Multi-scale modeling of metal-CNT interfaces

M. Claus*§, A. Fediai‡*††, S. Mothes*,§ A. Pacheco§, D. Ryndyk‡*††,
S. Blawid**, G. Cuniberti‡*†† and M. Schröter§
* Center for Advancing Electronics Dresden, TU Dresden, Germany, martin.claus@tu-dresden.de
§ Chair for Electron Devices and Integrated Circuits, TU Dresden, Germany
‡ Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden, Germany
** Laboratory for Devices and Integrated Circuits, Universidade de Brasilia, Brazil
†† Dresden Center for Computational Materials Science, TU Dresden, Germany

Introduction

It is well known that the metal-CNT interfaces in CNTFETs have been a key factor limiting the device performance. Efforts have been made to improve the understanding of physics at these interfaces and the contact length scaling behavior seen in experiments [1]. However, the related interface phenomena are not fully understood [1], which makes it difficult to improve the device performance.

Typically, the impact of the metal-CNT interfaces on the device characteristics is lumped into a resistance which is commonly labeled as the contact resistance R_c (including the contribution of both, the source and the drain contact).

While for digital applications the contact length is an critical parameter in terms of overall device size, for analog HF applications as described in [2] the contact length is in µm scale which allows an investigation of the metal-CNT interfaces in the long-contact-limit. As suggested in [3], contact engineering and thus a detailed understanding are mandatory for optimizing the device linearity of CNTFETs.

Results and Discussion

A multi-scale modeling and simulation framework for CNTFETs is employed to study the impact of different contact materials on the device behavior. By means of an atomistic simulation platform [4] which combines large-scale ab initio calculations with a Green function approach a good agreement between atomistic simulation studies and experimental data for Pd [1] and Al contacts has been observed demonstrating a strong correlation between metal-CNT coupling strength, contact length and the contact resistance. Fig. 1 and 2 show the local DOS for the investigated (17,0)-tube with Pd and Al contacts, respectively. Compared to Al, Pd does not change the DOS of the CNT underneath the metal contact significantly. Fig. 3 shows atomistically calculated transfer characteristics for the two different contact materials.

The atomistic simulation results are employed to adjust the contact model used within the transport studies at the device level [5] which offers greater flexibility regarding device architecture and materials and a significantly reduced computational burden. The greater flexibility is possible due to a simplified hetero-junction contact model [5] which has been verified by atomistic simulations. The key contact parameters are the interface potential step $\triangle\Phi$ (see also [6]), the Schottky barrier height Φ_sb, the DOS within the metal coated tube portion and direct tunneling of metal states to the channel [7]. Fig. 4, 5 and 6 show the impact of the contact model parameters on the contact resistance and on the transconductance. (For a ballistic channel and fully transparent contacts, the total device resistance approaches its ballistic limit of $R_\mathrm{q} = h/4q^2 \approx 6.4\,\mathrm{k}\Omega$.) These plots exemplify the challenges for contact engineering.

Acknowledgment

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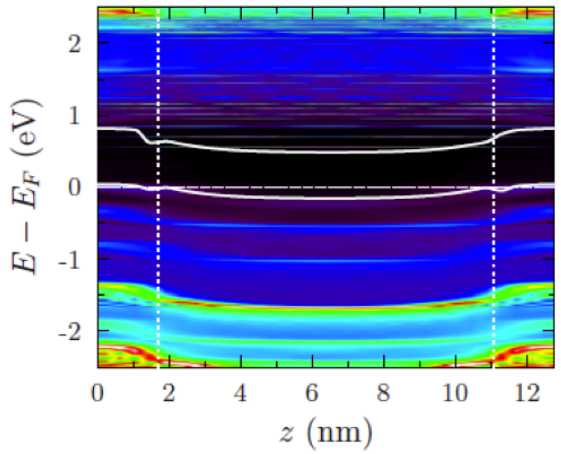

Fig. 1. Atomistically calculated local DOS for a 10 nm long CNTFET with Pd contacts.

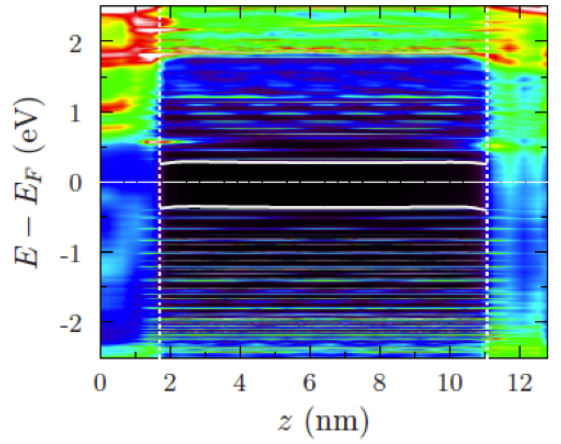

Fig. 2. Atomistically calculated local DOS for a 10 nm long CNTFET with Al contacts.

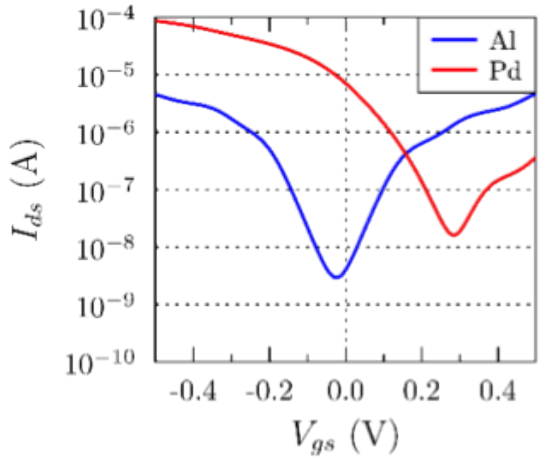

Fig. 3. Comparison of atomistically calculated transfer characteristics for Pd and Al contacted 10 nm long CNTFET.

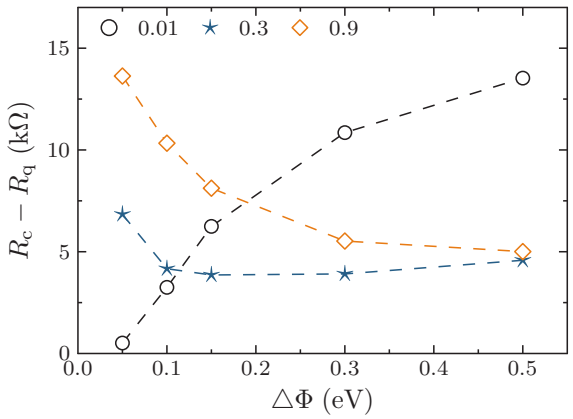

Fig. 4. Simulated contact resistance for different △Φ and different DOS (i. e. effective masses) within the metal coated tube portion.

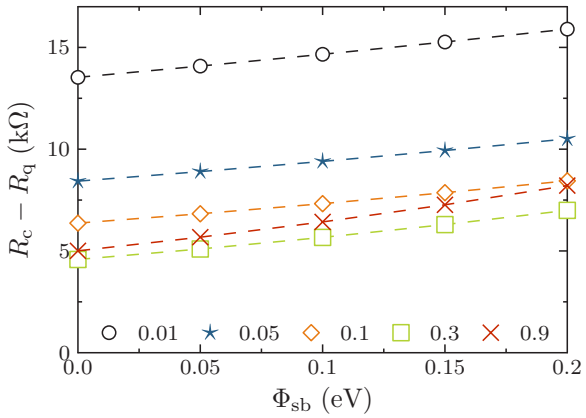

Fig. 5. Simulated contact resistance for different Schottky barrier heights and different DOS within the metal coated tube portion.

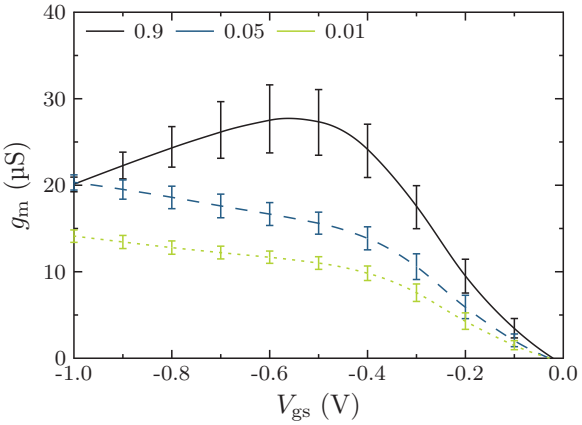

Fig. 6. Transconductance for different contact DOS (i. e. the contact effective mass). The error bars indicate the impact of the Schottky barrier heights which are changed in between 0 eV and 0.2 eV.