

# Variation of Contact Barrier Height in Metal-Semiconducting Carbon Nanotube Junctions using a Localized Gate

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## ABSTRACT

Electronic devices based on carbon nanotubes provide great promise for future use in integrated circuits. In previous work we have measured the local field effect in a metal-semiconducting carbon nanotube-metal device using a conducting-tip atomic force microscope. Based on those results we propose a consistent electrostatic model that incorporates the image force, electric field and tip potential and demonstrates how the latter reduces the potential barrier seen by thermionically emitted carriers in the metal-nanotube junction. Consistent with experimental data the model describes a position dependent change in the barrier height. This model complements tunneling effects models currently being formulated. Local gating has a much smaller effect on current through the junction than uniform gating using a backgate structure. This allows for an increase in current before tunneling current begins to dominate in the junction.

**Keywords:** Nanotubes, 1D junctions, Schottky barrier height

## 1 INTRODUCTION

Semi-conducting single-walled carbon nanotubes (SSWNT) are excellent candidates for constructing practical nano-scale electronic devices. Recent work has shown the potential of using these molecules as transistors, able to be turned on and off using an electrostatic backgate [1-5]. It is shown that the behavior of these devices is dominated by the contact region [4], [6]-[8]. Use of an electrostatic backgate has been shown to modulate current by affecting the behavior of the contact [9], [10], as opposed to early models that claimed the nanotube conductance was being altered. The mechanism of transmission between the metal electrode and the nanotube itself however is still not completely understood.

Tunneling has been proposed as the major method of carrier transport through the contact barrier [9], [10]. An electrostatic backgate moves the Fermi level within the device and shortens the width of the depletion region at the interface. This modulation of depletion width controls the amount of tunneling current that passes through the junction. Local gating techniques have also been shown to

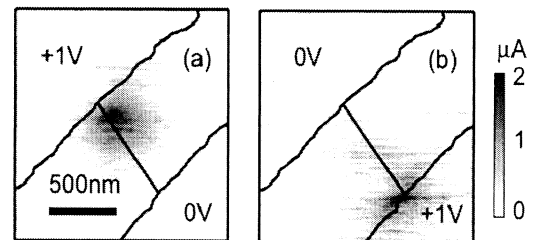


Figure 1: Current dependence on position of the AFM tip relative to the junction. It can be seen that far from the junction no effect on current is observable

modulate this current on a much smaller scale [4], [11], [12]. The small energy band gap indicates that prior to a sufficient adjustment of the Fermi level, thermionic emission must be the dominate method of transmission. This thermionic emission is due to the relatively small barrier height between the metal and the carbon nanotube.

We have previously used a Conducting-Tip Atomic Force Microscope (CT-AFM) to measure this local field effect in a Metal-SSWNT-Metal device [4][13][14], where we succeeded in modulating current due to the presence of the potential of the AFM tip. Figure 1 shows a scanning gate microscopy (SGM) current flow map that is strongly dependent on tip position. Here, the SSWNT is CVD-grown and contacted by two Cr/Au leads. The nanotube

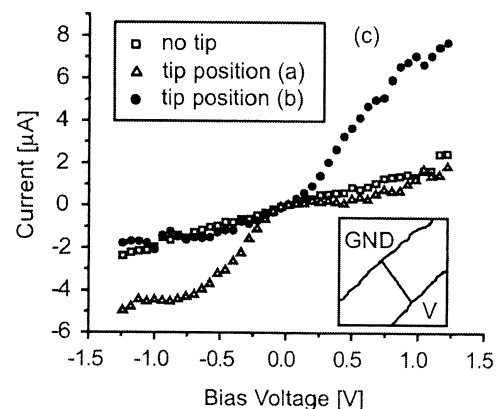


Figure 2: Current versus bias voltage of the device for different configurations of the AFM tip position

exhibits p-type behavior, so the contact with applied positive voltage is reverse biased while the other is slightly forward biased. The tip position is seen to have an effect only in the vicinity of the reverse biased junction, which indicates this junction dominates current flow. I-V data with and without the tip is shown in Figure 2. Measurements in the absence of the tip yield a symmetric I-V, however, the tip significantly increases current flow when the junction in its vicinity is reverse biased, thus giving rise to asymmetric I-V characteristics exhibited in the figure. Figure 2 also shows that the device itself is symmetric, i.e. switching contacts has the same effect as reversing applied voltage polarity.

Previous explanations of this behavior have mainly been qualitative and based on changing of the Fermi level due to the presence of the tip. Here, we present a formulation based on the electrostatic potential of the tip and its effect on the Schottky barrier height.

## 2 THEORY AND RESULTS

Schottky barriers are formed between metal electrodes and contacted semiconductor material [15]. Application of voltage, forward biases one junction (the cathode) for p-type semiconductor and reverse biases the other. The current through the entire device is dominated by the reverse bias junction with the main transport mechanism being thermionic emission of holes from metal to the semiconductor over the potential barrier. Experimental data indicates that the same occurs when metal contacts are made to SSWNT [5]-[10]. This barrier is nominally the difference between the metal Fermi level and the tube's valence band, but there has been considerable discussion in the literature with little agreement on the Fermi level's position near the junction [6],[16]. Nevertheless, we expect that the nominal barrier ( $\phi_{bp}$ ) is reduced by ( $\Delta\phi_{bp}$ ) a combination of image force and the electric field in the tube similar to the classical treatment of Schottky barrier height lowering in bulk materials. We propose here that the presence of the CT-AFM creates a position dependent electrostatic potential that alters the existing potential profile and modifies the maximum height of this barrier. This is similar to an electron-electron cloud effect that we have previously formulated within the context of metallic contacts to a two dimensional electron gas [17].

The potential due to the tip is modeled by considering the electric field generated by the charges on the surface of the tip. A conical shape is a good approximation for the tip, considering the ratios of tip radius, distance to grounded substrate and the distance from the surface of the silicon dioxide [19]. Due to the one dimensional nature of the nanotube, the derivation can be further simplified by modeling the tip as a line charge. The charge stored on the tip is approximated by:

$$dQ_d = \rho_L(l - (y - h))dy \quad (1)$$

where  $h$  is the tip distance above the sample,  $l$  is the length of the tip and  $\rho_L$  is a line charge density as shown in Fig 3. The maximum charge is stored closest to the SSWNT and then decreases with increasing distance. This charge exerts a force on the carrier, due to Coulombic interaction, described by:

$$dF = \frac{qdQ}{4\pi\epsilon R} \quad (2)$$

where  $R$  is the carriers distance from the line segment  $dy$ . Due to the nanotube's quasi-one dimensional nature only the electrostatic force in the lateral ( $x$ ) direction, i.e. direction of one-dimensional current conduction, will affect the carriers moving through the device. We can then find the total force in the  $x$  direction by integrating  $y$  from  $h$  to  $h+l$  to arrive at:

$$F_x = \int_h^{h+l} \frac{q\rho_L(l - (y - h))}{4\pi\epsilon} \cdot \frac{x_{tip} - x}{\left(\sqrt{(x_{tip} - x)^2 + y^2}\right)^3} dy \quad (3)$$

where  $x_{tip} - x$  is the carrier's distance from the tips  $x$  component. Using this force the potential observed by the carrier due to the presence of the tip is found by integrating from infinity to some value  $x$ :

$$E_{tip} = \int_{\infty}^d F_x dx = \frac{\rho_L q}{8\pi\epsilon} \left[ \sqrt{d^2 + h^2} - \sqrt{L^2 + d^2} + L \ln \left( \frac{L^2 + L\sqrt{L^2 + d^2}}{h^2 + h\sqrt{h^2 + d^2}} \right) \right] \quad (4)$$

where  $d$  and  $L$  are shown in Fig. 3.

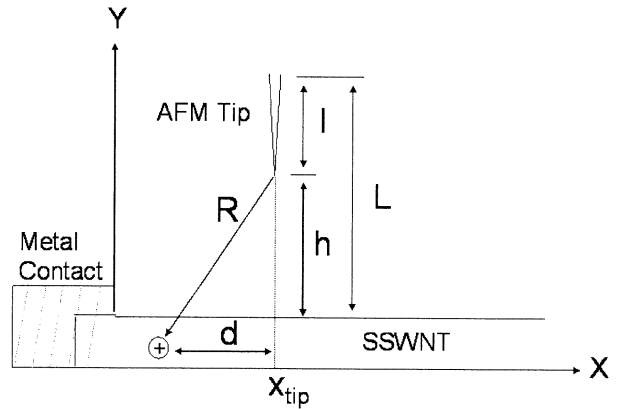


Figure 3: Description of layout and variables in the derivation of the modified Schottky Barrier Height.

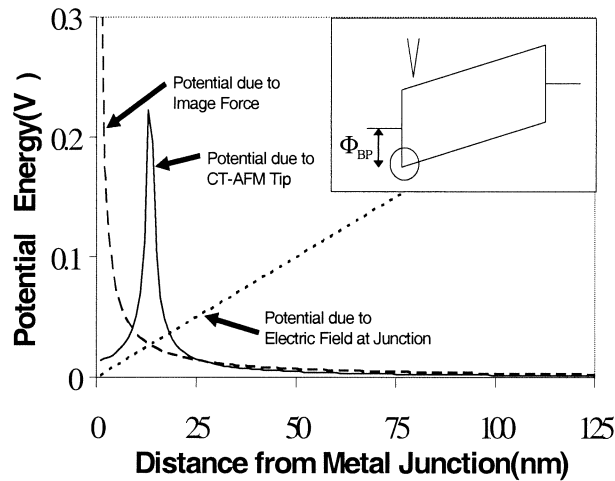


Figure 4: Plot of potentials of all three forces acting on a hole moving across the metal-SSWNT junction. The inset is a description of the energy band diagram of the device and marks the primary area of interest with the circle indicator

This potential is then combined with the electric field in the junction device and the image force to create a net potential that the carrier must travel through. The electric field is found by assuming that the entire length of the device is depleted resulting in a linear variation of the electric potential [20]. The image force is calculated in the classical manner. Thus a consistent electrostatic picture that incorporates the image force, electric field and tip potential is developed. This method shows a reduction in the barrier experienced by thermionically emitted carriers due to the presence of the biased tip. An important aspect of this formulation is that barrier reduction is a function of the tips position along the tube relative to the metal-SSWNT interface. This change in barrier height results in an

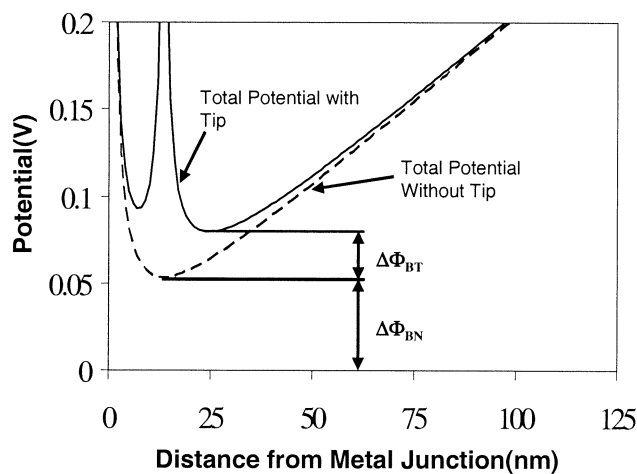


Figure 5: Calculated total potentials with and without tip present.

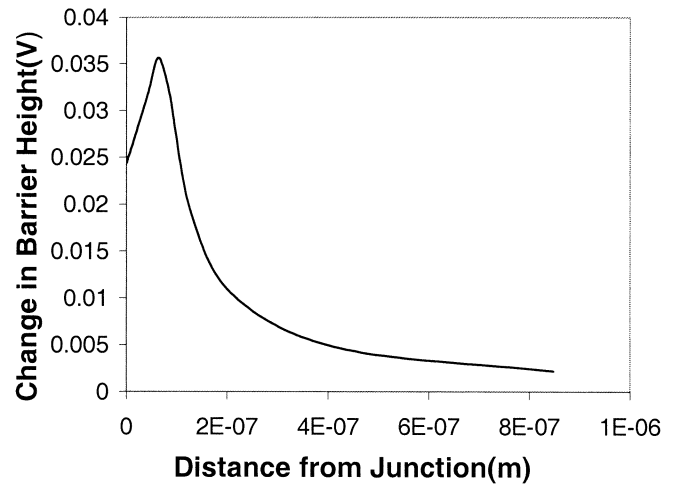


Figure 6: The calculated change in barrier height as a function of CT-AFM tip position. The maximum change takes place when the CT-AFM tip is in the vicinity of the former maximum barrier height

increase of current at the junction as observed in the data. Figures 4 and 5 show the result of this formulation using approximate values for the height, length and charge density. The image force potential, the electric field due to band bending and applied bias, and the potential due to the tip are calculated at the anode in Fig. 4; the cumulative effect is shown Fig 5. Clearly, the tip potential has the most effect when it is near the point where barrier height without the tip is at its maximum, and it diminishes when the tip is moved away from that point. As seen in Figure 6 the barrier lowering due to the tip ( $\Delta\Phi_{BT}$ ) is of the order of tens of meV, resulting in a current increase of  $\exp(\Delta\Phi/kT)$  which is consistent with experimental results when the charge density on the tip is kept small. This small charge density can be attributed to the dimensions of the tip, since it is an order of magnitude larger than the nanotube itself much of the charge is distributed symmetrically on either side and thus does not contribute greatly to the potential in the x direction.

### 3 CONCLUSIONS

We have developed an analytical model that describes the effect of an external potential on the barrier height seen by charge carriers that are emitted from metal to a semiconducting single walled carbon nanotube. This model is used to explain our experimental data that is obtained by utilizing a Conducting-Tip Atomic Force Microscope (CT-AFM) to measure the local field effect in a metal-nanotube-metal device. The model accounts for the forces exerted by the electric field due to band bending, image force, and the Coulombic force exerted by the AFM tip, demonstrating

how the barrier height can be reduced thus resulting in increase of conduction. The results are in good qualitative agreement with experimental data and, particularly, account for the dependence of the current on the AFM tip position.

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