# Self-energies: enabling multiphysics and multiscaling in optoelectronic quantum transport modeling

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***Abstract*—State of the art optoelectronic quantum transport methods either face prohibitive numerical load or significant physical approximations. This work introduces a good compromise in terms of an extension of Büttiker probes that can handle electron/hole recombination and generation in atomically resolved tight binding representations in the nonequilibrium Green's function framework.**

***Keywords—nonequilibrium Green's function method, quantum transport, carrier recombination, carrier generation, light emitting diodes***

## I. Introduction

Modern optoelectronic devices combine the small length scale of atoms and subatomic features with the typically several orders of magnitude larger scale of optical wave lengths. Even the pure electronic transport situation in optoelectronic devices [1-3] combines few nm or even smaller critical dimensions with larger range source and drain regions [4,5]. In other words, the physics of most modern optoelectronic devices combines multi-physics (e.g. electrons, phonons and photons) with multi-domain (subatomic and micrometer wave lengths) design aspects [6]. Self-energies within the framework of the nonequilibrium Green's function method are made to cover exactly such situations: Self-energies have been used to model the energy, momentum and heat exchange between electrons, phonons and photons [7-9]. They are used to embed active device areas into open or even field-periodic boundary surroundings [3,6,9]. Recently, it was shown how self-energies can be used to handle different physical situations in various device areas in numerically efficient, approximate ways [6]. In this work, we present an extension of the Büttiker probe self-energy model to handle various recombination and carrier generation effects in optoelectronic and band-to-band tunneling devices.

## II. Method

Throughout this work, charge transport is solved within the nonequilibrium Green's function method. The devices are atomically resolved in the empirical tight binding method. Open boundary conditions, carrier scattering, relaxation, generation and recombination is handled within the self-energy concept. Traditional approaches handle the scattering within the self-consistent Born approximation. The numerical load of this approximation is often preventive to handle optoelectronic devices in atomic resolution. To overcome this situation the Büttiker probe self-energy concept is extended to handle all scattering processes relevant in optoelectronic and band-to-band tunneling devices.

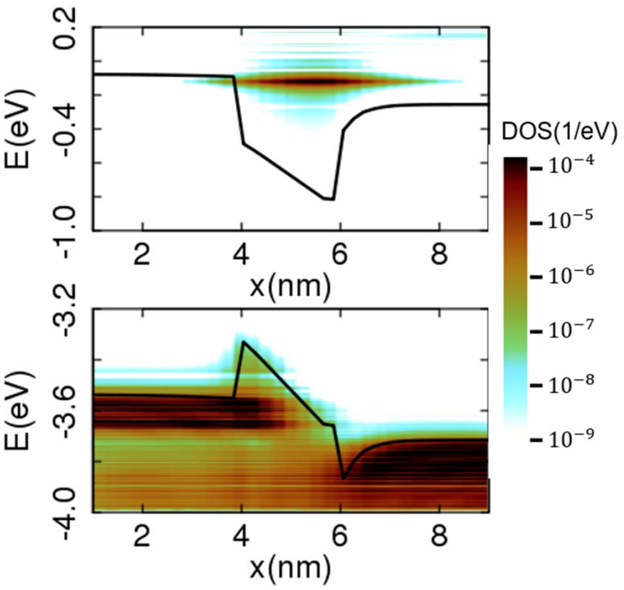


*Figure 1: Density of states (contour) in the conduction band (above) and valence band (below) of a 2nm $GaN/In_{0.13}Ga_{0.87}N/GaN$ quantum well typical for blue light emitting diodes. Electrons enter from the left, holes from the right according to the p/n doping structure.*

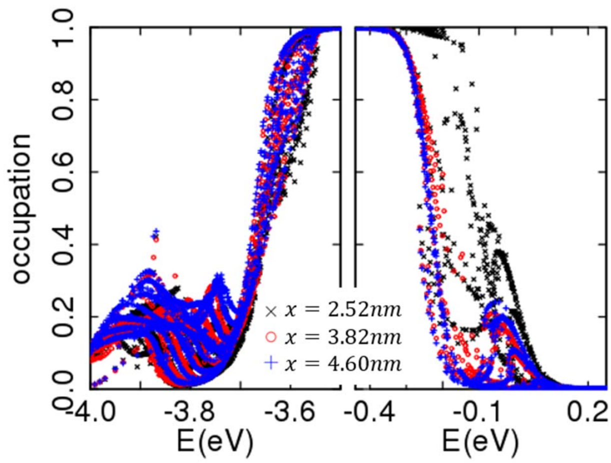


*Figure 2: Local occupancy of holes (left) and electrons (right) in the device of Fig.1 at various positions. The deviations from the Fermi distribution originate from the nonequilibrium situation.*

## III. Results

The quantum wells of light emitting diodes typically host a lot of electrons and holes that face thermalization. Figures

1 and 2 assess this assumption since they show the energy resolved density and occupation functions of a GaN/$In_{0.13}Ga_{0.87}N$/GaN quantum well typically found in blue LEDs. Electrons and holes are solved within a 20 band empirical tight binding model. Scattering is assumed with Büttiker probes of 10meV scattering strength. Electrons enter the simulation area from the left, holes from the right. Holes in the quantum well indeed follow a constant Fermi distribution function, whereas the electron distribution is spatially varying and deviates from the Fermi one.

Spatially varying distribution functions are one of the reasons for spatially varying recombination current densities – a measure essential for optoelectronic device performance

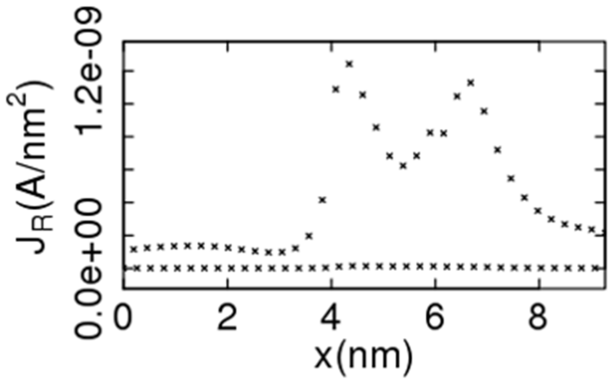


*Figure 3: Recombination current density of the quantum well of Fig.1. The atom type, the quantum mechanical confinement and nonequilibrium occupancy determine the effective Büttiker probe recombination current.*

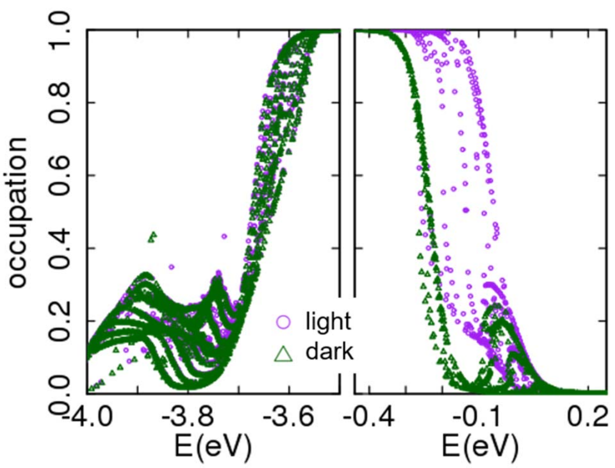


*Figure 1: Hole (left) and electron (right) occupancy functions in the quantum well of Fig.1 at the position of 4.6nm with (purple) and without (green) light illumination. The carrier generation leads to an increase in hole and electron occupancy. The higher density of states in the valence band weakens the observed occupancy increase compared to the electrons in the conduction band.*

predictions. Figure 3 shows the atomically resolved recombination current of the quantum well of Fig.1. Nitride atoms host significantly more recombination events than gallium and indium ones, which explains the oscillatory shape of the result.

Büttiker probes can be used to model light absorption and the carrier generation as well. This is exemplified in Fig. 4 which compares the electronic distribution function of Fig. 2 with the case when a carrier generation Büttiker probe is added.

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