Schottky barrier heights of Carbon Nanotube FETs: Theory versus Experiment.

M. M. De Souza,D. Casterman, S. Taioli,
EEE Department, University of Sheffield, Mappin Street, Sheffield S1 3JD, UK.
Email: m.desouza@sheffield.ac.uk

Single-wall carbon nanotube field-effect transistors (CNTFETs) have been shown to behave as Schottky barrier (SB) FETs. Factors controlling the SB height (SBH) are nevertheless not easy to establish. In [1], a range of CNTFETs with Pd, Ti and Al contacts were used to extract the SBHs via statistical sampling of on-current 'Ion' as a function of diameter, 'd'. These reveal a dependence of the SBH on type of metal and the diameter of the CNT. In particular, a breakdown of the linear dependence of 'Ion', versus diameter 'd', below 1 nm is observed.

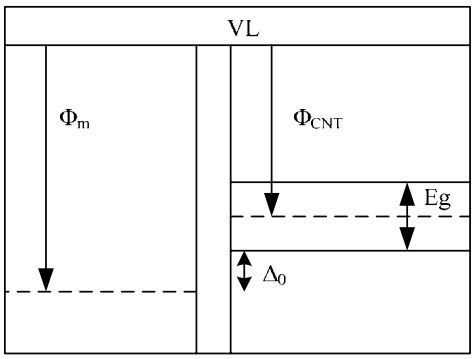

Fig 1. SB model using Eq (1).

The model for the SBH of a (p)-CNTFET proposed by Leonardo [2] is based upon the depletion induced by charge transfer from the CNT to the metal contact giving rise to a partial band re-alignment. Due to the fixed "depletion" imposed by the carbon nanotube geometry, in comparison to a conventional bulk device, a value of the SBH, lying between that of a simple model corresponding to Equation (1) below (Fig 1) and the bulk limited value of *Eg(d)*/2 is expected.

$$\Delta_0(d) = \frac{Eg(d)}{2} - \phi_m + \phi_{CNT}(d) \qquad (1)$$

where , Δ_0 is the Schottky barrier for holes, *d* is the diameter, *Eg* the bandgap, Φ_m and $\Phi_{CNT}(d)$ are respectively the work functions of the metal and the CNT. The model is obtained by including electrostatics in the evaluation of the depletion charge of the CNTFET.

We use theoretical Density Functional Theory (DFT) calculations [3] to evaluate the impact of nanotube diameter in the range 0.55-1.7 nm on the SB model. These studies of zig-zag nanotubes [4] reveal the SBH to be a function of the bandgap, and also independently, the workfunction of the CNT. Strong hybridization effects in the small diameter range upto 0.8 nm result in a significant deviation from the "1/d" rule, consistent with calculations of Zolmi et al [5] and the experimental data of [1]. Using the DFT extracted parameters, in Leonardo's model, yields a transition from Schottky to Ohmic behaviour at a nanotube diameter of ~0.9 nm for Pd contacted devices. In comparison, the transition was reported to occur at ~1.4 nm assuming a fixed semiconductor work function [1,2]. Furthermore, the theoretical variation of SBH predicted with diameter, to date, results in an overall magnitude which is at least one order smaller than that predicted by the IBM data [1].

Several reasons can be ascribed to this discrepancy. (a) Under-estimation of the bandgap due to many-electron corrections, not taken into account within DFT. Moreover, the impact of the GW correction on the semiconductor workfunction needs to be included, on a case-by-case basis. (b) A simplistic model was used in the extraction of the Schottky barrier height in [1]. A 1/d dependence of the bandgap was ascribed throughout the entire range of diameters which does not account for hybridisation at small diameters. (c) The functional form of the dependence of the SBH on the diameter [2] does not capture the behaviour in the entire range of diameters, particularly at smaller values.

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