Coupling Atomistic and Finite Element Approaches for the Simulation of Optoelectronic Devices

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***Abstract*—Multiscale methods coupling quantum mechanical/atomistic models such as envelope function and tight binding approaches with continuous media models e.g. for strain or electronic transport are very useful for an accurate simulation of modern and emerging electronic and optoelectronic devices based on nanostructured active regions. We present simulations using TiberCAD whose main focus is on providing an integrated multiscale/multiphysics simulation environment.**

I. Introduction

The functionality of many modern and emerging electronic and optoelectronic devices is based on nanostructures such as quantum dots, nanowires or carbon nanotubes. Structures containing quantum dots are particularly interesting for use as photodetectors, light emitters or as single photon sources. An accurate simulation of such devices has to go beyond the semi-classical models which are used to describe conventional devices. Fully quantum mechanical or atomistic approaches are needed to obtain a correct description of structural, electrical and optical properties. Usually, the active part of a device which needs such a treatment is small compared to the overall simulation domain. The computational cost of more accurate quantum mechanical models however forbids their application to the whole device. It is therefore necessary to adopt a multiscale simulation approach which couples the semi-classical models describing the surroundings of the active region to the quantum mechanical or atomistic models acting only on the nanostructured parts of the device.

It is the aim of the TiberCAD project [1], [2] to provide an integrated multiscale and multiphysics simulation environment capable of coupling different models on different scales in a unified and transparent way.

In this work we present simulations of the optical properties of nanostructures based on the envelope function approximation (EFA) and on the empirical tight binding (ETB) method.

II. Simulation models

Strain has a critical influence on the behaviour of heterostructures due to its effect on the band energies and the strain induced piezoelectric polarization. The latter is particularly important in nitride-based devices. The calculation of strain in lattice mismatched heterostructures is based on linear elasticity theory of solids, assuming pseudomorphic interfaces between different materials [3]. We assume small deformation such that the strain is a linear function of deformation and that Hooke's law can be used which linearly relates stress to strain. The strain and deformation field is found by minimizing the elastic energy of the system. As a result we obtain the strain tensor in any point of the structure, the shape deformation and the piezoelectric polarization, which depends linearly on strain. Self-consistent electromechanical simulations can be carried out by including the converse piezoelectric effect.

Transport of electrons and holes is treated in a semi-classical picture based on the drift-diffusion model. The particle fluxes are written in terms of the electrochemical potentials. The conduction and valence band edges and effective masses are obtained from bulk $\mathbf{k}\cdot\mathbf{p}$ calculations, including the corrections due to strain. For non-isothermal simulations the particle fluxes are modified to include the Seebeck effect.

Quantum mechanical models are used for the calculation of eigenstates of confined particles in nanostructures, either based on the envelope function approximation (EFA) or on atomistic approaches [4]. In the former the Hamiltonian of the system is constructed in the framework of single-band and multiband $\mathbf{k}\cdot\mathbf{p}$ theory [5], [6]. The atomistic approaches are based on the empirical tight binding (ETB) method. In this method the electronic states are written as a linear combination of atomic orbitals (LCAO), whereas in EFA the Bloch functions are used as basis. The atomistic structure, which is needed for ETB calculations, is generated internally in TiberCAD according to the macroscopic device description and crystallographic orientation. The generation algorithm allows for pseudomorphic heterostructures, and it is able to deform the atomistic structure according to the strain obtained from the continuous media elasticity model by projecting the deformation field onto the atomic positions. In a similar way, the macroscopic electrostatic potential calculated in the Poisson/drift-diffusion model is projected onto the atomic positions in order to couple the atomistic model to the continuous media models.

The solution of the eigenvalue problems resulting from the EFA and ETB models provides the energy spectrum, the particle densities and the probabilities of optical transitions. The particle densities are calculated by populating the electron and hole states according to the expectation value of the corresponding electrochemical potential $\bar{E}_F = \langle\psi_i|E_F|\psi_i\rangle$. The particle densities can be fed back to the Poisson/drift-diffusion model for self-consistent Schrödinger–Poisson/drift-diffusion calculations. In the case of ETB, the resulting density

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has to be projected onto the finite element mesh used for the continuous media models.

The implementation of both EFA and ETB in the same software in a consistent and transparent way opens the possibility of doing concurrent simulations using both models on exactly the same structure. This allows on the one hand to compare the results of the two methods, and on the other hand it could be used to tune the $\mathbf{k}\cdot\mathbf{p}$ parameters needed for the EFA calculation based on more accurate ETB results.

III. Simulation example

As an example we show some results of the simulation of a hexagonal $Al_{0.3}Ga_{0.7}N$ nanocolumn in p-i-n configuration with embedded GaN quantum dot (QDot). The column is assumed to be grown along the c-axis on top of an unstrained AlGaN layer. First we calculate strain based on linear elasticity. Additionally, we deform the mesh according to the found deformation field. Then we solve the Poisson/drift-diffusion model, applying an external voltage of 3.5 V between the top and the bottom of the column. The resulting electrostatic potential profile, which includes the effects of spontaneous and piezoelectric polarization, is then used for an EFA and a ETB calculation. The latter are restricted to the central part of the structure containing the GaN QDot. The trace of the strain tensor, representing the relative volumic change, is plotted in Fig. 1, together with the atomistic structure used for the ETB calculus. In Fig. 2 we show the emission spectra for the different polarizations as obtained from the EFA calculation. The first electron and hole states resulting from both EFA and ETB are plotted in Fig. 3.

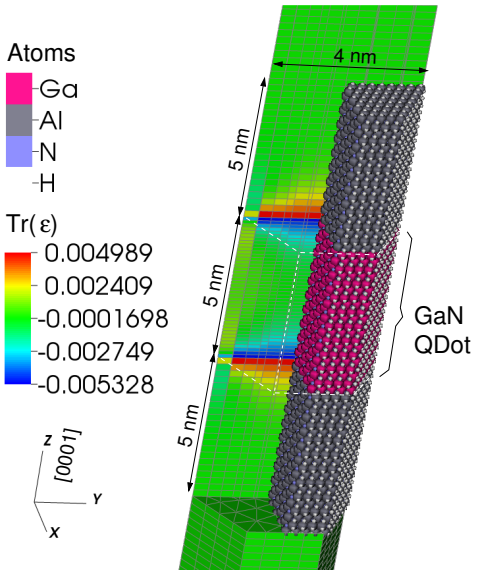

Fig. 1: Trace of the strain tensor and internally generated atomistic strcuture. The extension of the latter indicates the simulation domain for the quantum mechanical calculations. The total length of the nanocolumn is 35 nm.

References

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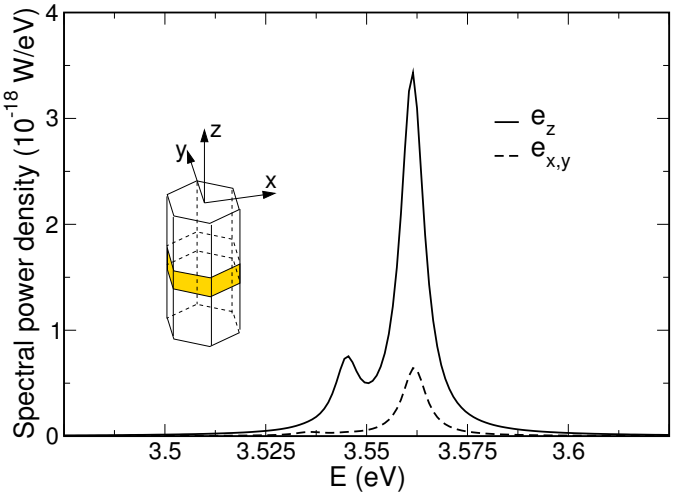
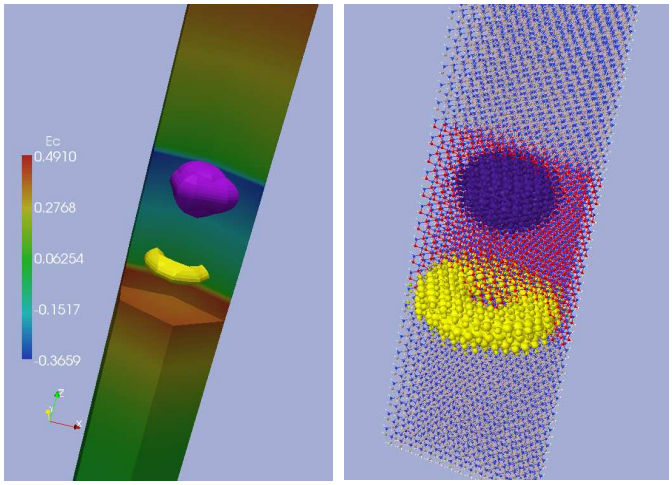


Fig. 2: The emission spectra for different polarizations calculated using EFA.



(a) (b)

Fig. 3: First electron (violet) and hole (yellow) states obtained at 3.5 V for the EFA (a) and for the ETB (b) calculations. The EFA result is plotted on top of the conduction band profile. The doughnut shape of the hole state is mainly due to strain.