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XXXV Cycle

Bridging scales in the modeling of optoelectronic nanodevices: from quantum to semiclassical approaches

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Research context and motivation

- Optoelectronic devices find an increasing importance in several applications, e.g., illumination, energy harvesting, data centres, cameras, etc.

- Modern optoelectronic technologies rely on highly nanostructured devices featuring quantum effects.
- A proper description of these kind of devices requires the use of quantum kinetic transport models which are computationally intensive.
- Moreover, TCAD tools acquire a dominant role here as they help to reduce prototyping costs.
- Scientific efforts have been made towards the implementation and optimization of quantum transport models for optoelectronic device simulation.

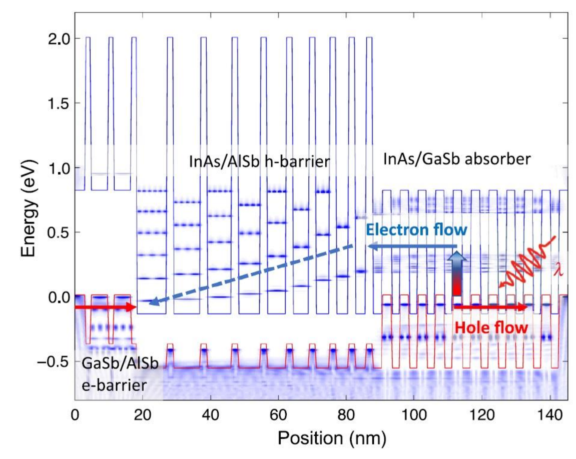

Figure. Interband cascade MWIR photodetector. An example of a highly nanostructured device.

F. Bertazzi et al. Nonequilibrium Green's Function Modeling of type-II Superlattice Detectors and its Connection to Semiclassical Approaches. Phys. Rev. Ap. 14 (2020)

Addressed research questions/problems

- Development of an in-house simulation code for the modeling of optoelectronic devices based on a multiscale approach, combining the NEGF formalism and a quantum corrected drift-diffusion model based on the direct solution of the Schrödinger equation.

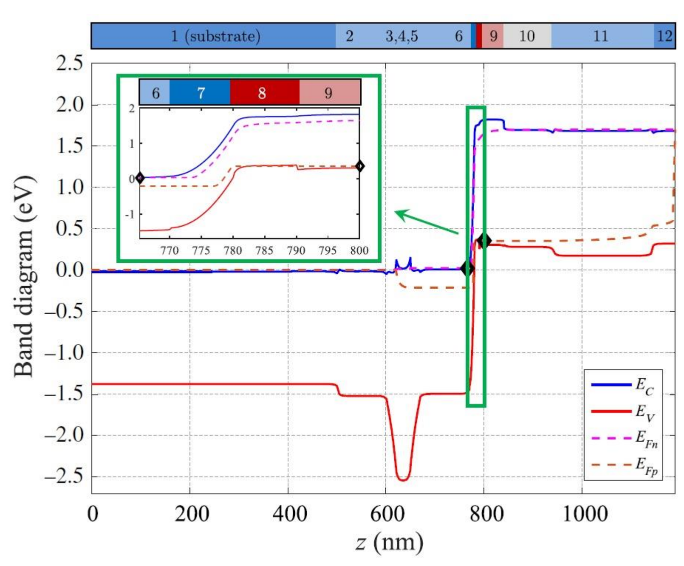

Figure. Section of a tunnel junction VCSEL, at 2.2 V bias. The tunnel junction is used to replace a long p-doped section, reducing the heating losses due to high resistivity. The modelling of this structure uses a multiscale approach by restricting the quantum kinetic simulation to the region inside the green square.

A. Tibaldi et al. *Analysis of Carrier Transport in Tunnel-Junction Vertical-Cavity Surface-Emitting Lasers by a Coupled Nonequilibrium Green s Function Drift-Diffusion Approach*. Phys. Rev. Ap. 14 (2020)

- Modeling of defects in LEDs. Shockley-Read-Hall and trap-assisted tunneling processes are included within a multiband quantum-kinetic simulation framework by means of an appropriate self-energy on equal footing of carrier dynamics.
- Modeling of Auger recombination and impact ionization phenomena. Carrier-carrier scattering is included within the GW approximation in NEGF.
- Study of light emission/absorption and transport properties in III-N LEDs and superlattice infrared photodetector structures. The effect of SRH and Auger is also studied, as both phenomena affect low and high bias operation leading to losses.

Submitted and published works

- A. Tibaldi, **J. A. Gonzalez Montoya**, F. Bertazzi, M. Goano, P. Debernardi. "*Bridging scales in multiphysical VCSEL modeling*". International conference on Numerical Simulation of Optoelectronic Devices (NUSOD), Hong Kong, 2018.
- F. Bertazzi, A. Tibaldi, **J. A. Gonzalez Montoya**, M. Goano, E. Bellotti. "*NEGF Modeling of Carrier Transport in Antimonide-based Type-II Superlattice Absorbers*". Photonics & Electromagnetics Research Symposium (PIERS), Rome, 2019.
- A. Tibaldi, **J. A. Gonzalez Montoya**, F. Bertazzi, M. Goano, M. Daubenschüz, R. Michalzik, P. Debernardi. "*Bridging scales in multiphysics VCSEL modeling*", Opt. and Quantum Electron, vol. 51, 2019, p. 231.
- A. Tibaldi, A. Gullino, **J. A. Gonzalez Montoya**, M. G. C. Alasio, A. Larsson, P. Debernardi, M. Goano, M. E. Vallone, G. Ghione, E. Bellotti, and F. Bertazzi. "*Modeling Tunnel Junctions for VCSELs: A Self-Consistent NEGF-DD Approach*". Photonics & Electromagnetics Research Symposium (PIERS), Sanya, 2020.
- F. Bertazzi, A. Tibaldi, M. Goano, **J. A. Gonzalez Montoya**, E. Bellotti. "*Nonequilibrium Green's Function Modeling of type-II Superlattice Detectors and its Connection to Semiclassical Approaches*". Phys. Rev. Appl., vol. 14, 2020, p. 014083.
- A. Tibaldi, **J. A. Gonzalez Montoya**, M. G. C. Alasio, A. Gullino, A. Larsson, P. Debernardi, M. Goano, M. E. Vallone, G. Ghione, E. Bellotti, F. Bertazzi. "*Analysis of Carrier Transport in Tunnel-Junction Vertical-Cavity Surface-Emitting Lasers by a Coupled Nonequilibrium Green's Function Drift-Diffusion Approach*". Phys. Rev. Appl., vol. 14, 2020, p. 024037.
- A. Tibaldi, **J. A. Gonzalez Montoya**, M. Vallone, M. Goano, E. Bellotti, F. Bertazzi. "*Modeling infrared superlattice photodetectors: from nonequilibrium Green's functions to quantum-corrected drift-diffusion*". Phys. Rev. Appl., vol. 16, 2021, p. 044024.
- **J. A. Gonzalez Montoya**, A. Tibaldi, C. De Santi, M. Meneghini, M. Goano, F. Bertazzi. "*NEGF modeling of trap-assisted tunneling in InGaN/GaN light-emitting diodes*". Phys. Rev. Appl., vol. 16, 2021, p. 044023.
- **J. A. Gonzalez Montoya**, A. Tibaldi, N. Roccato, C. De Santi, M. Meneghini, M. Goano, and F. Bertazzi. "*Trap-Assisted Tunneling in GaN-Based LEDs: A Nonequilibrium Green's Function Study*". GaN Marathon, Venice, 2022.

Novel contributions

- Quantum-kinetic treatment of the trap-assisted tunneling (TAT) phenomenon. For the case of isolated point defects, the nonequilibrium Green's functions (NEGF) approach is equivalent to a quantum-corrected drift-diffusion

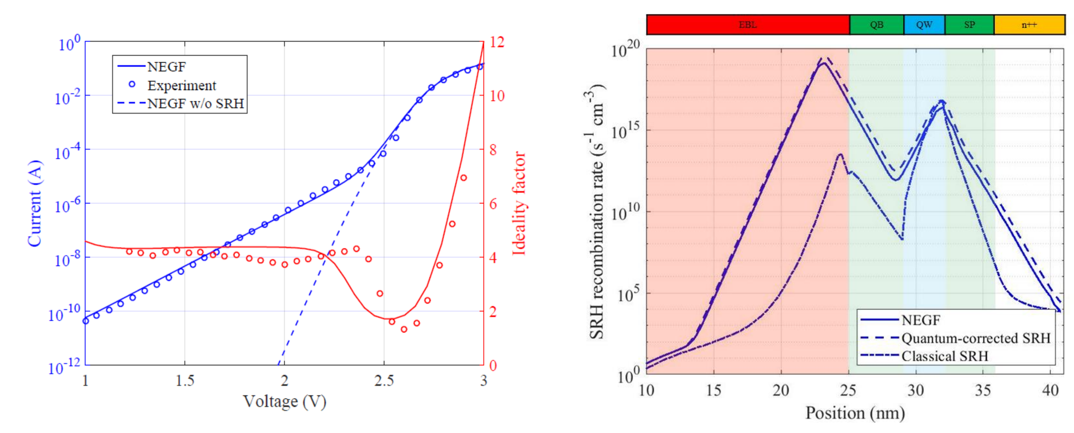

Figure. Left: I-V characteristic and corresponding ideality factor from NEGF and measurements of a 3 nm $In_{0.17}Ga_{0.83}N/GaN$ QW LED. Right: SRH recombination rate at 2.0 V. Recombination has increased noticeably with respect to the classical case. NEGF rate can be recovered with the usual SRH formula, and the quantum corrected charge.

- Quantum-kinetic treatment of Auger recombination in NEGF. Current work on the computation of Auger coefficients in type-II superlattices
- Simulation of modern optoelectronic devices (ICIPs,TJ-VCSELs, GaN LEDs)

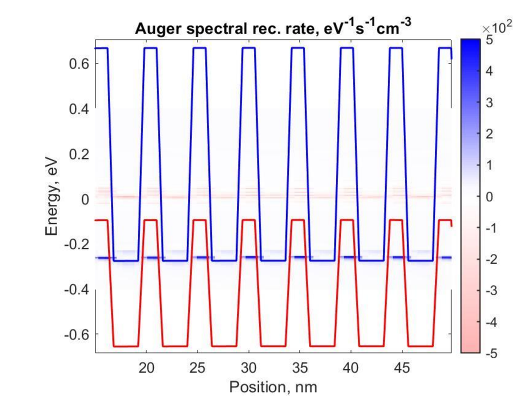

Figure. Spectrally resolved recombination rate at 0.1 V. Estimated e-e Auger coefficient $10^{-28} cm^6 s^{-1}$.

Adopted methodologies

- Quantum kinetic simulation approach based on the Nonequilibrium Green's Function formalism

Dyson and Keldysh equations

$$G^R(\underline{k},E) = [EM - H(\underline{k}) - \Sigma^R(\underline{k},E)]^{-1}$$

$$G^{\lessgtr}(\underline{k},E) = G^R(\underline{k},E)\Sigma^{\lessgtr}(\underline{k},E)G^A(\underline{k},E)$$

Carrier densities and current

$$n = \frac{1}{A}\sum_{\underline{k}}\int \frac{dE}{2\pi} iG^<$$

$$J = \frac{e}{\hbar A}\sum_{\underline{k}}\int \frac{dE}{2\pi}[(H-EM)G^< - G^<(H-EM)]$$

- Schrödinger-Poisson-Drift-Diffusion simulation approach

Schrodinger equation

$$H(\underline{k},z)\psi_n^{(i,\underline{k})}(z) = E_{i,\underline{k}}\psi_n^{(i,\underline{k})}(z)$$

Quantum correction and effective band edges

$$n(z) = \frac{1}{A}\sum_k\sum_i\left|\psi_n^{(i,\underline{k})}(z)\right|^2 f(E_F^{(n)},E_{i,\underline{k}})$$

$$n(z) = N_C\mathcal{F}_{\frac{1}{2}}\left(\frac{E_F^{(n)}-\tilde{E}_C}{k_BT}\right)$$

Drift-Diffusion equations

$$\partial_z^2\phi(z) = -\frac{e}{\varepsilon}[N_D(z) - N_A(z) + p(z) - n(z)]$$

$$\partial_z J_n(z) = eU_n(z)$$

$$J_n(z) = e\mu_e n\partial_z(\tilde{E}_C + k_BT\,logN_C + k_BT\,log\gamma_n)$$

+ FGR emission spectrum for the radiative recombination rate.

Future work

- Further investigation on the subthreshold behavior of GaN based LEDs presenting very high ideality factors using the multiband implementation of the SRH self-energy in NEGF.
- Investigation on the effect of SRH and Auger recombination in type-II superlattice absorbers, and the effect of lattice disorder in carrier transport.
- Full TJ-VCSEL simulation and comparison with experimental results.
- Investigation of droop mechanism in GaN based LEDs.

List of attended classes

- 02LWHRV – Communication (24/4/2021, 1 CFU)
- 01SHMRV – Entrepreneurial Finance (15/4/2021, 1 CFU)
- 01RISRV – Public Speaking (5/9/2022, 1 CFU)
- 01UNXRV – Thinking out of the box (25/7/2022, 1 CFU)
- 01SWPRV – Time management (12/2/2020, 1 CFU)
- 01UOCKG – Fractional Equations and Anomalous Diffusion (13/2/2020, 4 CFU)
- 02IUGKG – Il metodo Monte Carlo (30/10/2020, 6 CFU)
- 01RGBRV – Optimization methods for engineering problems (15/6/2020, 6 CFU)
- 01TBCRT – Ottimizzazione stocastica e apprendimento ottimale (25/6/2020, 3 CFU)
- 02MXBOQ – Passive Optical Components (6/7/2020, 8 CFU)
- 01UIYRV – Physics-based modeling of semiconductor devices (1/4/2020, 3 CFU)
- 01SFURV – Programmazione scientifica avanzata in matlab (25/5/2020, 4CFU)
- 01QFFRV – Tecniche innovative per l'ottimizzazione (26/2/2021, 4 CFU)
- 01NDLRV – Lingua italiana I livello (18/6/2021, 3 CFU)