Towards a multiscale modeling framework for metal-CNT interfaces

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***Abstract*—This paper gives a short overview on our recent investigations towards a multiscale modeling and simulation framework for metal-CNT interfaces. We employ three simulation approaches with well defined interfaces. For the simulation at device level we make use of a recently developed wave-function based effective-mass Schrödinger-Poisson solver which employs a hetero-junction like contact model to capture the physics in the contact region where the CNT is embedded into metal. The required model parameters are adjusted to TB and DFT simulation results. A comparison with experimental data for a short channel device shows the applicability of the proposed approach.**

I. Introduction

Very recently, astonishing experimental results for ultra-short Carbon nanotube transistors (CNTFETs) with channel lengths below 10 nm have been published in [1] disproving some theoretical claims made before regarding the scalability of CNTFETs (see [2] for a related discussion). It turned out and it has already been pointed out in e. g. [3] that the contacts need to be carefully described in order to predict the transistor characteristics correctly. Several attempts have been made to model the contact regions and to explain the experimental results in [1] (see [2] for a list of references). Here, we adopt a multi-scale simulation strategy to understand and to model the contact regions at different levels of complexity ranging from (*i*) a sophisticated atomistic simulation approach based on density functional theory (DFT) as implemented in CP2K [4], (*ii*) a tight-binding (TB) model as described in [5] to (*iii*) an effective-mass (EFM) Schrödinger-Poisson solver. More details about the mentioned EFM approach can be found in [6].

An appropriate treatment of the injection of charge carriers into the 1D transistor-channel is essential for predicting the terminal characteristics of CNTFETs. In fabricated transistors, CNTs are embedded into the contact metals [7]. Therefore, the charge carriers are not directly injected from the bulk metal into the transistor channel, but from the metal coated tube portions. Chemical bonding between the contact metal atoms and the CNT atoms can alter the CNT electronic structure considerably [5], [8]. While in DFT simulations the metal atoms of the contacts are included in the simulation of a transistor explicitly, they are considered in the TB approach only by a well-defined self-energy and properly chosen coupling parameters. In the EFM approach the extended metal coated tube region is reduced to a single point and included in the EFM simulations by means of QTBM-like boundary conditions comprising an effective dispersion relation, a potential step at the coated-to-uncoated CNT interface (as depicted in Fig.1) and an effective injection gap. Thus, the coated-to-uncoated CNT interface is modeled as a simplified heterojunction as first described by the authors in [2], [9], [10]. With the latter approach, the simulation of the transistor is thus reduced to the simulation of the channel region (excluding the extended contact regions) and properly defined boundary conditions.

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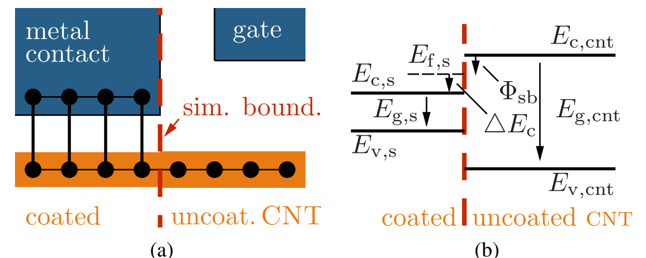


Fig. 1: **(a)** Schematic of the metal-CNT contact region and **(b)** band edge of the heterojunction in this region.

While going through the different abstraction level in the described multi-scale approach one replaces the physical rigor of the DFT method by the more flexible (in terms of reproducing experiments) and fast EFM approach at the cost of the number of model parameters which need to be adjusted. Here, we adopt the following methodology. From the equilibrium DFT-calculations the density-of-states (DOS) within the contact region is extracted and used to adjust the contact parameters of the TB (not shown here) and EFM model (see [6]). The remaining model parameters for the TB and the EFM simulators are adjusted to fit the experimental results published in [1]. In the last step, the current-voltage characteristics calculated with the TB method are used as a reference for the EFM simulations.

II. Results

From the experimental device structure described in [1], three similar structures compatible with the different simula-

tion methods are derived. In all simulations, the channel length is set to 9 nm. A sketch of the atomistic structure used in the DFT simulations is shown in Fig. 2. It comprises three regions: (1) deep contact, (2) interface region between metal coated and uncoated CNT, and (3) uncoated channel region. In fact, the heterojunction-like contact model shown in Fig. 1 captures the physics in region (2).

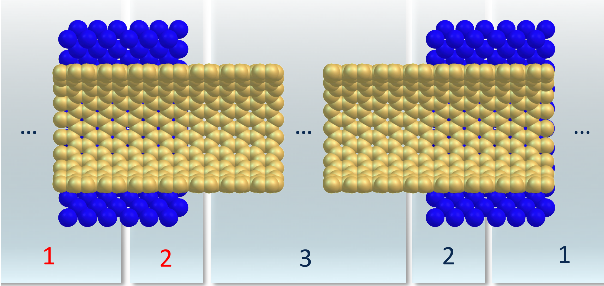


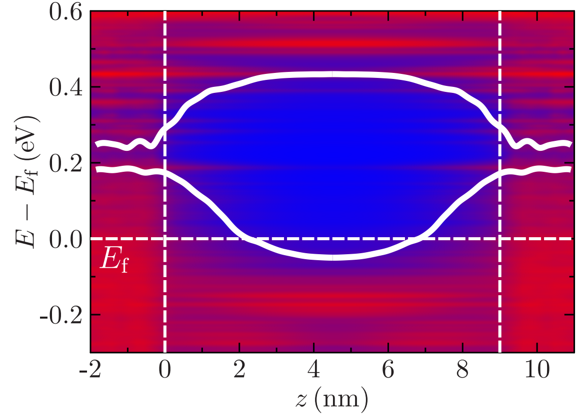
Fig. 2: Atomistic structure of a CNT partially embedded into contact metals.

Fig. 3 shows the local zero-bias DOS computed with the DFT and the EFM solver. In the EFM calculations, the mean local DFT-DOS in the contact region (see Fig. 4(a)) is used to describe the EFM boundary conditions by adjusting the injection band, the potential step and the effective dispersion relation needed for the employed QTBM boundary conditions. Additionally, effective bands are shown marking the region with a negligible DOS. Both calculations are in good agreement. Especially, the EFM results capture both, the injection gap as well as the available states (MIGS) nearby the contact regions in the channel correctly which validates the heterojunction-like contact model for the wave-function based EFM approach. However, to verify non-equilibrium current transport (which is very cumbersome to calculate with the DFT approach), we employ the TB approach to relate the DFT and with the EFM simulations.

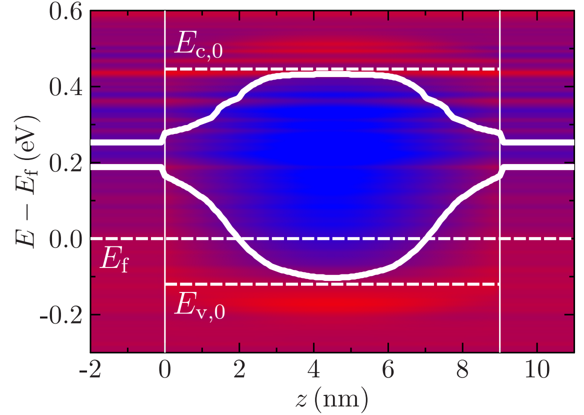
Fig. 4(a) shows a comparison between the mean local DOS of the DFT and the TB model in the metal coated tube portion. For the relevant energies around the Fermi level a good agreement between the DFT and the TB results is reached for a medium coupling strength which justifies the TB model.

The local DOS in the contact region significantly depends on the interaction strength between the metal and the C atoms. In the TB model, the interaction between them is empirically modeled with a coupling parameter [5]. Fig. 4(b) shows the related TB results for different coupling strengths. It is obvious that the effective injection gap depends on the coupling strength. The stronger the interaction, the smaller is the injection gap.

From the TB simulation results, effective dispersion relations are derived for the EFM approach allowing the calculation of the current voltage characteristics for different coupling strengths by means of the EFM approach. Two different effective masses are extracted from the reference data to match either the momenta or the group velocity of the injected carriers.



(a)



(b)

Fig. 3: Local DOS (logarithmic scale) along the transistor (including the contact region) projected to the C atoms calculated with (**a**) the DFT and (**b**) the EFM approach.

The simulation results of the TB and the EFM approach are in good agreement (not shown here).

A comparison of the EFM results with the experimental results published in [1] is shown in Fig. 5 for different coupling strengths. Obviously, the optimal coupling strength for a good fit should be neither very strong nor too weak.

It also has to be pointed out that the employed contact model and especially the effective dispersion relation has a significant impact on the bias-dependent charge injection and thus on the high-frequency capability of the device. Fig. 6 shows the quasi-static transit frequency f_T for the device analyzed in Fig. 5. Obviously, the peak value and the whole bias-dependence changes if the coupling strength between the CNT and the metal is changed.

III. Conclusion

In this paper a methodology to adjust the contact parameter of a wave-function based effective-mass Schrödinger-Poisson solver to TB and DFT simulation results has been presented. A comparison to experimental results shows the applicability of the approach. In addition, the DFT simulation results justify a

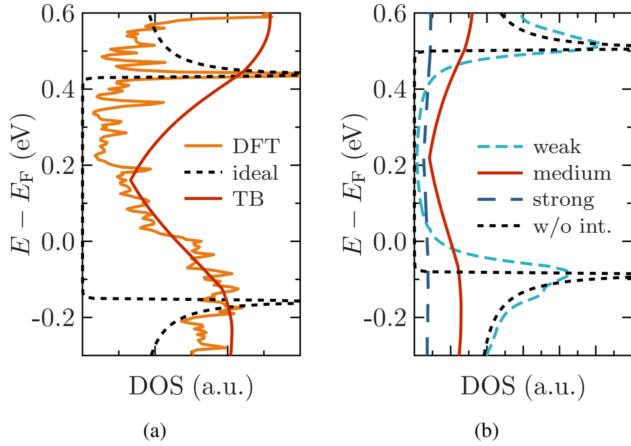


Fig. 4: (**a**) Mean values for the DOS in the contact region from the DFT and the TB approach. (**b**) TB calculated DOS in the contact region for different coupling strengths. Note that the DOS plots are partially scaled.

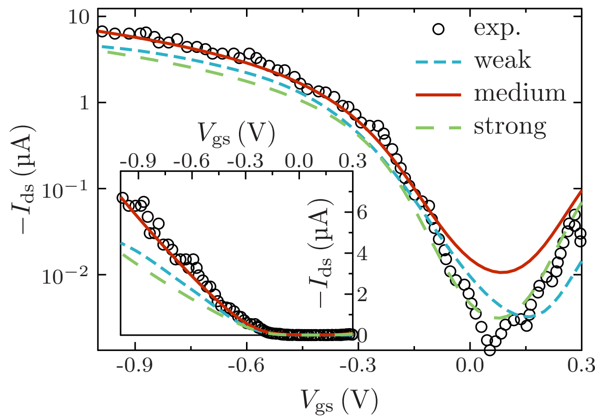


Fig. 5: Comparison between experimental [1] and EFM results for different coupling strengths ($V_{ds} = -0.4\,\text{eV}$).

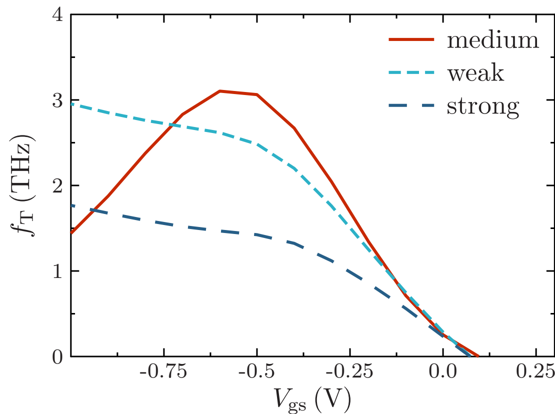


Fig. 6: Transit frequency calculated by means of the EFM approach for different coupling strengths ($V_{ds} = -0.4\,\text{eV}$).

recently published heterojunction-like contact model capturing the physics in the interface between a metal-coated to an uncoated CNT including an injection gap and a potential step at this interface and an effective dispersion relation for the QTBM-like boundary conditions.

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