

# Coupled Monte Carlo–drift-diffusion simulation of transport in III-N LEDs

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## INTRODUCTION

III-N LEDs have started a revolutionary change in the lighting industry, but many problems stand in the way of further improvements. One of the most serious problems is the efficiency droop, which has been studied and discussed for several years without a clear conclusion on its cause [1], [2]. The two most widely accepted possible explanations are a form of electron leakage [3] and direct or indirect Auger recombination [4]. One of the solution methods proposed to avoid droop is to use multi-quantum well (MQW) devices. However, in a typical device this does not help, since only one of the quantum wells (QWs) emits all the light [5], [6]. In spite of numerous theoretical and experimental attempts to explain the origins of the droop, discussion has not advanced for some time. The discussion is further complicated due to difficulties in fitting various theoretical and experimental results together. Therefore advanced physical models are needed for further investigations.

We introduce a coupled Monte Carlo–drift-diffusion (MCDD) device simulation method to study the efficiency droop in III-Nitride MQW LEDs. We apply the method to answer two relevant questions: (i) the importance of electron leakage in the efficiency droop of MQW LEDs and (ii) the causes of uneven carrier distribution between the QWs. The novelty of our work lies in applying the Monte Carlo (MC) method [7]: by employing a self-consistent MC simulation for the electron gas we gain accurate information of the droop mechanisms based on the device physics. This cannot be fully done by using the conventional DD model which relies on the assumption of carrier thermalisation. In this work, we also report the discrepancies between

the DD model and the more sophisticated MC method in these specific devices.

## METHOD, RESULTS AND DISCUSSION

In the MCDD method we model the electron gas by direct simulation of the Boltzmann equation with the MC method, which accurately describes nonequilibrium transport in nanodevices. We model the hole gas with the DD equations. The MC and DD are connected through Poisson's equation and the conventional ABC model for electron-hole recombination. The hole distribution is calculated with Fermi distribution, and the coupled simulation is run until convergence is reached, resulting in steady-state solutions.

Fig. 1 shows the MQW LED device including three QWs. Figs. 2, 3, and 4 show the band diagram, carrier densities, and recombination rate density in the structure, calculated with the DD model. Microscopic analyses using the MCDD method confirm the existence of the hot electron population. As demonstrated experimentally in the literature, our simulations confirm that only one QW emits almost all light.

Efficiency droop is still a very important open question in research of III-Nitride LEDs, and our numerical results help in understanding its origins in more detail. The MCDD method introduced in this work can be extended for more accurate studies of current transport in lasers and novel optoelectronic device concepts such as freestanding nanowires, plasmonic optoelectronic structures, and organic LEDs.

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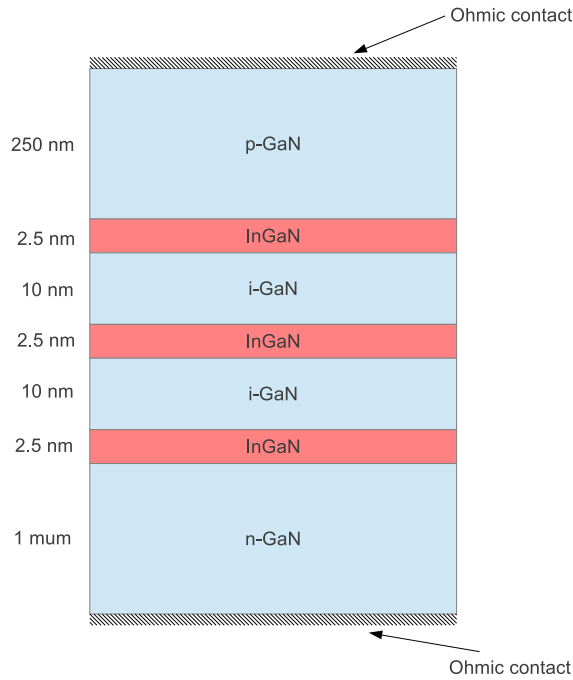


Fig. 1. The III-Nitride MQW structure simulated in this paper.

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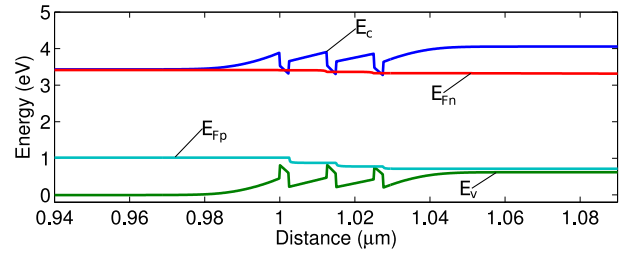


Fig. 2. Band diagram of a MQW LED with 3 QWs at 2.7 V, calculated with the DD model.

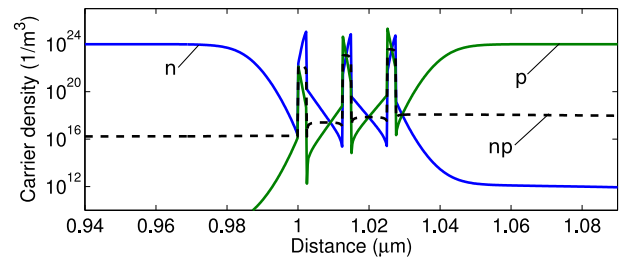


Fig. 3. Carrier densities of a MQW LED with 3 QWs at 2.7 V, calculated with the DD model.

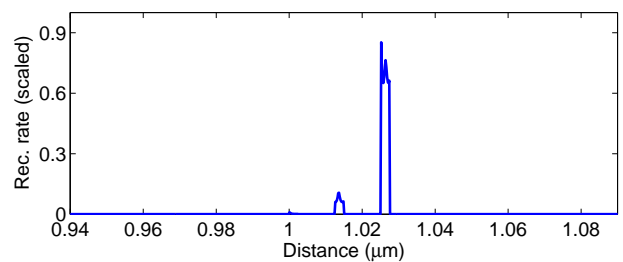


Fig. 4. Scaled recombination rate density in a MQW LED with 3 QWs at 2.7 V, calculated with the DD model. Only one of the QWs emits almost all the light, and one of the QWs is so dim that its recombination rate cannot even be seen on this scale.