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

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Introduction

III-Nitride (III-N) light-emitting diodes (LEDs) have started a revolution in general lighting and are on track to replace all the competing lighting technologies [1]. Even with the spectacular evolution of III-N LEDs into a very efficient technology, they still suffer from an efficiency droop, whose origin is not fully understood [2]. In addition, the device-level understanding of III-N multi-quantum well (MQW) MQW LEDs is still incomplete, the most obvious indication of which being the difficulty to fit simulated current-voltage characteristics to experiments.

Typically the full device-level models for III-N LEDs are based on the drift-diffusion (DD) model, which assumes quasi-equilibrium carrier distributions [3]. However, Iveland *et al.* and Binder *et al.* have recently measured clear indications of hot electrons and holes in LEDs already at typical operating conditions [4], [5]. Inspired by these measurements, we recently developed a Monte Carlo–drift-diffusion (MCDD) model to specifically study hot electrons. According to the MCDD simulations, a significant amount of hot carriers is generated by Auger recombination, and part of these hot electrons are visible even at the p-contact [6]. At certain conditions we also detected a significant difference between the MCDD and DD results [7].

In this work, we perform fully bipolar MC simulations for electrons and holes in realistic III-N LED devices taking into account all the relevant scattering and recombination processes and device physics.

Theory, Results & Discussion

A coupled MC simulation is performed for electrons and holes, resulting in device-level characteristics and distribution functions as a function of the bias voltage [8]. The initial values are taken from a standard DD simulation, and the bandstructure is an analytical model fitted to the full band structure shown in Fig. 2.

Figure 3 shows the electron densities from the DD and MC simulations for the LED structure with three QWs at strong injection. The largest amount of electrons is located in the rightmost QWs closest to the p-side, which is also responsible for most of the light emission. The electron densities from the DD and MC simulations also exhibit a slight difference between each other. This difference is a direct consequence of the fact that the MC simulations do not assume any quasi-equilibrium distributions for the carriers.

DD simulations typically result in unrealistically high turnon voltages for III-N MQW LEDs. The higher turnon voltage in the DD simulation originates from quasi-Fermi losses in the barrier layers between the QWs [9], which are illustrated by the band diagram shown in Fig. 4. The MC simulations for the sample structures of Fig. 1 enable studying how accounting for hot carriers increases the current density for a given bias voltage. The smaller turnon voltages given by the MC model clearly indicate that accounting for hot carriers is needed for complete understanding of the device physics of III-N LEDs.

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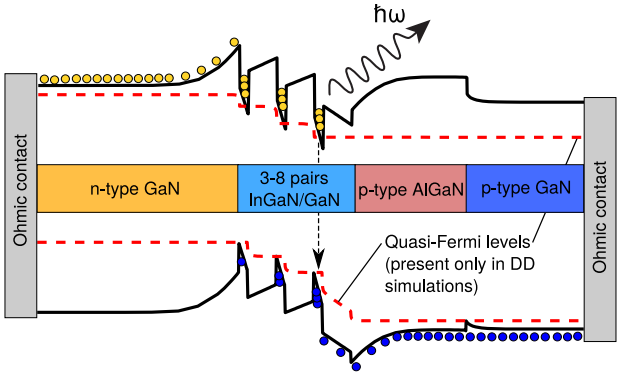

Fig. 1. The III-Nitride MQW structures simulated in this work.

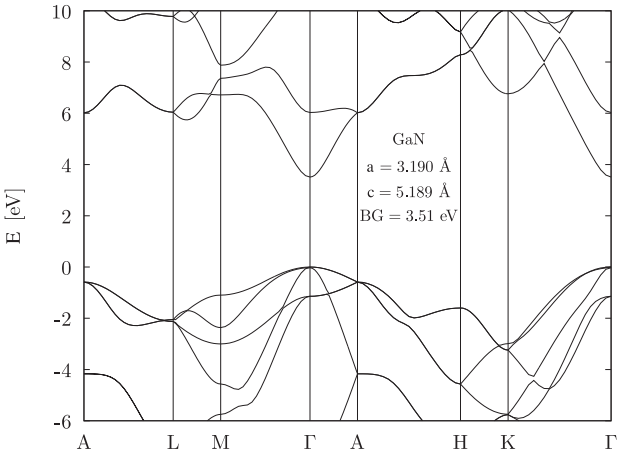

Fig. 2. The full bandstructure calculated from first principles.

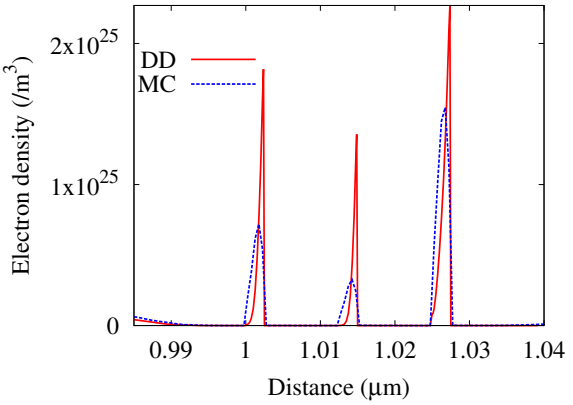

Fig. 3. Electron densities from the initial DD and final MC simulations for a structure with three QWs, at a current density of 400 A/cm^2.

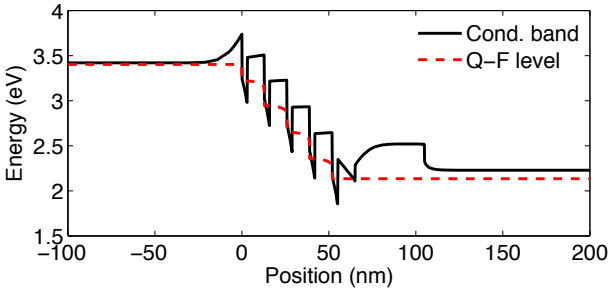

Fig. 4. Band diagram of the structure with 5 QWs from the DD simulation. The bias voltage is 4.5 V and the current density is 284 A/cm^2.

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References

[1] S. Nakamura and M. R. Krames, Proc. IEEE **101**, 2211–2220 (2013).
[2] J. Piprek, Compound Semiconductor **20**, 44–48 (2014).
[3] J. Piprek, J. Römer, and B. Witzigmann, Appl. Phys. Lett. **106**, 101101 (2015).
[4] J. Iveland, M. Piccardo, L. Martinelli, J. Peretti, J. W. Choi, N. Young, S. Nakamura, J. S. Speck, and C. Weisbuch, Appl. Phys. Lett. **105**, 052103 (2014).
[5] M. Binder, A. Nirschl, R. Zeisel, T. Hager, H.-J. Lugauer, M. Sabathil, D. Bougeard, J. Wagner, and B. Galler, Appl. Phys. Lett. **103**, 071108 (2013).
[6] T. Sadi, P. Kivisaari, J. Oksanen, and J. Tulkki, Appl. Phys. Lett. **105**, 091106 (2014).
[7] P. Kivisaari, J. Oksanen, J. Tulkki, and T. Sadi, J. Comput. Electron., DOI: 10.1007/s10825-015-0687-z (2015).
[8] P. Kivisaari, T. Sadi, J. Oksanen, and J. Tulkki, Proc. SPIE **9363**, 93631S (2015).
[9] P. Kivisaari, J. Oksanen, and J. Tulkki, J. Appl. Phys. **111**, 103120 (2012).