Monte Carlo simulation of hot electron transport in III-N LEDs

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***Abstract*—We study electron dynamics in a multi-quantum well (MQW) light-emitting diode (LED) using Monte Carlo simulation and show that at strong injection, Auger recombination in the quantum wells creates a hot electron population which is still visible at the p-contact 250 nm away from the MQW. The Auger-excited electrons also generate a leakage current that is notably larger than leakage predicted by drift-diffusion, indicating that electron leakage in III-N LEDs at strong injection is predominantly caused by Auger-excited hot electrons.**

I. INTRODUCTION

Deployment of III-N based light-emitting diodes (LEDs) in high-power applications is limited by the efficiency droop at strong injection. After several years of research, Auger recombination [1] and leakage current [2] are widely considered as the main causes behind it. In this work we use a coupled Monte Carlo–drift-diffusion (MCDD) model to simulate electron transport in a complete multi-quantum well (MQW) LED shown in Fig. 1. We show that Auger recombination generates a significant hot electron population and a large part of it gets trapped in the U sidevalley (close to the L point). The hot electron population also generates a fairly large electron leakage towards the p-contact, creating a secondary loss effect related to Auger recombination.

Our model uses the hole density obtained from the standard drift-diffusion (DD) model as a fixed charge density input in a self-consistent Monte Carlo (MC) simulation of the electron system. Poisson's equation is used for solving the self-consistent electric fields, and the standard ABC model is used for calculating recombination rates. The Auger recombination rates are also used to account for the hot electron generation. To our knowledge, our work is the first fully self-consistent MC simulation of electrons in a realistic III-N LED with current-spreading layers and contacts, as opposed to using MC models for electrons inside the active region [3].

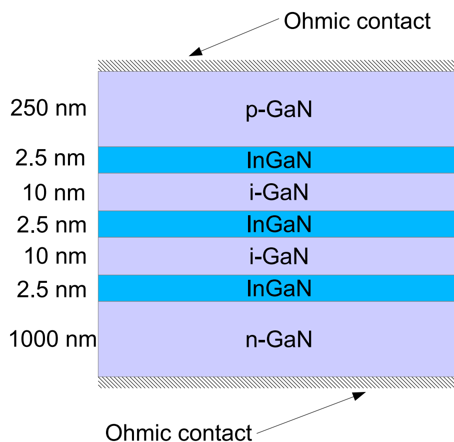

Fig. 1. III-N LED device simulated in this work. The n- and p-type doping densities are 10^{24} 1/m^3.

II. THEORETICAL MODEL

In the MCDD model, electrons in the conduction band are simulated with a self-consistent MC simulation of the Boltzmann transport equation (BTE). Before performing the MC simulation, electron, hole and recombination rate densities are solved numerically from Poisson's equation and the DD equations, using the ABC model to calculate recombination rates from the electron and hole densities as in Ref. 4.

After obtaining steady-state solutions from the DD simulation, hole density from DD is used as a fixed background charge density for solving Poisson's equation and recombination rate density during the MC simulation (for details about the MC simulation, see [5]). The MC simulation is performed self-consistently, calculating the trajectory of electron particles using a spherical non-parabolic multivalley model of wurtzite GaN and related compounds [6]. Most important electron-phonon, ionized impurity, alloy disorder, and carrier-carrier scattering probabilities are derived from Fermi's golden rule for transitions between different Bloch states, and they are used here to select transitions for electrons as a function of their energy. The electrostatic potential is updated during the MC simulation by solving Poisson's equation using the time-evolving electron density from MC and the hole density from DD as inputs. Electron and hole densities are also used to calculate recombination rates in the quantum wells (QWs) with the ABC model during the simulation, and the rates are used both to annihilate electrons due to recombination and to excite electrons due to Auger processes.

Net recombination coefficients used in the ABC model are given as $A = 10^7$ 1/s, $B = 4 \cdot 10^{-17}$ m^3/s, and $C = 10^{-42}$ m^6/s, which are very close to values reported in Refs. 7 and 8. The Auger coefficient is also comparable to values calculated from first principles in Ref. 9. The MC simulation is run for a long time of typically several tens of nanoseconds until a steady state is reached. The resulting distribution function f satisfies the BTE for the conduction band electrons. After reaching steady state, the simulation is continued and characteristics such as electron densities, energies and velocities are collected from the simulated electron ensemble.

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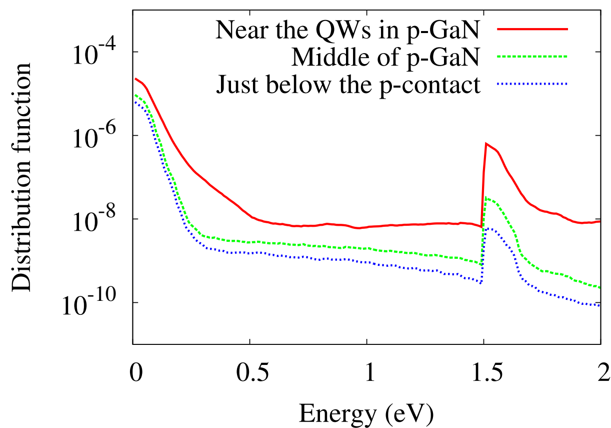

Fig. 2. Distribution function of electrons including the Γ_1 valley and the closest upper U valley in p-GaN at strong injection of 3.3 V, calculated using the MCDD model. The U valley is at 1.5 eV, and it has a notable population of electrons still next to the p-contact 250 nm away from the MQW.

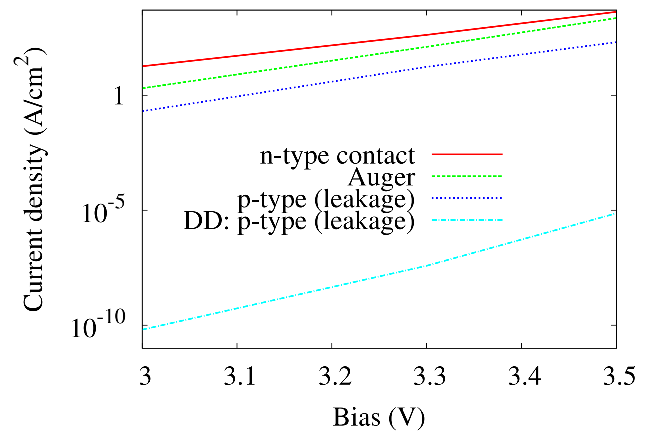

Fig. 3. Total electron current, electron current generated by Auger recombination, and electron leakage current calculated with MCDD. Also shown is the electron leakage current from the DD simulation.

III. Results

The MCDD model is deployed to simulate current transport in the LED device shown in Fig. 1 at different bias voltages. Fig. 2 shows the distribution function of electrons including the Γ_1 valley (valley minimum at 0 eV) and the closest upper U valley, whose minimum at 1.5 eV is close to the L point. The distribution function is shown for strong injection of 3.3 V in different positions in p-GaN above the MQW. The distribution function shows a significant hot electron tail in the Γ_1 valley, and in addition it shows a notable electron population in the U sidevalley. The U valley population decreases as electrons travel further away from the MQW in p-GaN, but it is still present close to the p-contact 250 nm away from the MQW. MCDD simulations without hot electron generation through Auger recombination (results not shown) show essentially no sidevalley population in p-GaN, and therefore the sidevalley electron population is predominantly caused by Auger recombination.

Fig. 3 shows the total electron current from MCDD, electron current generated by Auger recombination from MCDD, electron leakage current from MCDD, and electron leakage current from DD. Electron leakage current simulated with MCDD is many orders of magnitude larger than leakage current simulated only with DD, and majority of the leakage current in MCDD is caused by Auger excitation of electrons in the MQW region. This indicates that Auger recombination contributes to efficiency droop not only through annihilation of electrons in the MQW, but also through creating a notable electron leakage towards the p-type contact.

The present form of the MCDD model is a significant improvement to the widely used DD model and it allows a much more detailed simulation of the electron dynamics in a realistic LED device, predicting several new key features. The distribution function of Fig. 2 shows a significant hot electron population at strong injection roughly at the onset of a significant efficiency reduction. The current density at the simulated high injection level of 3.3 V is roughly 400 A/cm^2, which is very relevant for high output power applications. The hot electron leakage current caused by Auger recombination also significantly affects the device operation and cannot be captured by the DD equations. Therefore understanding hot electron effects on the device operation at strong injection will be very important in future studies.

IV. Conclusions

We studied hot electron transport in a III-N MQW LED device using a coupled Monte Carlo–drift-diffusion (MCDD) model and showed that at high injection levels, Auger recombination in the MQW region creates a population of hot electrons in the Γ_1 and U valleys. The hot electron population is still present at the p-type contact 250 nm away from the MQW. The hot electron population created by Auger recombination also results in a significantly larger leakage current than that predicted by the drift-diffusion simulation, indicating that electron leakage at strong injection is predominantly caused by Auger recombination.

Acknowledgments

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