceptually divided into four parts: section of the nanotube (D), which lies on the metal electrode (M), semi-infinite regions of the nanotube L and R [Fig. 1]. The Hamiltonian of the system can be written as,

$$H = H_c + H_m + H_{c-m} \text{ and} \tag{3}$$

$$H_c = H_D + H_L + H_R + H_{LD} + H_{RD} \tag{4}$$

where, $H_c$ is the pi-electron tight binding Hamiltonian of the nanotube. $H_{LD}$ and $H_{RD}$ are terms in the Hamiltonian coupling D to L and R respectively. $H_m$ and $H_{c-m}$ are the free particle and nanotube-metal coupling terms of the Hamiltonian. The Green's function $G^r$ is obtained by solving: $[E - H_D - \Sigma_L^r - \Sigma_R^r - \Sigma_m^r]\, G^r(E) = I$, where the self energy $\Sigma_\alpha = 2V_\alpha^\dagger\, g_\alpha^r\, V_\alpha$ ($\alpha \in$ **L**, **R** and **M**). $g_\alpha^r$ is the surface Green's function of terminal $\alpha$. The transmission probability $[T_{\alpha\beta}]$ is given by,

$$T_{\alpha\beta}(E) = Trace[\Gamma_\alpha(E) G^r(E) \Gamma_\beta(E) G^a(E)]\ , \tag{5}$$

where, $\alpha$ and $\beta$ represent two different terminals across which transmission is calculated and $\Gamma_\alpha = 2V_\alpha^\dagger \, Im[g_\alpha^r] \, V_\alpha$ is the coupling to terminal $\alpha$. Finally, this is a non self-consistent calculation.

**Results and Discussion**: We first present results for dependence of the threshold value of the metal Fermi wave vector on chirality, using armchair and zigzag tubes connected to the metal contact. We then discuss the dependence of the diameter dependence of conductance using the case of a zigzag tube as an example. Finally, the case of disorder in coupling between the nanotube and metal is considered. We consider only weak coupling between the nanotube and metal. The average value of the diagonal elements of the coupling strength $\Gamma_M$ are tabulated in Table 1 for the various values of the metal Fermi wave vector considered. We calculate the transmission versus contact length between nanotube and metal for various Fermi wave vectors in the metal and all atoms around the circumference of the tube are assumed to make uniform contact with the metal. We emphasize that our results are also fully valid in the case where only a sector of atoms along the cirumference of the nanotube make contact to the metal such as in Ref. 2.

In the case of armchair tubes, when the metal Fermi wave vector $k_f$ is smaller than $2\pi/3a_0$ ($0.85\mathring{A}^{-1}$), $T_{ML}$ does not change significantly with contact length as shown for $k_f = 0.75\mathring{A}^{-1}$ in Fig. 2(a). For values of $k_f$ above the threshold, the transmission monotonously increases with an increase in contact length. The monotonic increase is due to weak metal-nanotube coupling, in which case an increase in contact length simply results in an increase in the transition probability to scatter from metal to nanotube.[12] The transmission will eventually saturate with increase in contact length as there are only two conducting modes at the band center. For the configuration considered [Fig. 1], $T_{ML}$ can have a maximum value of unity. The second feature of Fig. 2(a) is the increase in transmission with increase in $k_f$. This can be understood by noting that electrons with a wave vector component along the nanotube axis that is larger than $2\pi/3a_0$ scatter from the metal to nanotube, and a larger $k_f$ implies a large number of available metal electron states. For the purpose of these calculations, we considered a (2,2) armchair tube; The essential physics would in principle be true for the

more realistic (10,10) nanotube also.

The case of zigzag tubes is different because bands at $E = 0$ cross at $k = 0$. Then, electrons in the metal electrode with any $k_f$ (no threshold) can scatter into a metallic zigzag tube. The results for a (3,0) tube are shown in Fig. 2(b). Here, there are two important points. The first point is that as there is no threshold metal Fermi wave vector, the transmission increases monotonically with contact length even for $k_f = 0.4\mathring{A}^{-1}$. The second point is that the transmission for $k_f$ equal to $0.75\mathring{A}^{-1}$ and $1.2\mathring{A}^{-1}$ are much smaller than that for armchair tubes [Fig. 2(a)]. The is because the nanotube wave vector around the circumference ($k_c$) of a zigzag tube is large, $k_c = 4\pi/3a_0$ for the crossing bands and this has the effect of making the overlap integral [Eq. (1)] small at E=0. As $k_f = 1.75\mathring{A}^{-1}$ is larger than the threshold for graphite, the transmission probability is larger, and comparable to that for armchair tubes [Fig. 2(b)].

What happens when the diameter increases? In the limit of large diameter, a nanotube is akin to graphene and the threshold $k_f$ to couple well with metal should approach $4\pi/3a_0$. Numerically, it is difficult to simulate a large diameter tube due to problems associated with the time and memory required to calculate $g_M^r$. So we instead compare a zigzag tube of two diameters to convey this point. Fig. 3 compares the transmission versus contact length of the (3,0) and (6,0) nanotubes; The (6,0) nanotube has double the diameter of the (3,0) nanotube. The (6,0) correspondingly has a smaller transmission and the trend of decrease in transmission will continue with further increase in diameter. Infact for large diameters, as the diameter increases the threshold value of $k_f$ is expected to change to $4\pi/3a_0$ in a manner that depends inversely on the nanotube diameter.

We now address the role of disorder. Disorder in either the nanotube, metal or nanotube-metal coupling will in general result in larger transmission when compared to the disorder-free case. Wave vector conservation is relaxed due to scattering from defects and transmission will increase with increase in contact length *even when the metal $k_f$ is below the threshold value*. We consider the case of disorder in nanotube-metal coupling ($H_{c-m}$). Disorder in all elements of the coupling between the nanotube and metal was introduced randomly. The

disorder in coupling of atom $i$ to the metal contact can be written as, $t_i = \alpha t^{av} + (1-\alpha) t_i^{rand}$, where $t^{av}$ is the average value of $t_i$ over all sites connected to the metal and $\alpha$ is a fraction between zero and unity. $t_i^{rand}$ is the random component whose average is equal to $t^{av}$. In Fig. 2(b), the two strengths of disorder correspond to $\alpha = 0$ and $\alpha = 0.5$ (smaller $\alpha$ corresponds to larger disorder), such that $t^{av}$ has the same value as that in Fig. 2(a). For an armchair tube in contact with a metal with $k_f = 0.75\mathring{A}^{-1}$, the transmission was very small and more importantly did not vary with contact length [Fig. 2(a)]. Introducing disorder changes this trend and causes a monotonic increase in transmission with length of contact [Fig. 4]. Similarly, for large diameter tubes, in the presence of disorder there should be significant transmission when $k_f$ is smaller than the threshold $4\pi/3a_0$. The requirement of wave vector conservation is also relaxed when the phase coherence length is small. So we expect the coupling to improve with decrease in phase coherence length.

**Conclusions**: In this paper, we addressed some aspects of the physics of a nanotube side-contacted to metal, a problem of current importance. The main result is that coupling of carbon nanotubes to metal depends on both chirality and diameter. Wave vector conservation of an electron scattered from the nanotube to metal plays a central role in determining the properties. The difference between small and large diameter nanotubes is that while in the former wave vector conservation is important only in the axial direction, in the latter it is important in both the axial and circumferential directions. As a result, small diameter armchair and zigzag tubes have a cut-off value of the metal Fermi wave vector equal to $2\pi/3a_0$ and zero, respectively. For chiral tubes, the cut-off value of the metal Fermi wave vector lies in between these two limits, with the value decreasing with increase in chiral angle. A large diameter nanotube is akin to a graphene sheet and the cut-off value of the metal Fermi wave vector in this case approaches $4\pi/3a_0$ with increase in diameter. Disorder in the metal, nanotube or their coupling relaxes the requirement of k-vector conservation and in general improves coupling. The groups of references 2 and 8 have shown increase in conductance with contact length. In this paper, we discussed two situations that could lead to this. The first situation requires the metal Fermi wave vector to be larger than the

threshold discussed and holds even when there is no disorder. The second situation requires disorder in coupling to the metal but there is no restriction on the value of the Fermi wave vector.

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[11] For a complete description of the formulation see: S. Datta, Electronic Transport in Mesoscopic Systems, Cambridge University Press, Cambridge, U.K (1995).

[12] Note that if the nanotube-metal coupling is strong, then the transmission probability would reach its maximum by contacting just only a few layers along the length. Further

increase in contact length will not result in a monotonic increases in transmission with contact length.

FIGURES

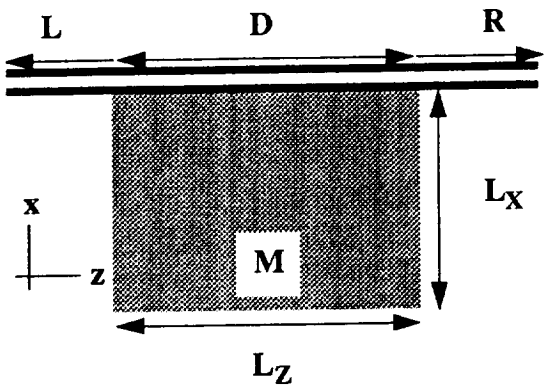


Fig. 1: A metal making contact to a nanotube. The $(x, z)$ dimensions of the metal form a rectangular cross section with lengths $(L_x, L_z)$. The $y$ direction is infinitely long.

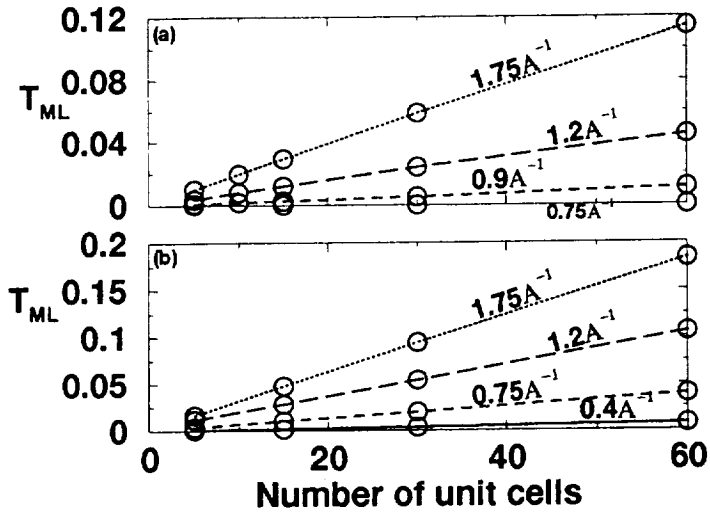


Fig. 2: Transmission probability for (a) armchair and (b) zigzag tubes versus contact length in number of unit cells of the nanotube. (a) The main point here is that for the metal Fermi wave vector smaller than the threshold $2\pi/3a_0$, coupling between the nanotube and metal is small and increasing the contact length does not change the transmission probability. For metal Fermi wave vector larger than $2\pi/3a_0$, the transmission probability increases with increase in contact length and also with increase in $k_f$ for a given contact length. (b) The main point here is that there is no threshold in the metal Fermi wave vector. Even in the case of a small value of the metal Fermi wave vector ($0.4\AA^{-1}$), the transmission increases with increase in the contact length, albeit the magnitude of transmission is small. As in the armchair case, the transmission probability increases with increase in $k_f$ for a given contact length. The $k_f = 0.4, 0.75$ and $1.2\AA$ values of $T_{ML}$ have been multiplied by ten times their real values.

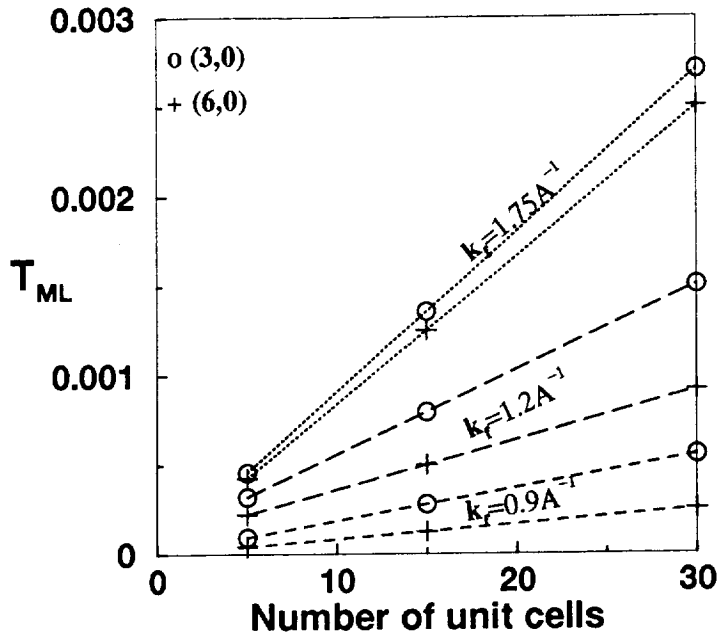


Fig. 3: Comparison of transmission probability of (3,0) and (6,0) nanotubes versus contact length in number of unit cells of the nanotube. The transmission probability decreases with increase in diameter and for a very large diameter tube (akin to a graphene sheet), the transmission probability will be appreciable only when the metal Fermi wave vector is larger than $4\pi/3a_0$.

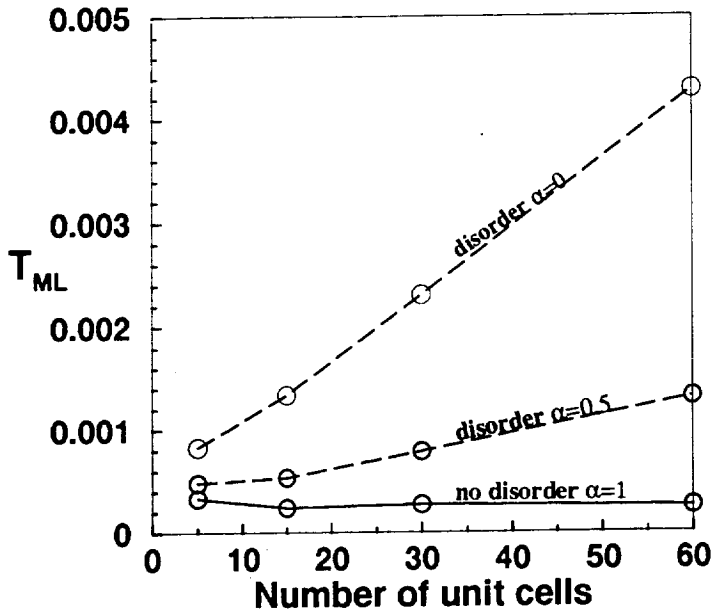


Fig. 4: Comparison of transmission probability versus contact length for a (2,2) armchair tube, with and without disorder in nanotube-metal coupling. The metal Fermi wave vector is $0.75\mathring{A}^{-1}$. Note that for the case without disorder, the transmission is poor and increasing the contact length does not help. Introducing disorder changes this picture and the transmission begins to increase with increase in contact length because k-vector conservation is relaxed.