Quantum transport modeling in III-Nitrides optoelectronic devices

Francesco Mercinelli

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Abstract

This work investigates quantum transport and quantum-corrected drift-diffusion models for the simulation and optimization of III-nitride optoelectronic devices. Their operation is strongly influenced by quantum confinement, tunneling through heterostructure barriers, trap-assisted tunneling, polarization fields and interband tunneling. These mechanisms cannot be fully described by conventional semiclassical drift-diffusion simulations, whereas a complete microscopic quantum-transport treatment is often too computationally demanding for realistic device structures and optimization studies. The objective of this thesis is therefore to establish a hierarchy of models ranging from microscopic quantum transport to computationally efficient quantum-corrected approaches, and to determine which physical information must be retained to describe the dominant transport and recombination mechanisms.

The non-equilibrium Green's function formalism is introduced as the microscopic reference, providing a unified description of the electronic structure, open boundaries, spectral carrier distributions, tunneling and scattering processes. A reduced effective-mass NEGF formulation based on Büttiker probes is also considered to lower the computational cost while preserving a spectral description of carrier transport. Two quantum-corrected drift-diffusion models are then formulated as further approximations: Poisson-Schrödinger drift-diffusion and density-gradient drift-diffusion. Both retain semiclassical current relations but modify the carrier densities and effective band edges to account for quantum confinement and tunneling-related charge redistribution. The Poisson-Schrödinger approach explicitly reconstructs the quantum local density of states from the Schrödinger eigenstates, whereas the density-gradient model introduces quantum corrections through differential relations involving the carrier densities.

The different levels of description are first compared for trap-assisted tunneling in a visible InGaN/GaN light-emitting diode. Starting from microscopic multi-phonon defect interactions, a quantum recombination rate with the algebraic structure of the conventional Shockley-Read-Hall expression is derived in terms of spectral capture and emission processes. Under strong electric fields, spectral states extend into the nominal bandgap and provide tunneling paths

between the extended bands and localized defects. Trap-assisted tunneling is therefore described through the quantum spectral charge and multi-phonon capture probabilities without introducing empirical field-enhancement factors, while the conventional SRH rate is recovered in the homogeneous semiclassical bulk limit. The NEGF calculation reproduces the experimental current-voltage characteristic and the increase of the ideality factor in the subthreshold regime over most of the investigated bias range. Among the reduced models, Poisson-Schrödinger drift-diffusion provides the closest agreement with NEGF because it retains the spectral information required by the capture process. Density-gradient drift-diffusion captures the qualitative behavior at a lower computational cost but exhibits larger deviations in the tunneling region.

The Poisson-Schrödinger framework is subsequently applied to the optimization of a 275 nm AlGaN UV-C LED. The electron-blocking region is investigated by comparing a conventional bulk layer with polarization-doped graded and superlattice designs. Both alternative structures improve hole injection while maintaining electron confinement, increasing the peak internal quantum efficiency from approximately 40% for the bulk EBL to 57% and 56% for the graded and superlattice EBLs, respectively. The p-side contact is then optimized to reduce the optical absorption associated with conventional p-GaN. A polarization-doped graded contact and a tunnel-junction contact are considered, with the tunnel junction analyzed through quantum transport because its operation relies on interband tunneling. The graded contact increases the peak wall-plug efficiency from 5.08% to 6.25%, while the optimized tunnel-junction contact reaches 8.78%. The latter provides the largest improvement in light extraction and external quantum efficiency, although its advantage depends on limiting the additional voltage drop introduced by the junction.

Overall, NEGF provides the detailed spectral description required to identify and validate quantum transport mechanisms, while Poisson-Schrödinger drift-diffusion retains the most relevant quantum information at a computational cost compatible with device-level optimization. The resulting modeling strategy provides a practical bridge between microscopic transport physics and the design of more efficient III-nitride optoelectronic devices.