Multiscale Approaches for Electronic Device Simulation

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Abstract— **Simulation of electronic devices relies to large extent on semi-classical models, especially the drift-diffusion model. Where quantum effects or atomistic details are particularly important, more involved models are used. Ideally, a combination of models on different scales would allow the simulation of the overall device structure. Here we present some approaches for combining continuum and atomistic models with the drift-diffusion model for the simulation of optoelectronic devices.**

I. Introduction

Semi-classical models are still used predominantly for the simulation of optoelectronic devices, since they have low computational cost and can provide reasonably accurate results, although in many cases quantum effects are playing a crucial role for the optoelectronic properties or in electronic transport. However, more accurate and possibly predictive simulation models are required, ideally without sacrificing completely the advantages of well-established semi-classical models [[1]-[3]].

In this work we illustrate our past and current efforts in combining drift-diffusion based device simulation models with continuum and atomistic quantum mechanical approaches, and with non-equilibrium Green's functions (NEGF). Our strategy follows a top-down approach, starting from the device level and enhancing the model locally where necessary. The interest is mostly devoted towards semiconductor hetero-structures, in particular based on III-nitrides and III-V, but also 2D materials. In such a context the semi-classical model can be corrected in a variety of ways, for example via a more accurate description of the local density of states including quantum confinement or atomistic details, or by correcting the local-equilibrium transport model by non-equilibrium or non-local effects, especially at hetero-interfaces or in quantum-confined structures [4].

The coupling of atomistic with semi-classical models is of particular interest in the simulation of short-period superlattices, tunneling structures and alloys, and has been used in recent years for the study of random alloy effects in alloy-containing quantum wells [5][6].

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II. Coupling of Atomistic and Continuum Models

Atomistic models are computationally expensive, and therefore usually only the active region of a device can be treated atomistically. However, in order to be able to obtain a simulation of the overall device, a consistent embedding of the atomistic model into the continuous media models is required. This allows to perform the simulation under realistic operating conditions and therefore to compare results with experimental data. We follow a top-down approach, where the atomistic structure is constructed automatically in the regions of interest, based on the assumption of pseudomorphic growth. We then use empirical tight binding (ETB) to calculate the single-particle states and optical properties. The ETB Hamiltonian is assembled using the electrostatic potential obtained from the semi-classical simulation at the operating point of interest, possibly self-consistently with a less computationally intensive quantum model like the effective mass approximation. For alloys, the atomic species are assigned randomly with spatially uniform or non-uniform probability, the latter to model effects of clustering. Figure 1. shows as an example an InGaN/GaN single-quantum well (QW) device, where the active regions (InGaN QW with pieces of the GaN barrier) are modelled atomistically.

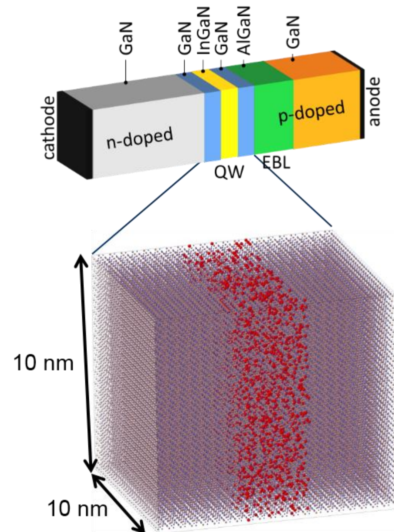

Figure 1. Simulation model of InGaN/GaN single-quantum well device, where the active region is modelled atomistically.

III. COMBINING NEGF WITH DRIFT-DIFFUSION

Non-equilibrium Green's functions are widely used for the calculation of quantum transport. However, it becomes computationally extremely demanding when including the relevant scattering processes. Moreover, some interband processes like Auger recombination, important in nitride LEDs, are very challenging and have not yet been implemented in NEGF.

It is of a certain interest to combine NEGF with the computationally inexpensive drift-diffusion model. One possible approach is to employ NEGF in regions where quantum transport is important and implement the coupling between the two via boundary conditions in regions where the local carrier distribution can be assumed to sufficient accuracy in a local equilibrium. Alternatively, a local recombination rate for the drift-diffusion model can be extracted from the NEGF scattering self-energies [4].

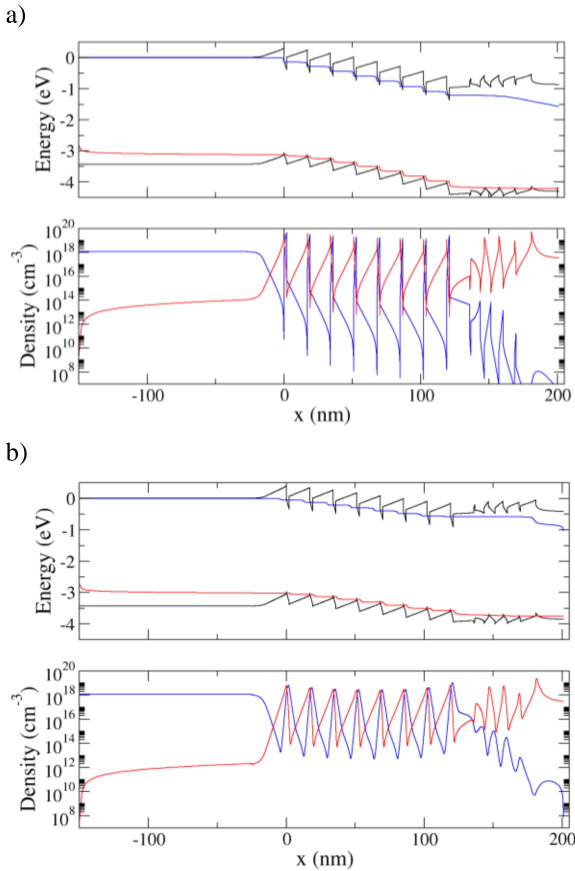

Figure 2. Simulation model of InGaN/GaN multi-quantum well device, fully classically in a), selfconsistent with Green's functions in b). The two simulations correspond to roughly the same device current. The top panels show the conduction and valence band edges and the quasi-Fermi levels, the bottom panels electron and hole denisties. Quasi-Fermi level and density of electrons are given in blue, of holes in red.

A further effective way of using Green's functions in the context of semi-classical models is to obtain quasi-equilibrium carrier densities in extended nanostructures like multi-quantum wells, by occupying the local density of states (LDOS) under assumption of a local quasi-equilibrium. This basically leads to a quantum-corrected drift-diffusion, however, the calculation of the carrier densities can be implemented in a computationally effective way by contour integration and reusing integration points. The advantage is that the density can be calculated effectively in large structures, as shown in Figure 2. In this example we simulated an InGaN/GaN multi-quantum well structure fully classically and self-consistently with the NEGF carrier densities on the whole structure, at approximately the same device current. The local quasi-Fermi levels, shown in the panels with the band edges, has been used to calculate the densities. As seen, the quantum densities can be obtained both in the quantum-confined and unconfined parts, which would be hard to achieve when calculating explicitly the eigenstates of the Hamiltonian. The importance of an accurate representation of the densities especially in the barriers, where it is lower, is given by the fact that this influences the effective barrier resistivity and thus forward voltage, which can be observed in the different drops in quasi-Fermi levels between individual QWs.

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