Electrical contacts to nanotubes and nanowires

F. Léonard and A. A. Talin

Sandia National Laboratories, Livermore, California, 94551 United States
fleonar@sandia.gov, aatalin@sandia.gov

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ABSTRACT

Recent experiments have indicated that the height of the Schottky barrier at carbon nanotube/metal contacts depends on the diameter of the nanotube and the metal workfunction. We provide a theoretical explanation for these effects based on self-consistent calculations of the charge and electrostatic potential at the carbon nanotube/metal interface. For Pd contacts, Schottky barriers are negative (ohmic contacts) for nanotube diameters larger than 1.4 nm. Our calculations are extended to Si nanowires, where it is shown that ohmic contacts are difficult to obtain.

1 Introduction

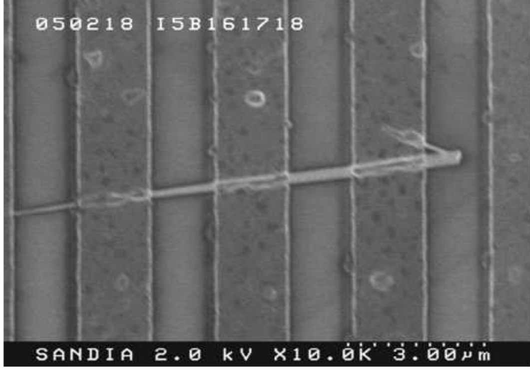
Semiconductor electronic devices play a key role in many modern day technologies. The advancement from the discovery of transistor action in semiconductors to the billions of transistors currently on a computer chip was made possible by many scientific and technological breakthroughs. One crucial development has been to understand and control the properties of electrical contacts to semiconductors. Indeed, forming low resistance electrical contacts has been the subject of decades of research and has allowed a thorough understanding of the properties of metal/semiconductor junctions. At such junctions, there is usually a Schottky barrier over which the carriers have to be excited to carry current. While some device concepts take advantage of the Schottky barrier, many device designs actually require an ohmic contact–examples are the source and drain contacts in MOSFETS. To eliminate the Schottky barrier, many strategies are used, the most common being heavily doping the semiconductor near the metal-semiconductor junction.

Alternatives to conventional semiconductor materials are actively being pursued, and an area that has attracted much attention is nanoelectronics, where the active device element is composed of a nanostructure such as a nanotube, a nanowire, a quantum dot, or a molecule. These nanostructures posses unique properties that may allow technological breakthroughs and performance improvements that will surpass conventional scaled-down devices. Despite the unique properties of nanostructures, the problem of electrical contacts still remains, and may be even more important since the contacts will be a significant fraction of the device size. Thus there is a clear need for understanding the properties of electrical contacts to nanostructures in more detail, and to devise ways to improve and control such properties. One problem however is that the physics concepts that were developed for traditional contacts are not applicable to metal/nanostructure interfaces because of the reduced dimensionality and the much different properties of nanostructures.

In this paper, we present a theoretical analysis of the properties of electrical contacts to carbon nanotubes and semiconducting nanowires[1]. This work is motivated by recent experimental work[2], [3] that found intriguing behavior at metal/nanotube contacts: the height of the Schottky barrier depends on the diameter of the carbon nanotube and on the metal workfunction. To explain this behavior we performed self-consistent calculations of the charge and the electrostatic potential at a metal/nanotube contact. From the calculated electrostatic potential, we extract the Schottky barrier and find that it depends inversely on nanotube diameter, including a cross-over to ohmic behavior at a nanotube diameter of about 1.4 nm, in agreement with experiments with Pd contacts. Furthermore, we show that the height of the Schottky barrier is sensitive to the metal workfunction. These calculations are extendded to semiconducting nanowires, where we find that forming ohmic contacts is difficult.

2 Modeling Approach

To illustrate the systems under consideration, Figure 1 shows Scanning Electron Microscopy images of electrical contacts to carbon nanotubes and GaN nanowires. In both cases, the nanostructure is first deposited on the SiO_2 substrate and the metallization is performed over the nanostructure. Thus, the nanotube or nanowires are embedded in the metal, forming an intimite contact, and affording better protection to the environment. (An alternative strategy is to first fabricate the elec-



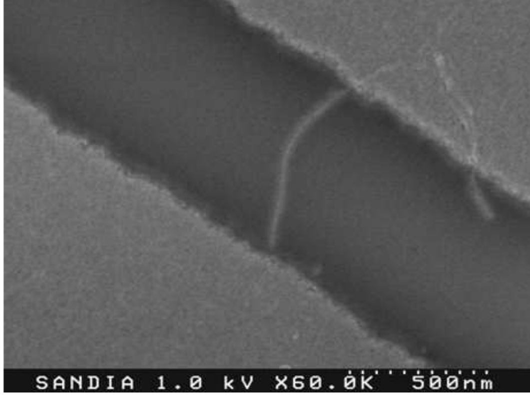


Figure 1: Examples of electrical contacts to nanotubes and nanowires. Panel (a) shows a SEM image of a GaN nanowire connected by 4 electrodes. Note that because the nanowire is tapered each contact has a different nanowire diameter. (b) SEM image of a carbon nanotube making contact to electrodes.

trodes on the substrate and then position the nanotube or nanowire on top of these electrodes. In that case the contact is not as intimate and the contact resistance is usually higher).To model the properties of such contacts, we consider a carbon nanotube or a nanowire fully embedded in a metal, as illustrated in Figure 2. In the case of the nanotube, there is a thin (van der Walls) separation between the nanotube and the metal, which is taken as 0.3 nm in the calculations. For the nanowire, we assume that the interface is circular with the nanowire making an abrupt interface with the metal. For both types of nanostructures we consider a perfect metal.

2.1 Carbon nanotubes

For a carbon nanotube, we express the charge on the nanotube as

$$\sigma_{NT} = eN_a \int D_{NT}(E + eV_{NT}) f(E - E_F) dE \quad (1)$$

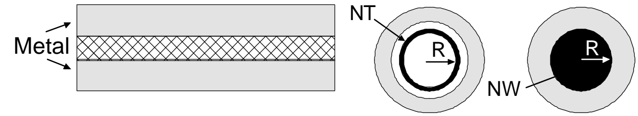


Figure 2: Sketch of the embedded nanotube or nanowire used for the calculations. Left picture shows a cross-section along the length of the nanotube or nanowire. Right pictures show radial cross-sections.

where $N_a = 4/\left(3\sqrt{3}a^2\right)$ is the atomic areal density ($a = 0.142$ nm is the C-C bond length), f is the Fermi function, and D is the density of states given by

$$D_{NT}(E) = \frac{2a\sqrt{3}}{\pi^2 d\gamma} \frac{|E|}{\sqrt{E^2 - (E_g/2)^2}} \quad (2)$$

with $\gamma = 2.5$ eV the tight-binding overlap integral, d the nanotube diameter and E_g the nanotube bandgap. The nanotube bandgap is given by

$$E_g = \frac{a\gamma}{d}. \quad (3)$$

The electrostatic potential on the carbon nanotube can be calculated using an image potential construction, and is given by

$$eV_{NT} = -\sigma \frac{ed}{2\varepsilon_0} \ln \frac{d + 2s}{d} \quad (4)$$

where ε_0 is the permittivity of free space and s is the separation between the nanotube and the metal. The procedure consists in solving self-consistently the equations for the charge and the potential for given values of the nanotube diameter and metal workfunction. Once the potential on the nanotube is determined, the Schottky barrier for holes (the most common experimental situation) is given by

$$\begin{aligned} \Delta &= E_F - E_v = E_F - E_v^0 + eV_{NT} \\ &= \Phi_{NT} - \Phi_m + \frac{E_g}{2} + eV_{NT}. \quad (5) \end{aligned}$$

where Φ_{NT} is the nanotube workfunction and Φ_m is the metal workfunction. A positive value of Δ indicates a Schottky barrier, while a negative value indicates an ohmic contact.

2.2 Nanowires

For a nanowire, there is a charge density throughout the nanowire, and the charge acquires a dependence on the radial coordinate r:

$$\sigma_{NW}(r) = eN_v \int D_{NW}(E + eV(r)) f(E - E_F) dE \quad (6)$$

where N_v is the volume density. The density of states is expressed as

$$D_{NW}(E) = \frac{\sqrt{2m^*}}{\pi\hbar} \frac{1}{\sqrt{E - E_g/2}} \tag{7}$$

where m^* is the effective mass. For Si nanowires, experiments have shown[4] that the bandgap depends on diameter as

$$E_g = 1.12 + \frac{4.33}{d^2} \tag{8}$$

where E_g is in eV and d is in nanometers. We use the Si volume density $N_v = 5 \times 10^{28}$ atoms/m^3 and take the effective mass to be equal to the free electron mass.

The electrostatic potential is calculated by solving Poisson's equation

$$\nabla^2 V(r) = \frac{\rho(r)}{\varepsilon} \tag{9}$$

where ε is the Si dielectric constant. This equation is solved numerically on a grid with the boundary condition of vanishing potential at the metal surface. Once the electrostatic potential through the cross-section of the nanowire is determined, we calculate the area averaged electrostatic potential

$$\overline{V} = \frac{\int V(r) r dr}{\int r dr} \tag{10}$$

and obtain the Schottky barrier from

$$\begin{aligned} \Delta &= E_F - E_v = E_F - E_v^0 + e\overline{V} \\ &= \Phi_{NW} - \Phi_m + \frac{E_g}{2} + e\overline{V}. \end{aligned} \tag{11}$$

3 Results

Figure 3 shows the calculated Schottly barrier height for electrical contacts to carbon nanotubes, assuming a metal workfunction 0.4 eV larger than the nanotube workfunction (for a nanotube workfunction of 4.7 eV, this would correspond to Pd contacts). The figure shows that the Schottky barrier decreases with increase in nanotube diameter, in agreement with the experimental observations[2], [3]. The Schottky barrier becomes negative at around 1.4 nm, signaling ohmic contacts for nanotubes with diameters larger than this value. The Schottky barrier can be shown to depend logarithmically on the nanotube diameter[1] due to partial charge transfer between the metal and the nanotube. As mentioned in the introduction, another intriguing conclusion from the experiments is that the Schottky barrier depends on the type of metal used for the contact. Figure 4 shows the dependence of the Schottky barrier on the metal workfunction for a 1.32 nm nanotube. The Schottky barrier

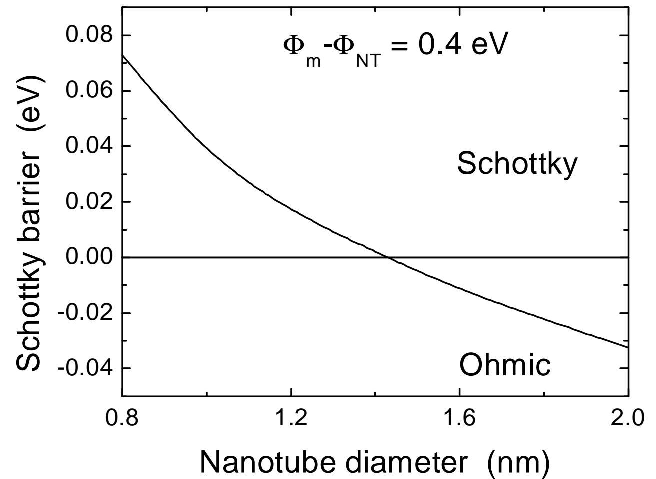


Figure 3: Calculated Schottky barrier at nanotube/metal contacts as a function of the nanotube diameter.

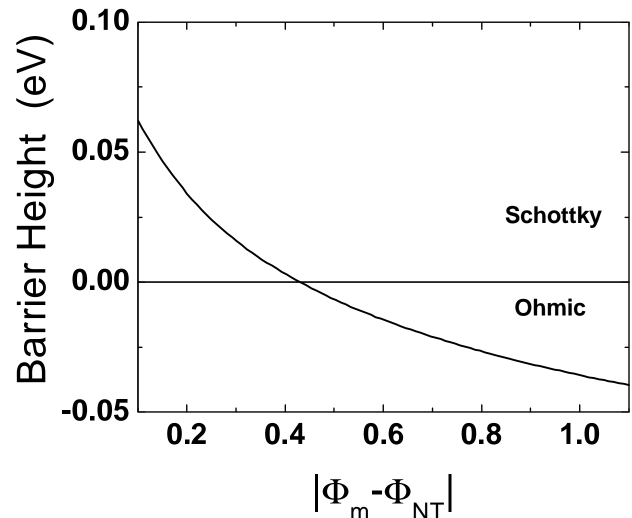


Figure 4: Calculated Schottky barrier height as a function of metal workfunction for a semiconducting carbon nanotube of 1.32 nm diameter.

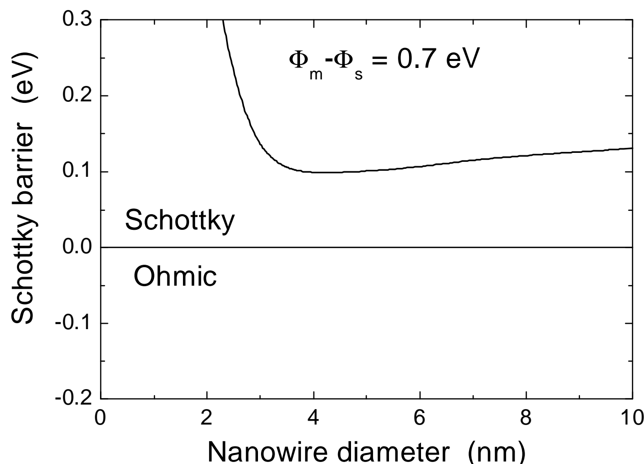


Figure 5: The calculated Schottky barrier heigth at contacts between metal and a Si nanowire.

decreases with increase in the metal workfunction, with a transition to ohmic behavior for metal workfunctions larger than about 5.15 eV.

While larger diameter carbon nanotubes show ohmic behavior, our calculations indicate that undoped Si nanowires always possess a Schottky barrier, as shown in Figure 5. The reason for this is two fold. First, the bandgap of large diameter Si nanowires approaches that of bulk Si (1.1 eV) in contrast to carbon nanotubes where the bandgap goes to zero at large diameters. Second, the bandgap of Si nanowires is proportional to d^{-2} (for carbon nanotubes the behavior is d^{-1}) so that it increases rapidly as the diameter is decreased, bringing the metal Fermi level in the bandgap. These small and large diameter behaviors in nanowires lead to the presence of a positive Schottky barrier at any diameter.

4 Conclusion

In conclusion, we have shown that the Schottky barrier at electrical contacts to quasi-one-dimensional nanostructures depends critically on the diameter of the nanostructure and the metal workfunction. Both of these concepts are quite different from what is expected in conventional metal/semiconductor contacts, highlighting the need to re-visit the physics behind contacts to nanostructures. While this paper focused on the basic properties of contacts, additional effects such as Fermi level pinning and the role of doping also show unusual behavior[1].

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