Three-Dimensional Analysis of Schottky Barrier Carbon Nanotube Field Effect Transistors

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Abstract

Two-dimensional (2D) and three-dimensional (3D) electrostatic analyses of Schottky barrier carbon nanotube field effect transistors (CNTFETs) are carried out. Comparisons between 2D and 3D simulation results for symmetric and asymmetric structures indicate that 2D simulations do not describe the behavior of the device accurately, suggesting that to understand and improve the behavior of CNTFETs 3D electrostatic analysis is required.

1 Introduction

Carbon nanotubes (CNTs) have emerged as promising candidates for nanoscale field effect transistors. It has been shown experimentally and theoretically [1, 2] that typical carbon nanotube field effect transistors (CNTFETs) operate by changing the transmission coefficient of Schottky barriers at the contact between the metal and the CNT, implying that for the analysis of CNTFETs accurate electrostatic simulation is required. Up to now most simulations have been performed using two-dimensional (2D) electrostatic analysis and some improvements based on these analyses were proposed [3]. In this work three-dimensional (3D) electrostatic analyses are carried out, the results of which indicate that 2D simulations do not describe the behavior of the device accurately.

2 Modeling

Assuming ballistic transport, we calculate the drain current using the Landauer-Büttiker formula [4]

$$I_{\mathrm{d}} = \frac{4\mathrm{q}}{\mathrm{h}} \int [f_{\mathrm{s}}(\mathcal{E}) - f_{\mathrm{d}}(\mathcal{E})] TC(\mathcal{E}) \mathrm{d}\mathcal{E}, \tag{1}$$

where $f_{\mathrm{s,d}}$ are equilibrium Fermi functions at the source and drain contacts and $TC(\mathcal{E})$ is the transmission coefficient through the device. The factor 4 in (1) stems from the twofold band and twofold spin degeneracy [5].

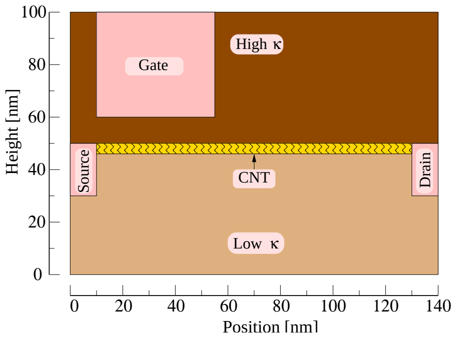

Figure 1: 2D sketch of the the asymmetric structure.

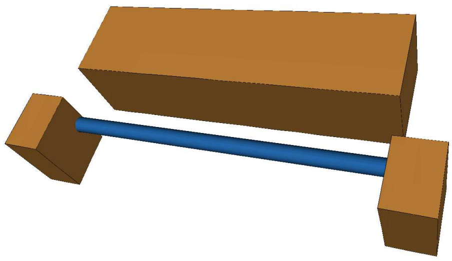

Figure 2: 3D sketch of the the symmetric structure.

We evaluate $TC(\mathcal{E})$ using the WKB approximation [2, 6, 7]

$$\ln TC(\mathcal{E}) = -2 \int k(x) \mathrm{d}x, \tag{2}$$

and an idealized band structure [8]

$$k = \frac{\mathcal{E}_\mathrm{g}}{\sqrt{3}\mathrm{a}\gamma_0} \sqrt{1 - \left(\frac{\mathcal{E} + \mathrm{q}V(x)}{\mathcal{E}_\mathrm{g}/2} \right)^2} \mathrm{d}x, \tag{3}$$

The symbol $\mathrm{a} = 0.246\ \mathrm{nm}$ denotes the lattice constant, $\mathcal{E}_\mathrm{g}$ is the band gap energy, $\gamma_0 = 2.5\ \mathrm{eV}$ is the transfer integral, and $V(x)$ denotes the electrostatic potential along the CNT. The integration in (2) is performed only within the classical turning points.
For electrostatic analysis the Smart-Analysis-Package (SAP) [9] was used. Since we focus on the subthreshold behavior of CNTFETs, we neglect charge on the CNT, which is considered to be a good approximation for the off-state regime [3, 5, 6, 10].

3 Results and Discussion

In this work we focus on ambipolar devices, where the metal Fermi level is located in the middle of the CNT band gap at each contact. All our calculations assume a CNT with $0.6\ \mathrm{eV}$ band gap, corresponding to a diameter of $1.4\ \mathrm{nm}$ [8]. We performed simulations for both symmetric and asymmetric structures. Fig. 1 shows the asymmetric structure for 2D simulations, in which the gate covers the CNT partially, whereas in the symmetric structure the gate covers the CNT completely. As discussed in [6] the asymmetric structure has the advantage of suppressing parasitic tunneling at the drain contact. For the 3D structure the gate, source, and drain were extended $20\ \mathrm{nm}$ into the third dimension, and the CNT was considered to be a cylinder with a diameter of $1.4\ \mathrm{nm}$, see Fig. 2. The relative permittivities of the materials above and below the CNT were set to 20 and 1 respectively. This can improve the subthreshold slope to some extent, since it increases the electric field along the CNT axis and therefore suppresses the Schottky barriers [6].
Fig. 3 shows current-voltage characteristics for both the symmetric and asymmetric structure using 2D electrostatic analysis. It can be seen that for the symmetric structure

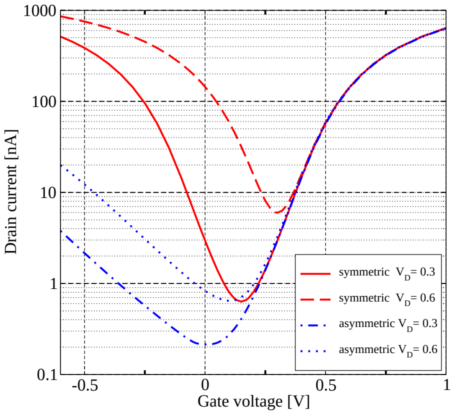

Figure 3: Drain current versus gate voltage from 2D simulations.

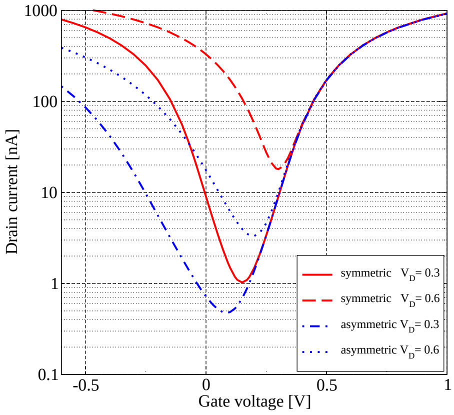

Figure 4: Drain current versus gate voltage from 3D simulations.

the current is symmetric with respect to the gate voltage, unlike for the asymmetric structure, where the current is expectedly not symmetric. This originates from the different transmission coefficients for electrons and holes. Thus a better off-current with respect to the symmetric structure is obtained, in agreement with [3].
Fig. 4 shows the current-voltage characteristics for 3D simulations. By comparing Fig. 3 and Fig. 4 it can be seen that the difference between 2D and 3D simulations increases as the gate covers the CNT partially. As can be seen in Fig. 4 the off-current for the asymmetric structure is higher than predicted by 2D simulations. For better comparison current-voltage characteristics of the asymmetric structure for both 2D and 3D simulations are shown in Fig. 5. The difference between drain currents can be well understood by comparing the band edge alignments resulting from 2D and 3D simulations as shown in Fig. 6.

4 Conclusions

2D and 3D simulations for symmetric and asymmetric structures of CNFETs have been performed. Our results show that 2D simulation is not accurate enough for predicting the behavior of CNTFETs and the difference between 2D and 3D analysis increases as the gate covers the CNT partially, suggesting that for accurate simulation of CNTFETs 3D analysis is required.

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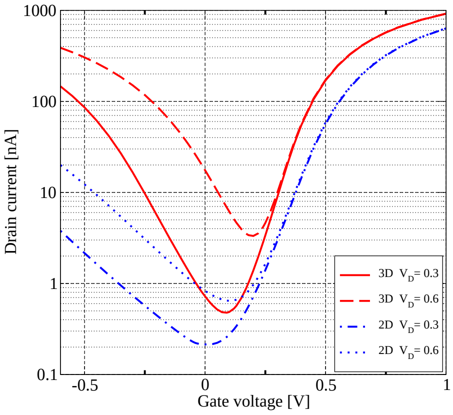

Figure 5: Comparison of drain currents from 2D and 3D simulations for the asymmetric structure.

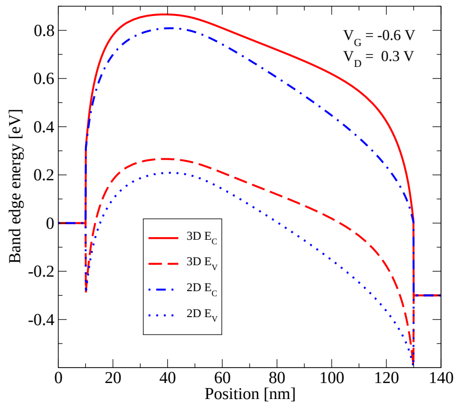

Figure 6: Comparison of band edges for the asymmetric structure from 2D and 3D simulations.

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