Scaling analysis of Schottky barriers at metal-embedded semiconducting carbon nanotube interfaces

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We present an atomistic self-consistent tight-binding study of the electronic and transport properties of metal-semiconducting carbon nanotube interfaces as a function of the nanotube channel length when the ends of the nanotube wire is buried inside the electrodes. We show that the lineup of the nanotube band structure relative to the metal Fermi-level depends strongly on the metal work function but weakly on the details of the interface. We analyze the length-dependent transport characteristics, which predicts a transition from tunneling to thermally-activated transport with increasing nanotube channel length.

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The nature of Schottky barrier formation and its effect on charge transport through metal-semiconductor interfaces have been actively investigated for decades due to their importance in microelectronics technology, but are not fully resolved despite the tremendous efforts from both the experimental and theoretical sides...
The self-consistent calculation proceeds by approximating the charge distribution as superposition of atom-centered charge distributions, \( \delta \rho(\vec{r}) = \sum_i \delta N_i \rho_i(\vec{r} - \vec{r}_i) \), where \( \delta N_i = (\rho S)_{i i} - N_i^0 \) and \( N_i^0 \) is the number of valence electrons on atomic-site \( i \) of the bare SWNT wire. \( \rho_i(\vec{r}) \) is a normalized Slater-type function, \( \phi(\vec{r}) \), whose exponent is chosen such that \( \int d^3\vec{r} \rho_i(\vec{r}) \rho_i(\vec{r}')/||\vec{r} - \vec{r}'|| = I_i - A_i \), where \( I_i, A_i \) are the atomic electron affinity (ionization potential). This gives \( \delta V(\vec{r}) = \sum_i \delta N_i V_i(\vec{r} - \vec{r}_i) \), where \( V_i = \int d^3\vec{r} \rho_i(\vec{r} - \vec{r}_i)/||\vec{r} - \vec{r}_i|| \) can be evaluated analytically.\(^{14,19}\) We take into account the image-potential effect by including within \( \delta V \) contributions from both atom-centered charges and their image charges (centered around the image positions), rather than imposing an image-type potential correction. The self-consistent cycle is completed by calculating the matrix elements of the potential \( \delta V_{nm} = \int d^3\vec{r} \phi_m^*(\vec{r}) \delta V(\vec{r}) \phi_n(\vec{r}) \) using two types of scheme: (1) If \( m, n \) belong to the same atomic site \( i \), we calculate it by direct numerical integration; (2) if \( m, n \) belong to different atomic sites, we use the approximation \( \delta V_{mn} = S_{mn} (\delta V_{mm} + \delta V_{nn})/2 \).

The calculated charge transfer and electrostatic potential change along the cylindrical surface of the SWNT for the Au/Ti/Pd-SWNT-Au/Ti/Pd junctions are plotted in Fig. 2. The electrostatic potential change is the difference between the electrostatic potentials within the SWNT junction and the bare SWNT, obtained as the superposition of contributions from the transferred charges (plus their image charges) throughout the junction. Here it is important to separate the electronic processes at the interface and inside the channel. The coupling with electrodes in the embedded part of the SWNT wire induces only a localized perturbation to the SWNT channel sandwiched between the electrodes, so the electronic states in the middle of the channel are essentially identical to those of the bulk (infinitely long) SWNT except for the shortest (2.1 nm) channel length studied here, leading to similar charge transfer both at the interface and in the middle of the channel. For such SWNT channels (longer than 4.2 nm), the potential change in the middle and consequently the band lineup scheme become independent of the channel lengths. Note that the transferred charge in the middle of the channel shows oscillatory behavior due to the interference of the image charges.
FIG. 3: (Color online) Fig. (a) shows cross sectional view of electrostatic potential change at the Au-SWNT wire-Au junction for SWNT channel length of 8.4 nm. The SWNT diameter is 0.8 nm. (b) shows the corresponding local density of states (LDOS) as a function of position along the NT axis for SWNT channel length of 8.4 nm. The plotted LDOS is obtained by summing over the 10 atoms of each carbon ring of the (10,0) SWNT. Note that each cut along the energy axis at a given axial position gives the LDOS of the corresponding carbon ring and each cut along the position axis at a given energy gives the corresponding band shift.

FIG. 4: Room temperature conductance of the metal-SWNT wire-metal junction as a function of SWNT channel length.
both the conduction band and valence band edges are nearly constant along the NT axis. From the LDOS in the middle of the channel, we can determine that for both the Au-SWNT-Au and Pd-SWNT-Pd junction the Fermi-level is located slightly below (by \( \approx 0.05(eV) \)) the midgap, while for Ti-SWNT-Ti junction it is located above (by \( \approx 0.15(eV) \)) the midgap. For the case of Au and Ti electrodes, these values are essentially identical to those obtained in the end contact scheme.

The physical principles of Schottky barrier formation at the metal-SWNT interface can be understood as follows: Since the electrochemical potential (Fermi-level) and therefore the electron occupation in the junction are determined by the electrodes in contact with the SWNT, the band lineup inside the SWNT channel is determined by the self-consistent charge transfer effect through the entire metal-SWNT-metal junction. Therefore, the metal Fermi-level position should be close to the middle of the gap since otherwise extensive charge transfer will occur inside the SWNT channel. Since the screening of the work function difference inside the SWNT junction is weak, the metal Fermi-level should be below (above) the middle of the gap since otherwise extensive charge transfer will occur inside the SWNT channel. Since the screening of the work function difference inside the SWNT junction is weak, the metal Fermi-level should be below (above) the middle of the gap since otherwise extensive charge transfer will occur inside the SWNT channel.

Given the potential shift across the metal-SWNT interface, we can evaluate the length and temperature dependence of the SWNT junction conductance using the Landauer formula

\[
G = \frac{2e^2}{h} \int dET(E)\left[-\frac{d}{dT}(E-E_F)\right] = G_{Tu} + G_{Th}
\]

and

\[
T(E) = \text{Tr}[\Gamma_L(E)\Gamma_R(E)G(E)]
\]

Here we have separated the conductance into tunneling contribution \( G_{Tu} = \frac{2e^2}{h} T(E_F) \) and thermal-activation contribution \( G_{Th} = G - G_{Tu} \). The result at room temperature is shown in Fig. 4. The tunneling conductance for all three junctions decreases exponentially with the SWNT channel length for channel lengths longer than 2.1(nm). A separation of contact and bulk effect on the tunneling resistance can thus be achieved using \( R = R_0e^{d/kT} \), where \( R_0 \) is the contact resistance and \( d \) is the inverse tunneling decay length. We find \( R_0 = 8.2, 0.68, 12.3(k\Omega) \) and \( d = 1.68, 1.37, 1.68(1/nm) \) for the Au-SWNT-Au, Ti-SWNT-Ti, and Pd-SWNT-Pd junctions respectively. Note that the contact resistance is different for the Au and Pd electrodes due to the different interface coupling, but the inverse decay length (a bulk-related parameter) is the same. The room-temperature conductance saturates with increasing SWNT length, because tunneling is exponentially suppressed and transport becomes dominated by thermal-activation over the top of the potential barrier, whose height is approximately independent of the SWNT channel length. For Ti-SWNT-Ti junction, this leads to a transition from tunneling to thermally-activated transport at roughly 4(nm). For Au/Pd-SWNT-Au/Pd junctions, this transition occurs at channel length of roughly 9(nm). Consequently we can say that transport through the SWNT junction is bulk-limited at low temperature, but is contact-limited at room temperature.

In conclusion, we have presented an atomistic real-space analysis of Schottky barrier formation at metal-SWNT interfaces with embedded contact. Further analysis is needed that treat both the gate and source/drain field self-consistently within the SWNT junction, to achieve a thorough understanding of nanotube-based devices.

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