Towards multiscale modeling of III-N-based LEDs

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***Abstract*—We present steps towards establishing a multiscale framework for simulating electronic and transport properties of nitride-based LEDs. Here, the connection between atomistic tight-binding calculations and continuum-based models will be discussed. We show how finite element and finite volume meshes are generated for this purpose. As a first application, the electronic structure of an InGaN quantum well is studied by means of tight-binding theory and a single band effective mass approximation and the results are compared. In this comparison, the only adjustable parameter is the effective mass in the continuum-based calculations, since local band edges are directly obtained from tight-binding. Finally, first LED device calculations, using a drift-diffusion model, are presented.**

I. Introduction

InGaN quantum wells (QWs) are the cornerstone of modern, energy efficient light emitting diodes (LEDs) operating in the blue spectral region. However, even though these systems have found widespread applications, several basic physical properties are still under discussion, for instance, the origin of the efficiency drop of devices emitting in the green spectral region. A key aspect that only has been targeted very recently is the impact of the alloy microstructure on the electronic, optical and transport properties of InGaN/GaN heterostructures [1], [2]. It has been shown that already random alloy fluctuations in an InGaN QW can lead to strong carrier localization effects. In standard continuum-based descriptions, such effects are not included. Thus, to simulate the characteristics of InGaN/GaN based LEDs, a multiscale approach is required [3]. Here the active region is modeled on an atomistic scale, thus accounting for (local) alloy disorder effects, while the GaN barrier and the contact region is treated on a continuum-based level. In this work we present steps towards such a framework, here connecting atomistic tight-binding (TB) theory and continuum-based electronic structure and drift-diffusion transport models.

II. Multi-scale Modeling Approach

Our multiscale approach is schematically depicted in Fig. 1. The starting point is an atomistic TB model, discussed in Ref. [1], which allows to account for fluctuations in the potential energy landscape due to (random) alloy fluctuations in an InGaN/GaN QW. By diagonalizing the TB Hamiltonian at each lattice site, local conduction (CBE) and valence band edges (VBE), including local strain and built-in potential effects, can be obtained. This data serves as input to construct a finite element mesh, using TetGen [4], that has as many

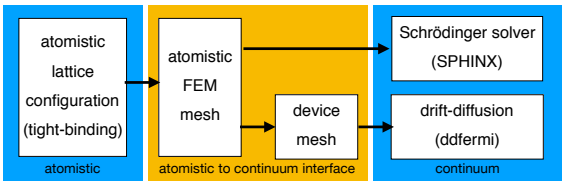

Fig. 1. Schematic illustration of the multi-scale workflow and the meshes underlying when connecting the different length scales/models.

nodes as atoms in the system; the values at these nodes are determined by the TB CBE and VBE energies at these sites. At the interface region between well and barrier, the nitrogen atoms see a mixed number of Ga and In atoms. Thus, in a finite element mesh this interface is also not sharp, even though we do not introduce any penetration of In atoms into the GaN barrier. An example mesh, using a virtual crystal approximation (VCA) in the TB model, is shown in Fig. 2 (a), which reveals this effect. Here, for a structure with 13,260 atoms, the resulting mesh has 13,260 nodes and 93,210 tetrahedra.

While such an approach allows to calculate electronic states of a QW system, for full device calculations also contact regions have to be added. As a test-bed we use a p-i-n diode structure, where the above described atomistic finite element mesh is used for the intrinsic device region. To that end, p- and n-doped GaN regions were added/attached to the active region using TetGen [4]. In doing so, the total number of nodes increases to 19,808. For device simulations, using finite volume methods, this mesh must be a boundary conforming Delaunay triangulation [4], which is generated here using TetGen. In the above case the resulting quality finite volume mesh has 24,472 nodes and 131,265 tetrahedra and is shown in Fig. 2 (b).

III. Results

Having introduced the general theoretical framework established here, we present some results obtained from the above test structure. In a first step, the electronic structure (electron and hole states) obtained from TB and single-band effective mass approximation (EMA) is compared. In a second step, we briefly discuss InGaN-based LED calculations in the frame of a drift-diffusion model utilizing ddfermi [5] with TB input for the active region.

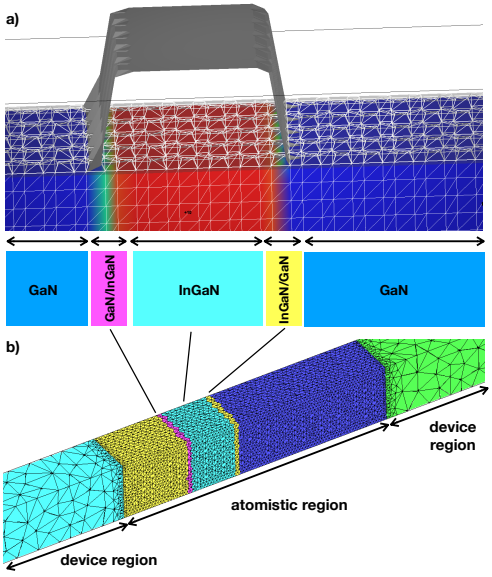

Fig. 2. (a) Atomistic finite element mesh along with the VBE profile on a crosssection (gray). Material domains and interface regions are indicated in the lower part. (b) Finite volume mesh generated for device simulations with contact regions (device regions) attached to the atomistic region.

A. Electronic states: Continuum vs tight-binding model

Here, our starting point is a 2.6 nm wide $In_{0.15}Ga_{0.85}N$/GaN single QW treated in VCA. To study the electronic states in a continuum-based model, we use an EMA for both electrons and holes. The EMA is implemented in the highly flexible plane wave code S/Phi/nX [6], which allows us to go to multiband approaches easily in future studies. To demonstrate the workflow, the calculations are performed in the absence of strain or built-in fields. We stress that using our multiscale frame, Fig. 1, the only adjustable parameter in the EMA is the effective electron/hole mass. The CBE and VBE profiles are directly obtained from the TB local band edges. The transfer/interpolation of data from the finite element mesh to a S/Phi/nX compatible grid is achieved by WIAS-pdelib. The results of the EMA can now be directly compared to TB data, summarized in Table I. For the holes we focus on heavy hole states only, noting that additional states come into play in the multi-band TB results, which have been excluded in the presented comparison. As Table I shows, excellent agreement between TB and EMA is found for both electrons and holes.

B. Drift-diffusion simulation

Using the device mesh discussed above, we have performed full drift-diffusion calculations employing ddfermi [5]. More specifically we studied the electrostatic potential and carrier densities inside the InGaN-based LED for different applied biases. In the equilibrium case we find the expected potential drop across the atomistic structure and the alignment of the Fermi levels.

IV. Summary and Outlook

In this work, steps towards the multiscale modeling of electronic, optical and transport properties of nitride-based heterostructures and devices have been presented. The starting point for our framework is atomistic TB theory, which provides input for continuum-based drift-diffusion calculations. To achieve this, we have established an interface that maps TB output in terms of local CBE and VBE onto a finite element mesh. This atomistic finite element mesh can now be embedded in a larger device mesh that accounts also for contact regions, thus allowing for device simulations. To this end, a quality finite volume mesh (boundary conforming Delaunay triangulation) is generated for device simulations by means of drift-diffusion models. Given that the overall atomistic to continuum frame is established, future studies will target the question of how alloy fluctuations affect the electronic and transport properties of nitride-based heterostructures and devices. Additionally, as shown above for electron and hole states, our presented approach includes a feedback loop, meaning that benchmarking and validation of the outcome of the continuum-based calculations against the results from atomistic modeling is possible.

TABLE I
Energies of the first 3 electron and hole states calculated within TB and EMA. For electrons an isotropic effective mass ($m_e = 0.18m_0$) has been used, while for the hole different masses in the growth plane ($m_h^x = m_h^y = 1.79m_0$) and along the c-axis ($m_h^z = 1.87m_0$) have been applied.

	Electrons		Holes	
State #	TB	EMA	TB	EMA
1	2.945 eV	2.948 eV	0.093 eV	0.093 eV
2	3.029 eV	3.029 eV	0.085 eV	0.085 eV
3	3.029 eV	3.029 eV	0.085 eV	0.085 eV

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