Doctoral Program in Electrical, Electronics and Communications Engineering (35^{th} cycle)

Full-band NEGF modeling of optoelectronic devices

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1 Motivation

Theoretical investigation in the field of optoelectronics has been limited to semiclassical transport models derived from the *Boltzmann transport equation* (BTE), and in particular to the *drift-diffusion* (DD) model, which is obtained from the zeroth-order moment of the BTE. Carrier interaction with electromagnetic waves is included in the form of generation-recombination rates of electron-hole pairs [1], and the dynamic evolution of the light field is modeled through an optical solver coupled to the electron system in the device by absorption/gain coefficients. Nevertheless, nanostructured material systems, which compose the active region of any modern optoelectronic device, are highly affected by the quantum nature of carriers, which could be engineered as, *e.g.*, in the case of carrier confinement in light-emitting diodes (LEDs), or tunneling in resonant tunneling diodes (RTDs) and tunneling-filed-effect transistors (TFETs). Thus, adequate quantum corrections should be added to the above picture in order take into account effects like the coupling of the extended bulk states (responsible of the current flow through the device) to the confined states, and tunneling-assisted recombination processes.

Overcoming the semiclassical description entails moving forward to genuine quantum kinetic approaches, able to provide a reliable approximation to the numerical simulation of optoelectronic devices, at least in what concerns their active region, and a thorough understanding of the physical mechanisms behind the microscopic phenomena with a high degree of fidelity. Quantum transport techniques come into play thanks to the development of theories like nonequilibrium Green's (NEGF) function formalism [2] and density matrix (DM) theory [3], suitable for the modeling of nanostructured devices in steady state and transient regimes, respectively. Leonid Keldysh in 1965 [4] firstly presented his theory of NEGF and opened the gate for this formalism to become a real computational tool. Recent technological breakthroughs permitted to produce full-operative complex optoelectronic devices like quantum cascade lasers (QCL) or vertical-cavity surface-emitting lasers (VCSEL), which brought the need of realistic simulation tools. This, together with the recent advent of large computer clusters with high computational

capabilities, has given the NEGF approach such great popularity for the numerical simulation of optoelectronic structures, mainly due to its relative simplicity and inherent capability to integrate the electronic transport and the optical domain into a single theory.

2 Description of the Work

In this thesis we aim to provide a deep insight into the relevant aspects of the nonequilibrium Green's function (NEGF) formalism and its application to the numerical simulation of optoelectronic devices, specifically oriented to LEDs and photodetectors. Our implementation is based on a multiband $\mathbf{k} \cdot \mathbf{p}$ representation of the electronic dispersion, which is essential for a realistic description of intra or interband tunneling processes and optical transitions. The present model, based on a finite-element space discretization in the longitudinal direction, is applied to the analysis of two nanostructured devices of particular relevance: GaN-based light emitting diodes (LED) and superlattice infrared photodetectors. In the first case, we investigate carrier transport in the subthreshold forward-bias regime where tunneling processes are relevant. The proposed model is shown to predict the subthreshold I-V characteristics and ideality factors from experimental data taken on a single quantum-well LED. As a second case study, we analyze the transport properties of superlattice infrared absorbers. The use of a genuine quantum-kinetic model is crucial here for an accurate description of the main ingredients determining the different transport regimes (*i.e.*, miniband transport, sequential tunneling, hopping). We attempt to demonstrate in this work an accurate, yet computationally feasible NEGF model of superlattice detectors by formulating the kinetic equations in terms of problem-matched maximally localized basis functions, numerically generated from few modes representing the main conductive channels of the nanostructure. A mobility study is also performed, providing a semiclassical interpretation of the obtained numerical results.

3 Results

Result are mainly presented in chapters 3 and 4 of the thesis. First, in chapter 3 we have presented a study of trap-assisted tunneling in GaN-based LEDs. The first step towards a quantum-kinetic description of defect recombination assisted by tunneling with NEGF is the determination of the associated scattering self-energy, for which we have provided a theoretical derivation starting from the perturbation expansion the device Green's function, and assuming that the isolated defect states interact with the extended states of the device by multiphonon emission. The multiband NEGF formulation of defect-mediated scattering is a novel result of this work. The first attempt toward a quantum kinetic description of Shockley-Read-Hall recombination with NEGF was made by *U. Aeberhard* in [5] using separated representations for the conduction and valence band Green's functions. Starting from this work, we have developed a more general theory adapted to our multiband $\mathbf{k} \cdot \mathbf{p}$ implementation. Starting from the principle of detailed balance of the capture and emission rates at the defect level, we have demonstrated that the net capture rate of electrons in the conduction band is equivalent to the semiclassical formulation from Shockley-Read-Hall, when the Green's function is assumed to satisfy quasi-equilibrium conditions. Here, the defect self-energy has been computed with three models: optical deformation potential, polar optical (Fröhlich model) and multiphonon theory, resulting in a good approximation of the semiclassical result in all three cases, and most importantly, they all give the same slope which characterizes the zero-field SRH recombination process.

Proceeding further, we have studied the enhancement of defect recombination due to tail state formation, when the structure is subjected to high electric fields. As a first approximation,

we have considered a GaN p-n diode with highly doped layers, with a single midgap defect level placed at the junction position where the electric field is maximum, observing the resulting recombination current. By separating the contributions of the SRH self-energy into direct and tunneling assisted components, we have demonstrated that the recombination rate obtained from the direct component is able to reproduce the results expected in a semiclassical situation (drift-diffusion simulation with the characteristic ideality factor of 2), while the full self-energy gives enhanced recombination with an ideality factor of 5.5. This result establishes a connection between NEGF and semiclassical SRH recombination models, and it also shows that the main contribution of the recombination current, giving rise to such high values of the ideality factor, comes from defect capture assisted by the tunneling of carriers into subgap states. Then, we moved to a more realistic case study: single quantum-well InGaN/GaN LED in the subthreshold forward bias regime. Experimental data taken from the literature [6] was used to contrast the simulation results. The computed ideality factors are in agreement with experimental data. Our calculations show that the standard SRH formula, computed with the correct quantum carrier densities, can reproduce NEGF results. This result suggests that trap-assisted tunneling can be described with drift-diffusion solvers complemented with appropriate quantum corrections for the calculation of the local density of states. Carrier densities may be estimated, *e.g.*, from localization landscape approaches, or more rigorously from the full eigendecomposition of the Schrödinger equation. Among possible quantum-corrected semiclassical approaches to study carrier transport in LEDs, the Schrödinger-Poisson drift-diffusion model seems promising. DD models, complemented with a quantum-corrected LDOS, may be the only viable approach to the numerical simulation of complex realistic structures. Additional work is needed to verify the accuracy of such quantum-corrected semiclassical models, especially in the high-injection regime, where out-of-equilibrium phenomena such as hot carrier transport become relevant.

In chapter 4 we have moved to the simulation of carrier transport in realistic infrared detectors based on type-II superlattice absorbers. We have started by describing a mode-space approach in which the NEGF equations are projected into a lower-order basis set of maximally localized problem-matched basis functions. This approach enables the multiband simulation of longer structures by reducing the memory requirements of the NEGF operators that need to be stored on each iteration of the self-consistent loop. Unlike other projection-based approaches, we propose an additional self-energy term taking into account the contribution of the remote basis set and allowing to conserve the total current. We have demonstrated the robustness of the method by modeling an interband cascade infrared photodetector (ICIP) of nearly 150 nm long using an 8-band $\mathbf{k} \cdot \mathbf{p}$ description of the electronic dispersion. An inspection of the spectrally resolved current density reveals the presence of miniband transport in the superlattice absorber, where current is generated due to the absorption of carriers. The optically generated electron current is then transformed into a hole current aided by the quantum-engineered hole and electron barriers that complement the device, and which serve as relaxation and tunneling phases. The crucial role of phonon relaxation can be also observed in the spectral scattering current plot, assisting the cascade of the minority electrons from the conduction miniband of the superlattice absorber across the graded superlattice acting as relaxation region. Overall, the mode-space approach, corrected to include the effect of the remote bands, is revealed to be an enabling tool towards the simulation of realistic T2SL photodetectors.

We proceeded further by performing a mobility study in an $InAs_{0.97}Sb_{0.03}/InAs_{0.55}Sb_{0.45}$ superlattice. Although macroscopic quantities such as carrier mobilities and lifetimes are admittedly not germane to the NEGF formalism, they represent critical ingredients needed in quantum-corrected drift-diffusion models which can be investigated with genuine quantum transport models to obtain a semiclassical perspective of the underlying phenomena. Our results show an almost linear low-field trend of the electron and hole velocities at $T = 200$ K,

up to a critical value of approximately 4 kV/cm. At high fields, it is expected that the minibands break into a Wannier-Stark ladder, where carrier transport occurs mainly by hopping assisted by phonon emission. In fact, the small spectral width of the first heavy-hole miniband HH1 ($\Delta_{v1} < 1$ meV) contributed to its subsequent breakdown even in the low-field limit, making hole transport highly dependent on the population of phonons assisting the hopping transitions. On the other hand, electron transport was observed to remain nearly unaffected by this effect, as most of the electron current corresponded to coherent propagation. In reality, disorder effects due to compositional or layer fluctuation can greatly impact the transport in superlattice structures. This was investigated by introducing random fluctuations in the layers width, which severely disrupted the hole miniband alignment. An inspection of the electron and hole low-field mobility over a wide range of temperatures revealed that μ_n displays a conventional phonon-limited dependence above 80 K, while μ_p is thermally activated in the whole energy range, mainly because of the dependence of hole transport in the phonon population assisting the hopping process. The hopping activation energy estimated from our calculations was $E_a = 15$ meV.

The last case study considered in this work consisted in a barrier IR detector made with type-II superlattices, specifically an nBn detector. This structures are of particular importance from an analytical point of view, because they provide the opportunity to analyze separately carrier transport of electrons and holes. In this case we have moved from the analysis of a single section of a device to the description of a full device using NEGF, including also space-charge effects and SRH recombination, which is a novel result. Compared with the previous analyses, we have followed a different route by including phonon scattering within the Büttiker probes formalism, in which local self-energies depend only on the diagonal of the Green's functions, hence reducing the amount of quantities that must be stored on each iteration. Under illumination conditions, we have observed that the barrier was able to successfully block the majority carrier current, while the minority carrier current rapidly recombined after crossing the barrier. The carrier extraction efficiency of the structure was found to be 25%.

References

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