Carrier transport in (In,Ga)N quantum well systems: Connecting atomistic tight-binding electronic structure theory to drift-diffusion simulations

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***Abstract*—Understanding the impact of the alloy microstructure on carrier transport in (In,Ga)N/GaN quantum well systems is important for aiding device design. We study the impact that alloy fluctuations have on uni-polar carrier transport for both electrons (n-i-n junction) and holes (p-i-p junction) using a multiscale framework. To do so we connect an atomistic tight-binding model to a 3D macroscale drift-diffusion solver, *ddfermi*, which includes quantum corrections through the localization landscape theory. Results indicate that for electrons, alloy fluctuations lead to a higher current at a fixed bias compared to a calculation without alloy fluctuations. In contrast, alloy induced hole localization effects results in a reduced current.**

***Index Terms*—III-Nitrides, multiscale modelling, transport, quantum wells**

I. Introduction

Due to, in principle, flexible bandgap engineering, the semiconductor alloy (In,Ga)N has attracted significant attention for optoelectronic device applications in the visible spectral range [1]. III-Nitrides have properties which differ from other III-V materials: they form preferentially in the wurtzite crystal phase, and (In,Ga)N/GaN heterostructures grown along the [0001]-direction (c-axis) exhibit strong built-in polarization fields [2]. These fields lead to a red-shifting of emission wavelength and decreases the overlap between electron and hole wavefunctions. On top of this, (In,Ga)N alloys exhibit strong carrier (hole) localization effects which is not found in other III-V alloys (e.g. InGaAs) [3]. Carrier localization has been shown to be important for electronic, optical and transport properties of (In,Ga)N/GaN quantum well (QW) systems [3], [4].

The most frequent approach to modelling transport properties of these systems is using a 1D virtual crystal approximation; this is the method used in most commercial software packages. A 1D model cannot capture localization effects, as describing the in-plane variation of alloy composition is impossible. Therefore, to simulate these systems ideally a 3D framework is required. Here we present a full 3D model which includes alloy fluctuations as well as quantum corrections. To disentangle transport properties from other effects such as recombination we first look at uni-polar transport for both electrons and holes.

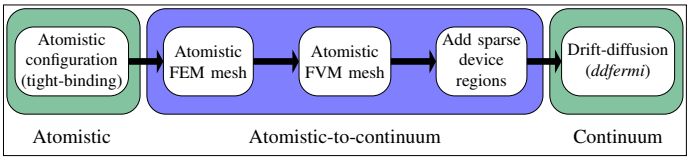

Fig. 1. Schematic of workflow connecting atomistic tight-binding model to continuum-based drift-diffusion.

II. Theoretical framework

In this work we connect an atomistic tight-binding (TB) model to a 3D continuum-based drift-diffusion framework utilizing *ddfermi* [4], [5]. An overview of the workflow is shown in Fig. 1. Starting from atomistic tight-binding theory, we construct a local Hamiltonian at each lattice site which is used to extract an (alloy disordered) energy landscape describing the valence band and conduction band confining potentials [4]. The energy landscape generated on an atomistic level accounts for (local) strain and polarization effects. The locally fluctuating band edges are placed on an atomistic finite volume method (FVM) mesh, which is then embedded within a sparser device mesh. This mesh contains information about device regions where alloy fluctuations are not critical, e.g. n- or p-doped GaN regions, which allows the simulation to be ultimately scaled up to full device modelling while maintaining a feasible numerical burden. Localization landscape theory has been used to efficiently include quantum corrections by generating an effective confining potential [6].

To investigate the impact of alloy fluctuations on carrier transport, random alloy calculations are compared to a virtual crystal approximation (VCA). In a VCA any spatial fluctuations in QW alloy composition are neglected, and piecewise-constant effective material parameters are used within this region; this is a 3D analogy of the 1D simulations available in many commercial software packages.

III. Results

In this section we present results on the impact of alloy fluctuations on uni-polar carrier transport through a single $In_{0.1}Ga_{0.9}N$ QW which is embedded within a GaN barrier.

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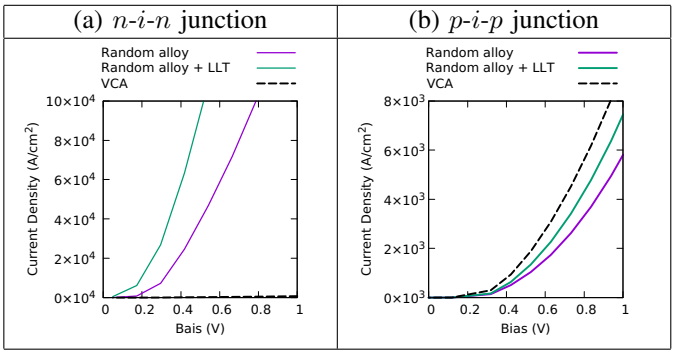

Fig. 2. Current density-voltage curves for (a) electrons in an n-i-n junction and (b) holes in a p-i-p junction. Results are shown for a single quantum well using a random alloy calculation *excluding* quantum corrections (purple), a random alloy calculation *including* quantum corrections via localization landscape theory (LLT) (green) and a virtual crystal approximation (VCA) (black, dashed).

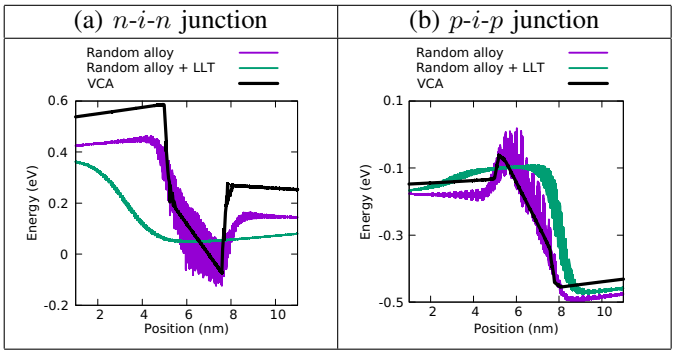

Fig. 3. Band edge profile along transport direction (c-direction) at equilibrium (0 V) for (a) the conduction band edge of an n-i-n junction and (b) the valence band edge of a p-i-p junction. Results are shown for a single quantum well using a random alloy calculation *excluding* quantum corrections (purple), a random alloy calculation *including* quantum corrections via localization landscape theory (LLT) (green) and a virtual crystal approximation (VCA) (black).

Results are discussed for electrons (Sect. III-A) and holes (Sect. III-B).

A. Uni-polar electron transport

Our results show that in the case of electrons, a VCA gives a significantly lower current density than the random alloy calculations (cf. Fig. 2 (a)) [4]. Including alloy fluctuations leads to a softening of the potential barriers at the QW interfaces which is not captured in a VCA. This is visible in Fig. 3 (a) where the conduction band edge of a single QW at equilibrium is shown. Quantum corrections result in a further softening of this barrier which leads to an increase in current in both the VCA (not shown) and random alloy calculations.

B. Uni-polar hole transport

Holes show contrasting results: the current density of a VCA exceeds the current density in a random alloy calculation (cf. Fig. 2 (b)) [7]. The valence band edge fluctuations (cf. Fig. 3 (b) (purple)) and the high hole effective mass lead to strong alloy-disorder-induced carrier localization within the QW region in the random alloy case. The coupling of the valence band edge, Fermi levels and charge densities with the device potential leads to a depletion of holes in the barrier material. In turn, this results in an increased resistance in the barrier due to fluctuations in the QW. The inclusion of quantum corrections via localization landscape theory reduces these strong fluctuations, and thus leads to an increased current, however, the random alloy current does not exceed the current of the VCA at a given bias point.

IV. Conclusion and Outlook

We have presented here a framework to connect an atomistic tight-binding model to a macroscale drift-diffusion solver, *ddfermi*. Applying this to uni-polar transport for both electrons and holes has revealed that alloy fluctuations results in an increase in electron transport due to the softening of the potential barrier compared to a virtual crystal approximation. In contrast, due to alloy-disorder-induced localization effects, hole transport is reduced. In all cases, quantum corrections lead to an increase in current due to the smoothing of the fluctuations and potential barrier.

Equipped with this framework we extend our study to a p-i-n junction. We will present results on the impact of alloy fluctuations on charge carrier distribution and recombination processes across a multi-QW in an LED.

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