Bipolar Monte Carlo simulation of hot carriers in III-N LEDs

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***Abstract*—We perform fully bipolar Monte Carlo simulations of electrons and holes in III-Nitride multi-quantum well light-emitting diodes (LEDs) to investigate the effects of hot carriers. Our results show how accounting for hot carriers affects the current-voltage characteristics and device efficiency. We also discuss the effects of bandstructure details on the simulation results. Further simulations with versatile QW and EBL configurations are needed to confirm the relationship between hot carrier effects and current-voltage characteristics.**

I. Introduction

Recent measurements and theoretical reports have reinforced the discussion of the efficiency droop of III-Nitride (III-N) light-emitting diodes (LEDs) [1]–[5]. However, discussion of the detailed physical mechanisms behind the droop is barred by large contradictions between different interpretations of recent measurements. To enable the next breakthroughs in explaining droop, future experiments must be supported by very sophisticated device models that enable quantitative interpretation of the measurements. As the efficiency droop is essentially a device-level phenomenon, it is also essential to have theoretical models that can account for all the important aspects of the full LED device.

Even the most sophisticated device simulation tools of III-N LEDs today are based on the drift-diffusion (DD) model, which assumes quasi-equilibrium distributions for electrons and holes. Therefore they are not capable of fully interpreting the measurements reported in Refs. [1], [2], as both measurements indicate the presence of nonequilibrium hot carriers. In addition, the DD model generally seems to overestimate the bias voltages needed for a given current density in multi-quantum well (MQW) LEDs. It has recently been suggested by Li in Ref. [6] that accounting for hot electrons would correct the overestimated bias voltages. However, current transport through indium fluctuations [7] and tunneling through traps [8] have also been suggested as alternative explanations.

We have earlier reported a Monte Carlo–drift-diffusion (MCDD) model, in which the electron distribution is simulated within a full III-N MQW LED device using Monte Carlo (MC) methods [3], [9], [10]. Even though the MCDD model has provided notable insight to the physics of hot electrons in LEDs, the hole distribution in MCDD is still based on a drift-diffusion simulation. Especially at certain conditions, the MCDD and DD models exhibit large differences in their predictions for device characteristics, indicating a breakdown of the DD model [10]. Therefore it is necessary to also account for nonequilibrium hole transport with the MC model.

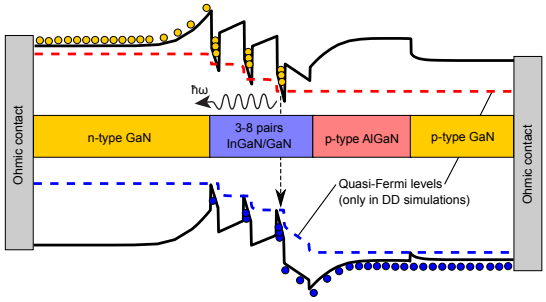

Fig. 1. The III-N MQW LEDs simulated in this work using the Monte Carlo model.

In this work we perform fully bipolar MC simulations for electrons and holes in III-N LEDs [11]. In the bipolar MC model, only the initial values for the MC simulation result from the DD model, so that both the electron and hole distributions result from an MC simulation. In the present work, we study hot carrier effects in the structures shown in Fig. 1 using the bipolar MC model, focusing especially on the effects of the number of QWs on the resulting hot-carrier effects and device characteristics.

II. Theoretical model

Electron and hole dynamics are studied using the MC model, in which the semiclassical Boltzmann's transport equation (BTE) is solved by a direct simulation of the carriers. More information of the MC framework can be found in Ref. [10]. The initial values for the spatial electron and hole distributions are taken from a DD simulation, and the MC simulations are performed for a number of bias voltages. Recombination rates are calculated based on the time-dependent electron and hole densities from the MC simulation using the A, B, and C coefficient for Shockley-Read-Hall, radiative, and Auger recombination. Intraband scattering processes include deformation potential and electrostatic acoustic and optical phonon scattering (including intravalley processes), ionized impurity scattering, carrier-carrier scattering, alloy disorder scattering, and carrier-carrier scattering. Material parameters are based on Ref. [12] with the exception of the intrinsic

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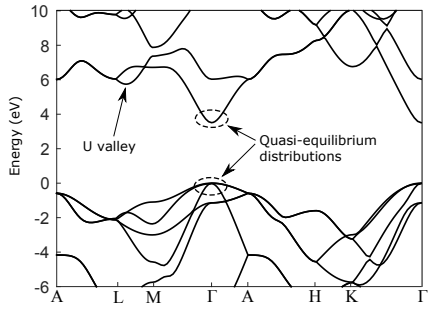

Fig. 2. The full bandstructure of GaN calculated from first principles. To perform MC simulations, we fit an analytical multivalley model to the full bandstructure.

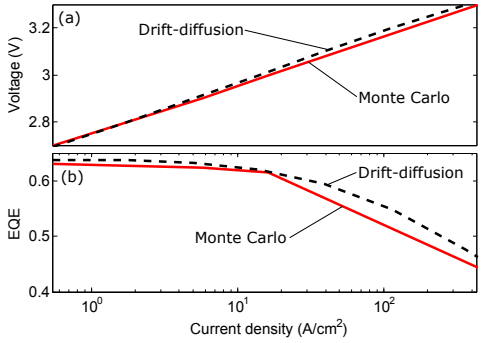

Fig. 3. (a) The current-voltage characteristics and (b) the external quantum efficiency of the structure with three QWs and no EBL, as resulting from DD and MC simulations.

polarization values, which are scaled by 50 %. To study the effects of the bandstructure details, we perform calculations using the bandstructure model of Ref. [13] as well as analytic bandstructures fitted to our first-principles bandstructure calculations.

III. Results

Figure 2 shows the full bandstructure of GaN calculated from first principles. Fitting an analytic multivalley bandstructure model to Fig. 2 allows comparing the MC simulation results with those calculated with the bandstructure model of Ref. [13]. Figure 3 shows (a) the bias voltage and (b) the external quantum efficiency (EQE) of the structure with three QWs and no electron-blocking layer (EBL), resulting from the DD and MC simulations. For this simple structure, the MC simulations exhibit a slightly smaller turnon voltage than DD. However, more simulations are needed to find out how this difference generally behaves in structures with an EBL and more QWs. The EQE from the MC simulation is also slightly lower than from DD. The differences between MC and DD in both (a) and (b) result from hot-carrier effects.

Figure 4 shows distribution function of electrons in the p-type GaN in the structure with three QWs and no EBL at a bias voltage of 3.3 V. Electron distribution at the U valley at 1.5 eV decreases steadily as a function of distance with respect to the thermal electron distribution close to the band edge at 0 eV. Results shown in Figs. 3-4 are still calculated using the bandstructure of Ref. [13].

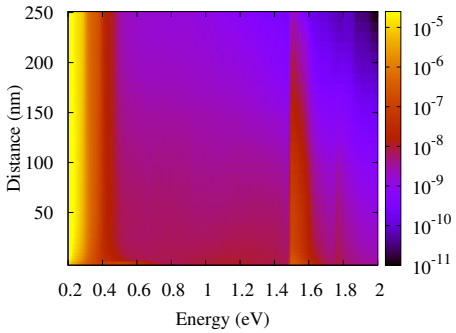

Fig. 4. Electron distribution function in the p-type GaN of the structure at a bias voltage of 3.3 V.

IV. Conclusions

We have developed a fully bipolar MC simulation model for III-N LED devices. Initial results for a simple structure reveal differences between the DD and MC results, and these differences are expected to increase in more complex LED structures. Differences between the DD and MC models indicate that accounting for hot carriers is needed to understand all the important device-level details of LEDs. However, further simulations are needed to confirm the relationship between hot carrier effects and current-voltage characteristics.

Acknowledgments

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