Multi-scale hybrid band simulation of (Al,Ga)N UV-C light emitting diodes

Robert Finn[†], Patricio Farrell[*], Timo Streckenbach[*], Julien Moatti[‡],
Stefan Schulz[†,§], Thomas Koprucki[*], Michael O'Donovan[*],
[†]Tyndall National Institute, University College Cork, Cork, T12 R5CP, Ireland
[*]Weierstrass Institute (WIAS), Mohrenstr. 39, 10117 Berlin, Germany
[‡]Univ. Bordeaux, CNRS, Bordeaux INP, IMB, UMR 5251, Talence F-33400, France
[§]School of Physics, University College Cork, Cork, T12 YN60, Ireland
Email: odonovan@wias-berlin.de

***Abstract*—Aluminium gallium nitride alloys are used for developing light emitting diodes operating in the UV part of the electromagnetic spectrum. These devices suffer from a low efficiency. To gain insight to this question we develop a 3-D modified drift-diffusion model which takes into account both alloy disorder effects and valence band mixing, and investigate the device efficiency. Results show that the current injection efficiency is strongly influenced by the chosen doping profile.**

***Index Terms*—UV-C emitters, electronic structure, drift-diffusion, disordered energy landscape, carrier transport**

I. Introduction

Due to its wide tunable direct bandgap which can span from visible ($E_G^{GaN} \approx 3.45$ eV) to UV-C wavelengths ($E_G^{AlN} \approx 6.00$ eV), the semiconductor alloy aluminium gallium nitride (Al,Ga)N is of particular interest for light-emitting devices operating in the UV part of the electromagnetic spectrum [1]. At high AlN contents (UV-C, emission wavelength < 280 nm) devices suffer from a low quantum efficiency [1]. Simulation tools play an important role for understanding the origin of this decrease, and engineering device design to improve efficiency. For this, modeling frameworks should capture the relevant physical effects which impact device characteristics.

The valence states of (Al,Ga)N alloys require particular attention. Firstly, alloy disorder leads to carrier localization which modifies the density of states and the carrier density distribution in a quantum well (QW) [2]. The in-plane distribution of a hole ground state of a c-plane QW, computed using tight binding (TB) in the presence of alloy disorder, is shown in Fig. 1 (top right). The state is localized in a small region of space due to alloy fluctuations – without alloy disorder the wavefunction would be homogeneously distributed across the shown area. Modifications of the wavefunctions will impact recombination processes in a device [3]. Additionally, perturbations of the electronic structure also impacts carrier transport, where alloy disorder introduces low-energy pathways which enable percolation currents in a device [3]. Thus alloy effects impact both the transport and recombination properties.

This work received funding from the Leibniz Competition 2022 (UVSimTec, K415/2021), the Sustainable Energy Authority of Ireland and Taighde Éireann – Research Ireland (17/CDA/4789, 12/RC/2276 P2 and 21/FFP-A/9014), and the Leibniz competition 2020 (NUMSEMIC, J89/2019).

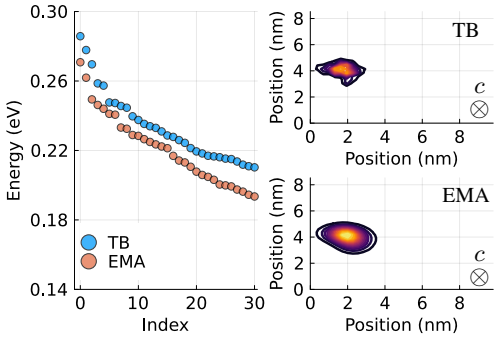

Fig. 1. Left: Hole energies of the first 30 states calculated from tight binding (TB) (blue) and a hybrid single band effective mass approximation (EMA) (orange) for a 2 nm $Al_{0.75}Ga_{0.25}N$ quantum well including alloy disorder. Right: 2-D slice of the TB (top) and EMA (bottom) ground state charge density for the chosen configuration within the quantum well.

Secondly, wavefunctions which contribute to emission can be constructed from states which facilitate emission of transverse electric (TE) or transverse magnetic (TM) light [2]. Unstrained bulk AlN emits primarily TM polarized photons, whereas bulk GaN emits mainly TE polarized photons. In (Al,Ga)N-based heterostructures the relative contribution of each depends on (among other factors) alloy composition, heterostructure properties (e.g. QW width) and carrier density.

To account for alloy disorder in a 3-D drift-diffusion (DD) device simulation the atomistic TB Schrödinger equation can in principle be coupled with the DD equations. This, however, is numerically prohibitive, as it requires solving a (large) eigenvalue problem self-consistently with the DD equations. Instead, we develop a framework which accounts for mixing between TE and TM emitting states in an approximation of a single band model, while also including alloy disorder. To further reduce the numerical demand, the atomistically treated QWs are embedded in a sparse mesh which describes regions where alloy disorder is of secondary importance.

II. Theoretical framework

To consider alloy disorder effects in DD, an energy landscape is extracted from TB via a local diagonalization of the TB Hamiltonian [4]. The energy landscape thus includes local

variations in composition, strain and polarization potential on an atomistic scale. The energy landscape is mapped onto a finite volume mesh which contains a node for every atom in the system, and is then embedded in a sparse mesh. Quantum corrections are included via localization landscape theory which approximates the single band effective mass approximation (EMA) of the Schrödinger equation [5].

As previously mentioned, the valence states of (Al,Ga)N alloys can be comprised of either TE or TM emitting states. This in principle requires a multi-band model, however to treat this with an EMA we construct a hybrid effective mass which is informed by the fraction of TE or TM emission:

$$\frac{1}{m_d(x_{\text{AlN}}, P_{\text{TE}})} = \frac{P_{\text{TE}}}{m_d^{\text{HH}}(x_{\text{AlN}})} + \frac{1 - P_{\text{TE}}}{m_d^{\text{CH}}(x_{\text{AlN}})} \quad . \tag{1}$$

Here m_d is the hybrid effective masses in the direction d (in- or out-of-plane), x_{AlN} is the AlN composition of the quantum well and P_{TE} is the fraction of TE emission which is computed from TB calculations [2]. m_d^{B} is the effective mass of the band B for the TE emitting band (B = HH) or TM emitting band (B = CH), which are a harmonic average of the AlN and GaN bands weighted by the alloy composition.

The model has been calibrated against TB. The separation between energy eigenvalues is similar in the EMA and TB. As this energetic separation depends on the inverse effective mass, this indicates the choice of mass is suitable (Fig. 1 left). The band offset within the QW was adjusted by a constant to ensure that absolute scale of the electronic structure is well represented. The position of the ground state is also in good agreement (c.f. Fig. 1 right, top and bottom) however we note that the EMA predicts a weaker localization compared to atomistic TB.

We apply this advanced framework to a UV-C emitting LED which contains five $\approx$ 2 nm $Al_{0.75}Ga_{0.25}N$ QWs separated by $\approx$ 7 nm $Al_{0.85}Ga_{0.15}N$ barriers. Recombination is treated using an ABC model which includes non-radiative Shockley-Read-Hall (R^{SRH}) and Auger-Meitner (R^{AM}) recombination as well as radiative recombination (R^{Rad}). An AlN electron blocking layer and p-GaN cap are included to prevent electron overshoot and aid hole injection into the QW regions. These are Mg-doped with a density of 10^{19} cm^{-3}. The software `ddfermi` is used to model the device using DD [6], and `AMGCL` is used to solve the system of equations [7].

III. Results

The band edge diagram of the structure (including quantum corrections as an effective confining potential from LLT) is shown in Fig. 2 (left). Alloy disorder impacts the energy landscape used in the DD calculations. This is shown in an in-plane slice through the QW closest to the p-side (Fig. 2 (right)). The fluctuations impact the carrier density, recombination and current density, and thus also the device efficiency. The efficiency is studied in terms of the carrier injections efficiency η^{CIE} (probability of injected carriers recombining within QWs) and radiative recombination efficiency η^{RRE} (probability that a recombination in the QWs will emit a photon); the internal quantum efficiency is thus $\eta^{IQE} = \eta^{CIE} \times \eta^{RRE}$. Our results show that η^{CIE} is strongly influenced by the doping profile, and the chosen doping activation energy. Without a suitable doping profile the electrons overshoot the active region leading to a lower internal quantum efficiency.

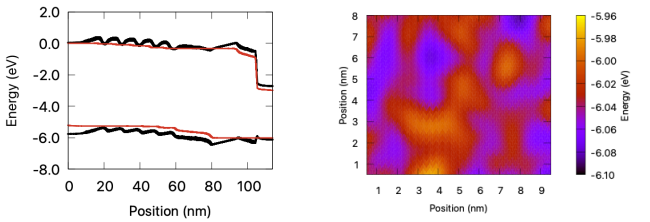

Fig. 2. Left: Band edge diagram of the LED structure studied in this work under bias. Right: In-plane valence band edge energy showing the impact of alloy disorder: The valence band energy varies by over 100 meV in the 10 $\times$ 9 nm^2 area. The data is shown for a slice through the right-most quantum well of the stack (on the p-side).

IV. Conclusion

In this work we present a framework to study device characteristics of (Al,Ga)N-based UV-C emitting LEDs. Optical polarization and disorder effects are considered. The framework builds on a hybrid band electronic structure model which is benchmarked against TB. Our results show that the doping profile is an important aspect for engineering higher device efficiencies in (Al,Ga)N-based UV-C LEDs.

References

[1] H. Amano, R. Collazo, C. D. Santi, S. Einfeldt, M. Funato, J. Glaab, S. Hagedorn, A. Hirano, H. Hirayama, R. Ishii, Y. Kashima, Y. Kawakami, R. Kirste, M. Kneissl, R. Martin, F. Mehnke, M. Meneghini, A. Ougazzaden, P. J. Parbrook, S. Rajan, P. Reddy, F. Römer, J. Ruschel, B. Sarkar, F. Scholz, L. J. Schowalter, P. Shields, Z. Sitar, L. Sulmoni, T. Wang, T. Wernicke, M. Weyers, B. Witzigmann, Y.-R. Wu, T. Wunderer, and Y. Zhang, "The 2020 UV emitter roadmap," *Journal of Physics D: Applied Physics*, vol. 53, p. 503001, sep 2020.

[2] R. Finn, M. O'Donovan, T. Koprucki, and S. Schulz, "Theoretical study of the impact of carrier density screening on Urbach tail energies and optical polarization in (Al,Ga)N quantum well systems," *Preprint at 10.48550/arXiv.2501.16808*, 2025.

[3] R. Finn, M. O'Donovan, P. Farrell, J. Moatti, T. Streckenbach, T. Koprucki, and S. Schulz, "Theoretical study of the impact of alloy disorder on carrier transport and recombination processes in deep UV (Al,Ga)N light emitters," *Applied Physics Letters*, vol. 122, p. 241104, 06 2023.

[4] M. O'Donovan, D. Chaudhuri, T. Streckenbach, P. Farrell, S. Schulz, and T. Koprucki, "From atomistic tight-binding theory to macroscale drift–diffusion: Multiscale modeling and numerical simulation of unipolar charge transport in (In,Ga)N devices with random fluctuations," *Journal of Applied Physics*, vol. 130, no. 6, p. 065702, 2021.

[5] C.-K. Li, M. Piccardo, L.-S. Lu, S. Mayboroda, L. Martinelli, J. Peretti, J. S. Speck, C. Weisbuch, M. Filoche, and Y.-R. Wu, "Localization landscape theory of disorder in semiconductors. III. Application to carrier transport and recombination in light emitting diodes," *Phys. Rev. B*, vol. 95, no. 14, p. 144206, 2017.

[6] D. H. Doan, P. Farrell, J. Fuhrmann, M. Kantner, T. Koprucki, and N. Rotundo, "ddfermi – a drift-diffusion simulation tool," tech. rep., Weierstrass Institute (WIAS), doi: http://doi.org/10.20347/WIAS.SOFTWARE.DDFERMI, 2020.

[7] D. Demidov, "AMGCL: An Efficient, Flexible, and Extensible Algebraic Multigrid Implementation," *Lobachevskii Journal of Mathematics*, vol. 40, no. 5, pp. 535–546, 2019.