Modeling Semiconductor Carbon Nanotube Rectifying Heterojunctions

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Abstract

We present a method of modeling the effective mass, band offset and current in a heterostructure electronic device constructed from two carbon nanotubes of different diameters.

1 Introduction

A carbon nanotube (NT) may be a single walled (SWNT) or a multi-walled (MWNT) tube, with length reaching up to 1mm (Saito et al. 1998). Each wall of the NT consists of a seamless cylindrical tubule formed from a 2D graphite sheet(graphene). The SWNT unit cell, shown in Fig. 1, is a cylindrical segment defined by two fundamental tube indices, n and m, which determine the tube's diameter and wrapping angle. A SWNT may be a metal or a semiconductor and typically ranges from 1 to 20 nm in diameter (Saito et al. 1998). SWNTs are further seperated into those which are optically active (chiral), and those which are not (achiral). These properties and others such as the bandgap (Saito et al. 1998), and, as found in this work, the effective mass, all are determined by the tube indices n and m. The same properties are exhibited by each wall of a MWNT, but typically larger diameters, up to 100nm, are observed. Since the lower conduction and upper valence bands of a MWNT will be determined by the outer wall, we will model their electrical transport properties considering the outer wall as an isolated SWNT.

Nanotubes of different diameter can be connected seamlessly by the incorporation of a small number of defects, which are usually pentagonal or heptagonal rings (Saito et al. 1998). The versatile electronic and structural properties and small diameter of carbon nanotubes offer great potential and interest to the nanoelectronics community (Martel et al. 1998, Deckker 1999). One structure of particular interest was a rectifying heterojunction that was recently fabricated (Papadopoulous et al. 2000) by the connection of two semiconducting MWNTs of different diameters.

We have developed a theory for explaining electronic properties of a heterojunction formed by nanotubes of different diameters. The model describes how to predict the effective mass, band offset and junction current based solely on the diameters, and thus the fundamental tube indices n and m, of the connected tubes.

2 Effective Mass and Band Structure

To get the dependence of the current on the choice of NT heterojunction, we will need to determine how the effective mass, m^*, of each tube depends on its diameter. For this we will use a π orbital tight-binding method (Saito et al. 2000), to first calculate the band structure. We find that this leads to a single analytical form for the hole and electron effective masses in any semiconducting NT which depends on the tube diameter

$$d(n,m) = \frac{a_{cc}\sqrt{3(n^2+m^2+nm)}}{\pi}. \tag{1}$$

The effective mass, $m^*(d)$, as a function of tube diameter is found to depend on the tube chirality according to:

$$m^*(d) = \begin{cases} \frac{29}{2} m_e \left(\frac{a_{cc}}{d}\right)^{\left[\frac{\pi}{2}+\frac{26\pi}{7}\left(\frac{a_{cc}}{d}\right)-\frac{37\pi}{3}\left(\frac{a_{cc}}{d}\right)^2\right]} & chiral \\ \frac{2}{3} m_e \left(\frac{a_{cc}}{d}\right) & achiral\ , \end{cases} \tag{2}$$

where m_e is the electron mass and $a_{cc} = 1.42\mathring{A}$ is the carbon-carbon bond length.

3 Band offset

We also present the first calculation of the band offset for a nanotube heterojunction using the average bond energy method of Wang et al. (1992). The average bond energy (E_b) can be used as a reference point to calculate the valence band offset between side 1 and 2 of a heterojunction according to

$$\Delta E_v = (E_{b1} - E_{v1}) - (E_{b2} - E_{v2}), \tag{3}$$

where E_v are the energies of the respective valence band maximums. We incorporate the wavefunction overlap between nearest neighbors and include the effects of σ-π mixing on the π-orbital band structure to calculate the difference in the average bonding energies. This difference, $E_{b1} - E_{b2}$, is found to be negligibly small. This indicates that very little charge moves across the junction in the formation of the heterojunction but since we are dealing with a very small interface, a significant amount of band bending will still most likely occur. Using the dependence of the bandgap on diameter, we arrive at the band offset which depends on the diameters of the tubes

$$\Delta E_v = E_{v2} - E_{v1} = \gamma a_{cc}\left(\frac{1}{d_1(n_1,m_1)} - \frac{1}{d_2(n_2,m_2)}\right). \tag{4}$$

Here $\gamma = 3.03$eV is the nearest-neighbor π transfer integral within the tight-binding bandstructure calculation.

Based on experimental evidence of large hole concentrations in nanotubes (Martel et al. 1998), the p-p nanotube heterojunction junction is shown in Fig. 2.

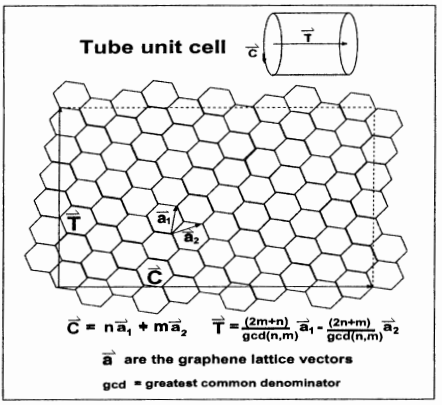

Fig. 1 Unit cell

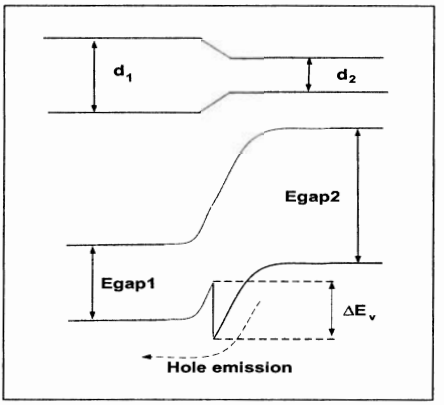

Fig. 2 Tube band-edge diagram

4 Current

To obtain the current across the NT junction with an applied forward bias, we adapt the heterojunction thermionic emission model (Milnes and Feucht 1972) to nanotubes. For the NT with large hole doping, the hole concentration is inversely proportional to the β power of the tube diameter, $N \propto \frac{1}{d^\beta}$,where $\beta \simeq 4$ (Papadopoulous et al. 2000). The dielectric constant will then scale as $\epsilon \propto N$ (Papadopoulous et al. 2000). Using this and equations we derived for effective mass (2) and band offset (4), we derive the following equation for the forward bias current across the junction, as a function of diameters, d_1 and d_2, of the connected tubes:

$$I_{d_1 d_2}(V) \propto I_o(d_1, d_2) \exp\left(\frac{qV + \frac{\gamma a_{cc}(d_1 - d_2)}{d_1 d_2}}{k_b T\left(1 + \left(\frac{d_1}{d_2}\right)^{2\beta}\right)}\right)\left(1 - \exp\left(\frac{-qV}{k_b T}\right)\right), \quad (5)$$

where

$$I_o(d_1, d_2) = \frac{1}{d_2^\beta \sqrt{m^*(d_2)}}\left(\left(\frac{d_2}{d_1}\right)^\beta \sqrt{\frac{m^*(d_2)}{m^*(d_1)}}\right)^{\frac{1}{\left(1+(\frac{d_1}{d_2})^{2\beta}\right)}}. \quad (6)$$

Using the experimental data of Papadopoulous et al. (2000) for a $\frac{d_1}{d_2} \simeq \frac{60}{40}$ NT junction, we find a good fit for β=3.3 as shown in Fig. 3(a). The dependence of the IV curve on the diameter ratio of three selected heterojuncions is illustrated in Fig. 3(b). As expected the current is clearly seen to turn on at lower forward bias voltages for heterojunctions with smaller diameter ratios and thus smaller band offsets.

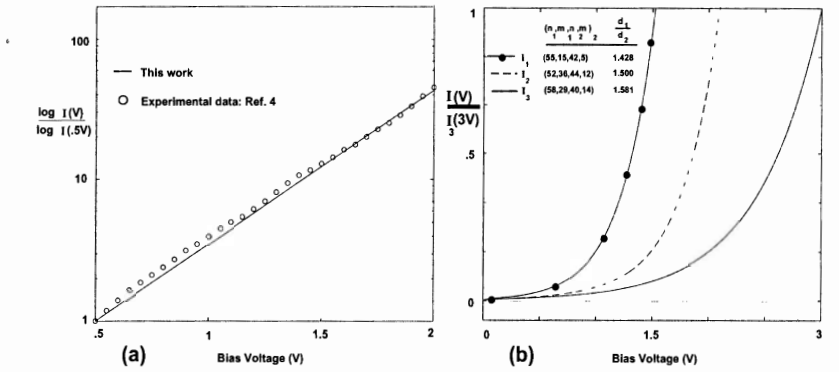

Fig. 3 Forward bias IV characteristics for SWNT junctions including , (a), the comparison of a $\simeq \frac{60}{40}$ diameter junction with experiment and , (b), the comparison of various junctions.

5 Conclusion

In this work we have developed expressions for the effective mass of any semiconducting carbon nanotube, and the band offset and forward bias current of a carbon nanotube heterojunction, in terms of the tube diameters. This allows a convenient prediction of how the electrical characteristics of a semiconductor-semiconductor NT junction vary as the component nanotubes are altered.

References

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