Connecting atomistic and continuum models for (In,Ga)N quantum wells: From tight-binding energy landscapes to electronic structure and carrier transport

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***Abstract*—We present a multi-scale framework for calculating electronic and transport properties of nitride-based devices. Here, an atomistic tight-binding model is connected with continuum-based electronic structure and transport models. In a first step, the electronic structure of (In,Ga)N quantum wells is analyzed and compared between atomistic and continuum-based approaches, showing that even though the two models operate on the same energy landscape, the obtained results differ noticeably; we briefly discuss approaches to improve the agreement between the two methods. Equipped with this information, uni-polar carrier transport is investigated. Our calculations reveal that both random alloy fluctuations and quantum corrections significantly impact the transport, consistent with previous literature results.**

I. Introduction

A key building block for energy efficient light emitting diodes (LEDs) operating in the blue spectral region are (In,Ga)N quantum wells (QWs). To guide the design of LEDs, understanding the fundamental electronic, optical, and transport properties is an essential ingredient. It is important to note that III-N materials exhibit very different properties compared to other III-V materials, as e.g. (In,Ga)As. This starts with the underlying wurtzite crystal structure, ranges over to strong electrostatic built-in fields, and finally is reflected in strong carrier localization effects. The last aspect is tightly linked to alloy fluctuations [1]. Standard continuum-based models, e.g. effective mass approximations (EMAs), underlying the workhorse of LED transport calculations, namely drift-diffusion (DD) solvers, do not capture such effects. Atomistic models, which can capture alloy fluctuations on a microscopic level and when coupled to fully quantum mechanical solvers, e.g. non-equilibrium Green's function methods [2], are in general numerically too expensive to target a full device. Recent studies building on modified continuum models have shown the strong impact of alloy fluctuations on the transport properties of (In,Ga)N LEDs [3]. All this highlights that the modeling of III-N-based LEDs is intrinsically a multi-scale problem [4].

We establish such a framework by connecting atomistic tight-binding (TB) theory with continuum-based models. Here, we generate local band edge energies from TB [5], which account for random alloy fluctuations and the obtained landscape can serve as input for modified continuum-based electronic structure and transport calculations. In doing so (i) strain and polarization field fluctuations are directly included in the TB band edges, (ii) a direct comparison of the electronic structure obtained from TB and EMA can be targeted and (iii) the approach can be connected to localization landscape theory (LLT) to account for quantum corrections in DD studies [3].

II. Multi-scale simulation framework

Our multi-scale simulation framework starts from the atomistic TB model introduced in Ref. [1]. Using the TB Hamiltonian, local conduction (CBE) and valence band edge (VBE) values are calculated. Having obtained TB band edge data at each lattice site, we employ TetGen [6] to construct a finite element mesh that has as many nodes as atoms in the system; the values at the nodes are given by the TB CBE and VBE energies. The generated mesh is then used as input for electronic structure calculations in the frame of a single-band EMA, implemented in the flexible plane wave solver Sphinx [7]. The approach has been extended to evaluate LLT [3] on the established mesh and the determined energy landscape is employed in carrier transport calculations. Here, also contact regions are added and described by a coarser grid compared to the active region; the required mesh is generated using TetGen [6]. As a test-bed, we study n-doped/intrinsic/n-doped (In,Ga)N systems. The carrier transport calculations are performed using ddfermi [8].

III. Results

In the following sections, we present results obtained within the above detailed framework both for the electronic structure, Sec. III-A, but also for transport properties, Sec. III-B.

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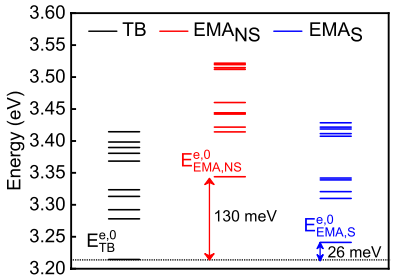

Fig. 1. The ten energetically lowest electron states (averaged over 10 alloy configurations) in an $In_{0.1}Ga_{0.9}N$/GaN QW. Tight-binding results in black, single-band effective mass approximation, with and without a shift of the conduction band edge energy, are given in blue and red, respectively.

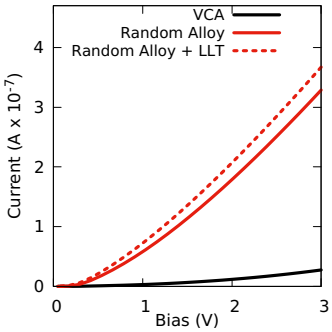

Fig. 2. Current voltage characteristics of a unipolar single $In_{0.1}Ga_{0.9}N$ QW device. The calculations have been performed using a virtual crystal approximation (VCA, solid black) and when accounting for random alloy fluctuations. In the random alloy case, results with (dotted red) and without (solid red) quantum corrections via localization landscape theory are presented.

A. *Electronic states: Continuum vs. tight-binding model*

Figure 1 depicts the energies of the ten lowest electron states in an $In_{0.1}Ga_{0.9}N$ QW; the results are averaged over ten different random alloy configurations. The TB data, E_{TB}, present the benchmark for the continuum-based calculations. Results from single-band EMA studies, $E_{\mathrm{EMA,NS}}$ and $E_{\mathrm{EMA,S}}$ (explained below/Fig. 1), operating on the TB energy landscape are also given. In principle, since band offsets, strain and polarization fields are included in the TB energy landscape, the only free parameter in the EMA is the effective electron mass, which has been determined by a comparison with VCA results [5]. However, as Fig. 1 shows, a noticeable difference in the ground state energies $E^{e,0}_{\mathrm{TB}}$ and $E^{e,0}_{\mathrm{EMA,NS}}$ is observed, while the energy separation between excited states is very similar. As discussed in Ref. [5], there are several ways forward to improve the agreement, including adjusting the band offset in the EMA calculations, as shown in Fig. 1 by $E_{\mathrm{EMA,S}}$.

We note that for hole states a similar behavior is observed [5], indicating that care must be taken when employing a modified continuum-based model to capture carrier localization effects in (In,Ga)N heterostructures. However, our approach allows to establish an improved continuum model that can then be used in carrier transport calculations.

B. *Drift-diffusion simulation*

Using the TB energy landscape, and including the band offset corrections required for the EMA (see above), we have simulated the I-V curve of an n-doped/intrinsic/n-doped single $In_{0.1}Ga_{0.9}N$/GaN QW device. In Fig. 2 we compare results obtained within VCA and when accounting for random alloy fluctuations. In the latter case, quantum corrections via LLT can also be taken into account. Figure 2 clearly shows that random alloy fluctuations and quantum corrections significantly increase the current above the turn-on voltage compared to VCA. This finding is consistent with previous results on (In,Ga)N based devices [3], highlighting again the importance of alloy fluctuations and quantum corrections for an accurate description of carrier transport in such structures.

IV. Summary and Outlook

By connecting atomistic TB theory with continuum-based models we have developed a multi-scale framework that targets both the electronic structure but also carrier transport in (In,Ga)N-based heterostructures and devices. Our calculations show that even when operating on the TB determined energy landscape, a noticeable difference in electron (and hole) ground state energies is observed between atomistic and continuum-based models. However, by modifying the carrier confinement in the EMA, good agreement with the TB model is achieved, at least in terms of energies. Building on the benchmarked EMA, uni-polar electron transport in an (In,Ga)N QW device has been investigated, revealing that alloy fluctuations and quantum corrections significantly impact the I-V curves of the device. The developed multi-scale simulation framework allows us now to target full LED structures.

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