NEGF Quantum Transport for Green MQW Nitride LEDs

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***Abstract*—This work presents a non-equilibrium Green's function (NEGF) based simulation of blue and green single and multi-quantum well light emitting diodes (LEDs). The simulations provide insight into transport phenomena like tunnelling, hot carrier and back-scattering and the behavior of the density of states above the active region. It is shown that the electron density in the quantum wells is largely in equilibrium in contrast to the quantum well barrier.**

I. Introduction

Simulation tools based on the quantum-mechanically consistent non-equilibrium Green's function(NEGF) method have been used successfully to investigate resonant tunneling diodes[1], quantum cascade lasers[2] and transistors[3]. In the case of nitride LEDs, drift-diffusion based tools have been used to investigate phenomena such as Auger induced efficiency droop[4], the role of indium fluctuations in efficiency drop in green LEDs[5] and acceptor activation[6]. However, such tools lack a consistent quantum mechanical treatment of transport processes, which can be provided by NEGF. NEGF has already been used in multi-physics simulations of nitride LEDs which employ a combination of NEGF and drift-diffusion methods[7] or a combination of equilibrium and non-equilibrium reservoirs[8]. Full NEGF simulations of GaAs/AlGaAs[9] and nitride LEDs[10] have used the carrier-carrier scattering method shown by Golizadeh[11] which has some current conservation issues. Here we present blue and green multi-quantum well simulations with the Buettiker method[12], [13] of carrier-carrier scattering.

II. Methodology

The LED structure is coupled to leads through which carriers can enter or leave the device. The non-linear Poisson equation for the electrostatic potential and the Dyson and Keldysh equations for the Green's functions are solved self consistently based on the formalism presented in [14]. Here, we replace the tight binding basis band structure by an effective mass model with envelope wave functions[9]. The local density of states, carrier and current densities can be extracted from the Green's functions.

The scattering models[10] included are acoustic and polar optical phonon scattering, electron-electron scattering, ionized impurity scattering and photon scattering. Non-radiative recombination processes are not included in the simulation as models for their implementation in NEGF do not exist. The space discretization is fixed and non-uniform. The energy discretization is non-uniform with iterative refinements and the the k-space is discretized over 60 equidistant points. All simulations are performed at room temperature (T=300K). Piezoelectric polarization has been included and related constants can be found in [15].

Electron-electron scattering is based on the Buettiker model presented in [12] and [13]. Since transport in LEDs is bipolar, we have two sets of probe Fermi levels. The iterations to find the probe Fermi levels to ensure current continuity are performed separately for electrons and holes.

III. Results

The LED structures we have simulated have the p and n doped injection regions of thickness 25nm and doping 1E18 cm^{-3}. The doping concentrations in our simulations refer to the density of ionized dopants. The electron blocking layer (EBL) is 10nm thick $Al_{0.13}Ga_{0.87}N$ and is p-doped at 1E18 cm^{-3}. The p and n barrier regions are 10nm each. The p-barrier is doped at 1E18 cm^{-3} while the n-barrier is doped at 1E16 cm^{-3}. The active region for blue emission consists of two 3nm thick $In_{0.2}Ga_{0.8}N$ quantum wells separated by a 5nm thick GaN barrier n-doped at 1E16 cm^{-3}. For green emission, the mole fraction of indium is increased to 30%.

Figure 1 shows the local density of states for electrons and holes at k=0 for a green MQW LED. The distinction between bulk and quantum states can be clearly seen. It is interesting to note that the conduction band states in the p-barrier are also quantized. The continuum states above the quantum wells and the barrier are also quantized and do not follow the bulk square root distribution.

Electrons tunnelling between the injection region and the quantum well in a blue MQW LED at a high bias voltage can be seen in figure 2. It also shows high energy electrons injected by the cathode not being captured by the quantum well. These hot electrons are partially back-scattered at the barrier between the quantum wells. The partially transmitted electrons travel across the active region and are subsequently back-scattered at the EBL.

Figure 3 shows the energetic distribution of electrons in the active region in the blue LED obtained by NEGF and compares

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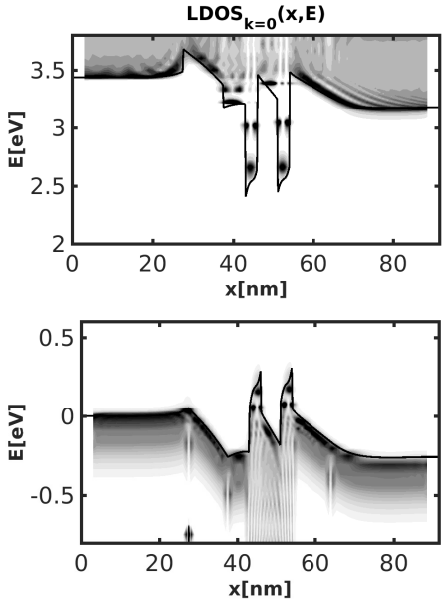

Fig. 1. LDOS in the conduction band(upper) and valence band(lower) in green MQW LED at 3.1V

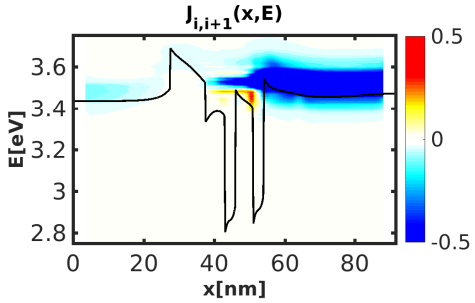

Fig. 2. Electron current in blue MQW LED at 3.4V. Positive and negative values indicate electron flow in positive and negative x-directions respectively.

it to analytically calculated equilibrium density distribution calculated by (1)

$$\frac{dn}{dE} = N(E)F(E) \tag{1}$$

where N(E) is the density of states and F(E) is the Fermi function. The NEGF and analytical distribution match well in the quantum wells up to around 3.6eV. Above 3.6eV, the density of states is not purely two dimensional. This can also be seen in the green LED LDOS in figure 1. In the barrier, the distribution is clearly in non equilibrium as the NEGF and analytical distribution do not match well. NEGF shows a density below the conduction band in the barrier, indicating tunnelling.

IV. Conclusions

While computationally demanding, using NEGF throughout the device can provide interesting insights on LED behaviour. In particular, the density of states and transport phenomena like tunneling through barriers and hot carrier scattering can be observed.

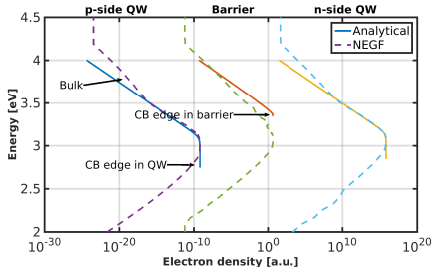

Fig. 3. Energetic distribution of electron density calculated analytically(solid) and by NEGF(dotted) in a blue LED in the p-side quantum well(left), the quantum well barrier(middle) and the n-side quantum well(right) at 3.1V.

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