The Non-Equilibrium Green's Function Method for Semiconductor Light Emitting Diode Simulation

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The non-equilibrium Green's function (NEGF) method is applied to carrier transport of a semiconductor light emitting diode (LED). NEGF is one of the most rigorous quantum transport methods where the occupation of states is calculated based on scattering self energies [1, 2]. Microscopic scattering processes and carrier coherence can thereby be treated in a consistent way. In optoelectronic devices, the close by arrangement of multiple hetero interfaces creates potential wells or barriers similar to the carrier phase or momentum relaxation length. The NEGF method can serve as a rigorous tool to investigate the device principles of operation in such quantum-well, -wire or -dot structures [3, 4].

1. Simulation model and setup

The simulation model is adapted to semiconductor multi-layer structures which can be described as one-dimensional in space with open contacts at the ends. The two-band effective mass Hamiltonian contains the energy of the electrons, photons, phonons and their respective coupling terms. In particular optical spontaneous emission is described as a non-local scattering process with coupling to an empty modal light field. As device example, a Gallium Nitride single quantum-well LED emitting at around 430nm is investigated. The thin InGaN active region (3nm) and AlGaN electron blocking layer (10nm) possess polarization charges at their respective interfaces, which cause a strong modulation of the potential. In order to calibrate the scattering parameters, single material resistor structures have been calculated prior to the LED simulation, and their effective mobility compared to literature data.

2. Results

The NEGF calculation of the single QW LED is compared to semi-classical drift-diffusion results. Carrier capture and escape in the QW show similar behaviour, carrier leakage and the electron blocking layer show signatures of non-equilibrium carrier distributions and tunneling currents, which are not part of the drift-diffusion description. Issues and challenges of the NEGF method for LED analysis will be discussed.

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