Multi-scale modeling of metal-CNT interfaces

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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 dimensions are relaxed which allows an investigation of the metal-CNT interfaces in the long-contact-limit. As suggested in [3], a detailed understanding of the contact physics is 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 energy dependent transmission probability through 10 nm long CNTFET channel with 20 nm long contacts.

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 [3], [5] which has been verified by atomistic simulations. The key contact parameters are the potential step $\triangle\Phi$ (see also [6]), the Schottky barrier height Φ_sb at the interface between metal-coated and uncoated CNT portion, 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 with 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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References

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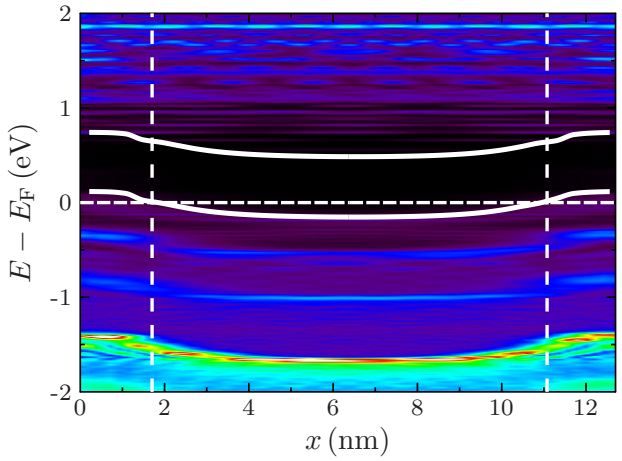

Fig. 1. Atomistically calculated local DOS for a 10 nm long CNTFET with Pd contacts.

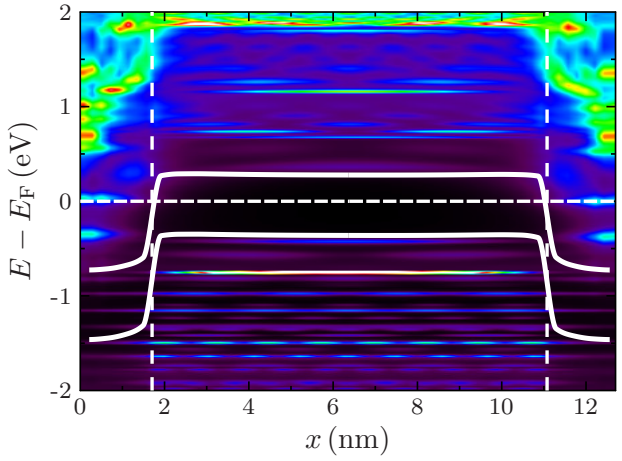

Fig. 2. Atomistically calculated local DOS for a 10 nm long CNTFET with Al contacts.

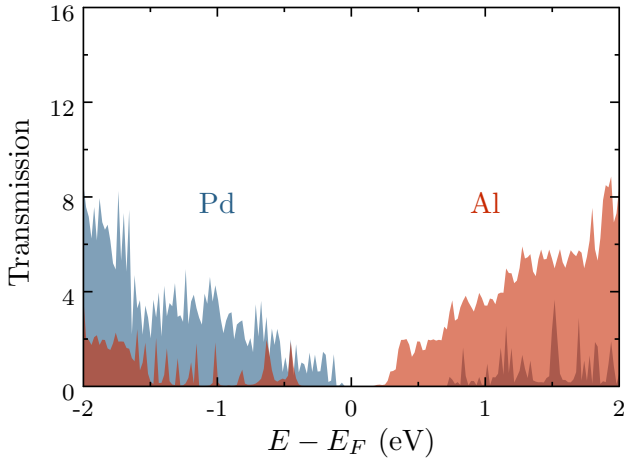

Fig. 3. Atomistically calculated transmission through Pd and Al contacted 10 nm long CNTFETs with 20 nm long contact regions.

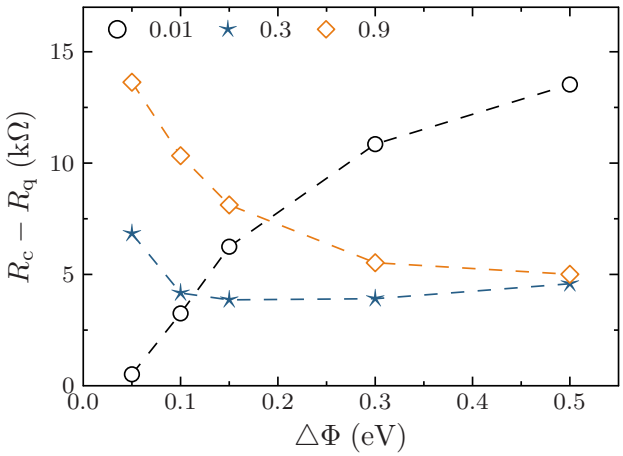

Fig. 4. Simulated contact resistance for various △Φ and effective masses (see legend) in the contact regions.

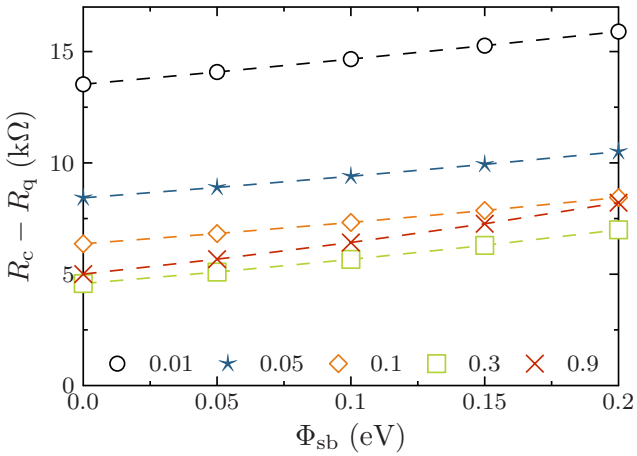

Fig. 5. Simulated contact resistance for various Φ_{sb} and effective masses (see legend) in the contact regions.

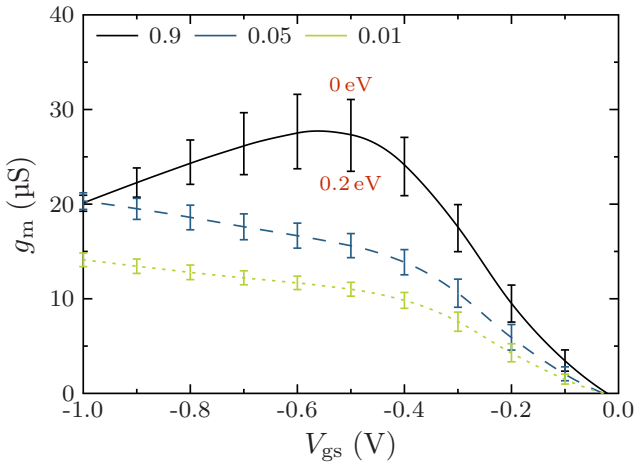

Fig. 6. Transconductance for various effective masses in the contact region. Error bars indicate impact of Φ_{sb} (0 eV – 0.2 eV).