3-D simulations on realistic GaN-based light-emitting diodes

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ABSTRACT

Comprehensive multiscale models have been employed to simulate the realistic GaN based light-emitting diodes (LED) using 3D finite-element analysis. The advanced features include drift-diffusion model for carrier transport, self-consistent Poisson-Shrodinger and K·P models for multi-quantum well band structure, quantum tunneling model for heterojunction, spontaneous and piezoelectric polarization models for built-in electric field, heat flow model for self-heating and ray-tracing model for photon extraction. All the advanced capabilities have been integrated into our software APSYS[1]. In this paper, we present the 3D simulations on the InGaN/InGaN LEDs. Based on the detailed simulation results, we were able to analyze the impact of micro- and nano-scale physical effects such as current crowding, carrier leakage, built-in interface charge and self-heating on the internal efficiency of the device. The macro-scale effect of the geometry on photon extraction was analyzed using 3D ray-tracing technique. Results of different structures will be given to demonstrate the power of the software in handling complicated realistic LED geometries. The simulation results can be used to optimize the design of quantum well layers, blocking layer materials and electrode geometries etc.

INTRODUCTION

Extensive experimental effort has been devoted to achieve high-efficiency III-nitride light-emitting diodes (LEDs) by improving the quality of III-nitride materials, optimizing multi-quantum-well (MQW) device structure and efficient light-extraction packaging [2-3]. Compared with a growing number of expensive and time-consuming experimental studies, in-depth simulations on the performance of LEDs are rarely reported. Although basic theoretical models are available for LED simulation, it still lacks detailed understanding of microscopic process, which restricted the design and optimization of LED device structure. For GaN based LEDs, computer simulations are very useful for device design issues such as current leakage, light extraction, current crowding and thermal effects. Kim *et al.* [4] have reported a 2D simulation analysis of InGaN/GaN LED, but the 3D effects on the current spreading and light extraction were not addressed. Piprek et al. [5] have done the simulation and analysis of AlGaN/GaN UV-LEDs using APSYS software.

In this paper, we use our advanced APSYS software to simulate comprehensively the real 3D GaN LEDs with different structures. Most important physical models are included for the simulations, which provide complete description of the LED operations. The presence of InN-composition modulation within the InGaN quantum wells has been taken into account to explain the EL spectrum and the I-V characteristics for the first time. We show that the classic drift-diffusion equation is not sufficient to describe the carrier transport of InGaN MQW structures and the contribution of quantum dot to the carrier transport and spontaneous emission has to be considered.

THEORETICAL MODELS

The simulations have been performed with the software package APSYS, which is a finite-element based device simulator. The advanced features include drift-diffusion model for carrier

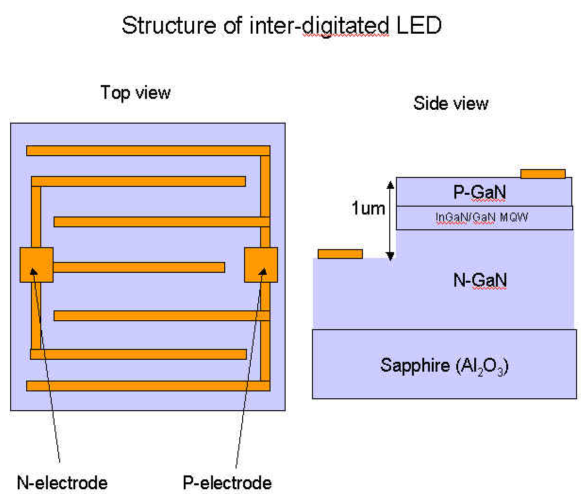


Figure 1(a) Inter-digitated LED.

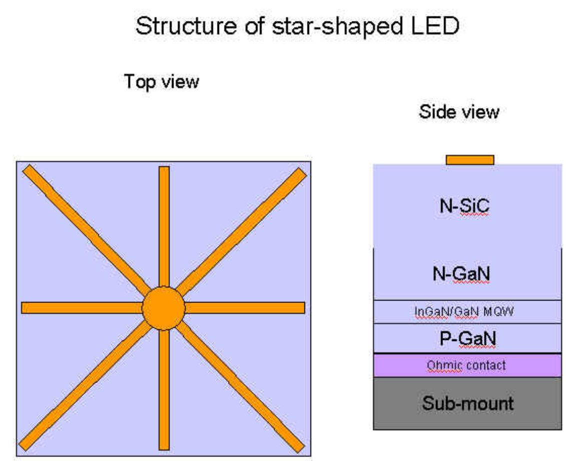


Figure 1(b) Star-shaped LED.

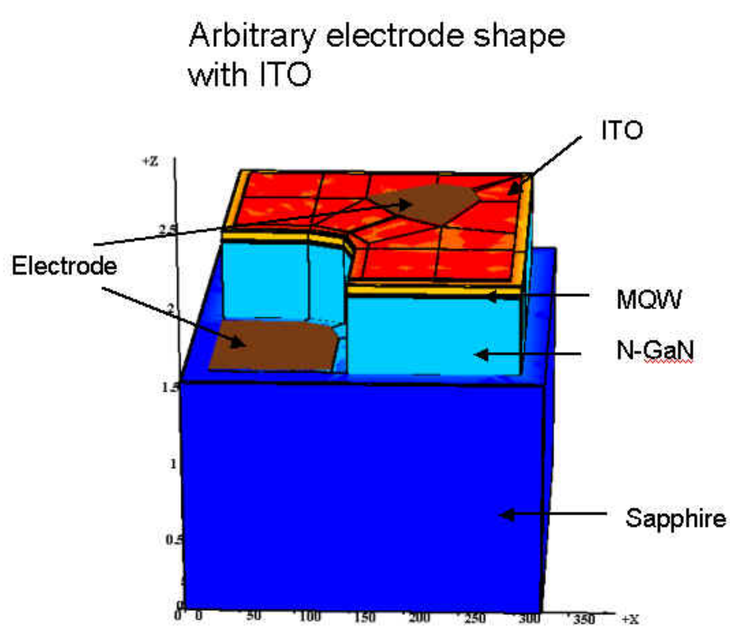


Figure 1 (c) Arbitrary electrode shape using ITO transport, self-consistent Poisson-Shrodinger and K·P models for multi-quantum well band structure, quantum tunneling model for heterojunction, spontaneous and piezoelectric polarization models for built-in electric field, heat flow model for self-heating and ray-tracing model for photon extraction. For details of the physical models implemented in APSYS, refer to Ref. [1].

The spontaneous and piezoelectric charge were calculated using fixed charge model by Fiorentini *et al.* [6]. This model did not take into account the screen effect of carriers and overestimated the value of the interface charge. It is noted that using 10%-50% of the calculated charge results in better agreement with experiments [5].

LED DEVICE STRUCTURE

The structures that we have simulated successfully are shown in Figure 1. The first 3D structure is inter-digitated electrodes. It has been demonstrated that the inter-digitated mesa pattern improves the optical power due to a more uniform current distribution and light extraction. The device was grown on sapphire substrate, the multi-quantum-well (MQW) active layers are composed of InGaN/InGaN with In composition of 10-30%. The chip size is about 1x1 mm^2, and the quantum well thickness is about 2nm. The second design is the so called star-shaped electrode which was fabricated by wafer bonding. The light extraction from top is enhanced due to transparent high refractive index SiC. Because SiC is conductive, the electrode can be directly deposited on top of it so that electrons and holes can be injected vertically, resulting in more uniform carrier distribution. The third structure uses transparent indium-tin-oxide (ITO) as contact, which has been proved more efficient for light extraction. These device structures are popular in commercial applications, and obviously only with 3D simulations can we accurately describe the electric and optical characteristics of these structures. Any attempts using 2D simulations will not be sufficient.

RESULTS AND DISCUSSIONS

The characteristics of the devices have been studied by 3D simulations, which include current-voltage curve, light power-current, 2D/3D distribution of potential, electron and hole concentration and lattice temperature, band diagram at different biases, spontaneous emission. Spectrum, ray-tracing and so on. Some results is presented here to demonstrate the power of the simulator. Figure 2 is current distribution for a inter-digitated structure, which shows clearly the current crowding under the contact. Figure 3 shows a typical I-V curve for the LED device and Figure 4 is the internal efficiency. Figure 5 shows the extracted power distribution versus angle in polar coordinate obtained using ray-tracing, which is very useful for package design.

Quantum dot effects

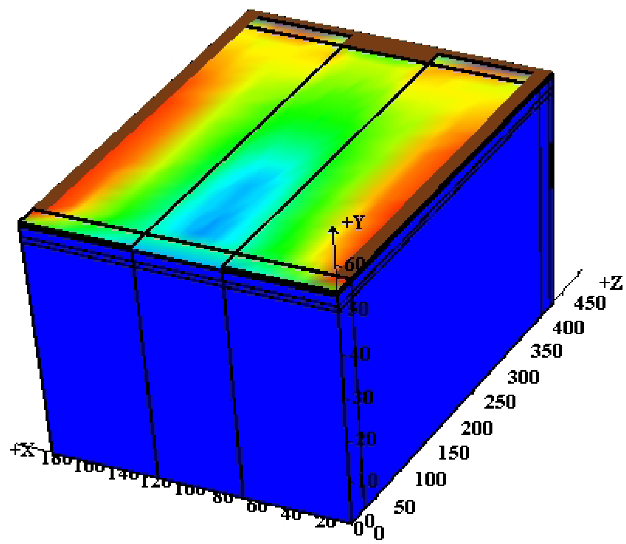
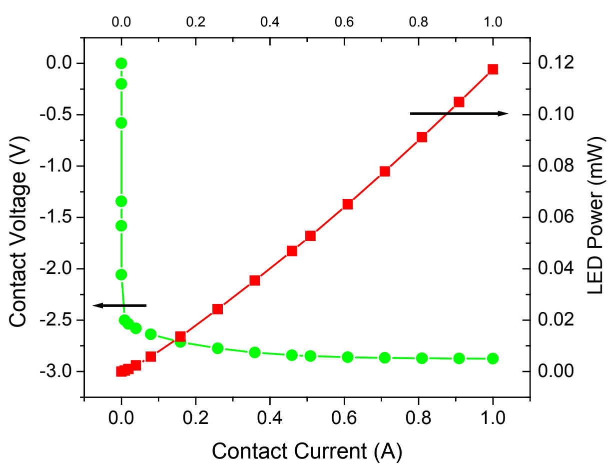


Figure 2 Current distribution shows the carrier crowding under the contact.



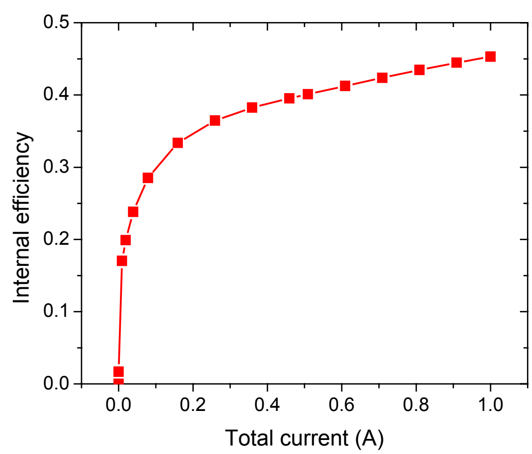


Figure 3 Current-voltage relation and LED light power as function of current.

Figure 4 Internal efficiency with current.

It is well known that the presence of InN-composition modulation within the InGaN quantum wells has significant effects on the LED internal efficiency and EL spectrum [2, 7]. The InN composition inhomogeneity could be due to inherent InGaN phase segregation or could be driven by the large lattice mismatch between InGaN and GaN. In-enriched regions act as quantum dot-like structures and therefore quantum transport should be taken into account in addition to drift-diffusion transport mechanism. The quantum dot-like structures have stronger confinement and higher In composition with respect to the quantum well, and act as the efficient radiative centers with emission wavelength very different from that of the quantum well emissions.

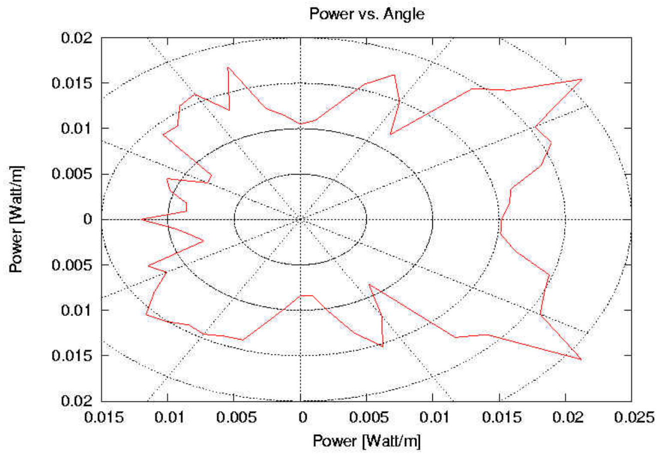


Figure 5 Extracted optical power distribution versus angle in polar coordinate

We report briefly the simulations on an InGaN/InGaN LED and compare the results with experiments. Experimental details have been published elsewhere [8], and the theoretical models for quantum transport and quantum dot emission will be given in another paper [9]. The quantum transport considers the carrier flying over the small quantum dots and the escaping from the confinement of quantum dots. We have included four different quantum dot sizes with diameters from 2-7nm. Spontaneous emission from both quantum well and quantum dots are taken into account.

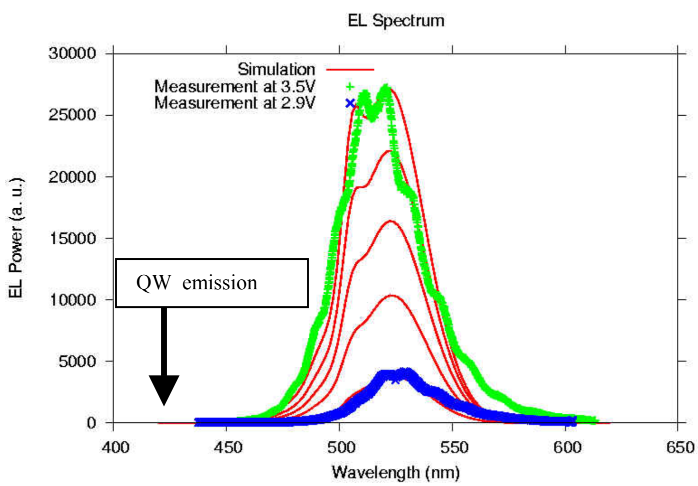


Figure 6 Calculated and experimental EL spectrum at different bias conditions. Arrow indicates quantum well emission.

Figure 6 shows that the spontaneous emission from MQW is about 420nm, far away from the experimental results. All the EL power comes from the quantum dot emissions, in very good agreement with experiment. Figure 7(a) is the I-V characteristic calculated with and without quantum transport. We here found out that simple drift-diffusion mechanism is not adequate for InGaN/InGaN MQW system where quantum dot structures are found inside the quantum wells due to In segregation. It is noted from Figure 7(b), drift-diffusion mechanism does not considers the escape and capture of carriers, and therefore the internal efficiency is overestimated to be close to 100%. The internal efficiency calculated by quantum transport is decreasing with current, because more carriers escape from or simply fly over the dots as more carrier are injected. The same trend has also been observed in experiments.

CONCLUSIONS

We have demonstrated the capability of our advanced software package APSYS in design and 3D simulation of realistic GaN based LEDs on typical LED structures from commercial applications. The software package incorporates most important multi-scale physical models and the output from the simulation give a full description of the characteristics of LED. We also showed that for InGaN MWQ LEDs, quantum transport and quantum dot spontaneous emission are essential for predicting the current-voltage relation and EL spectrum.

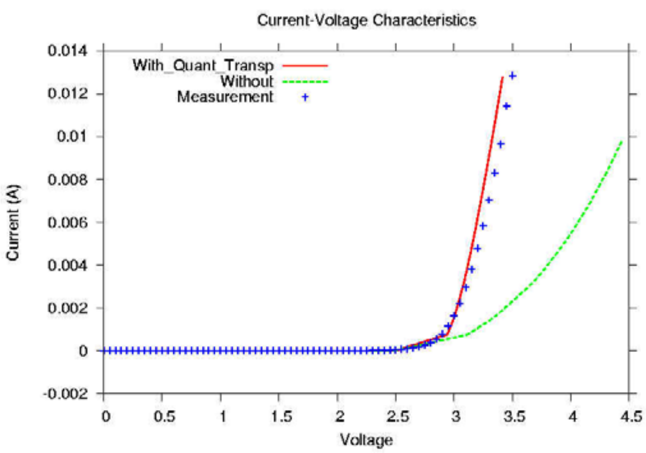


Figure 7(a) Current-Voltage characteristics

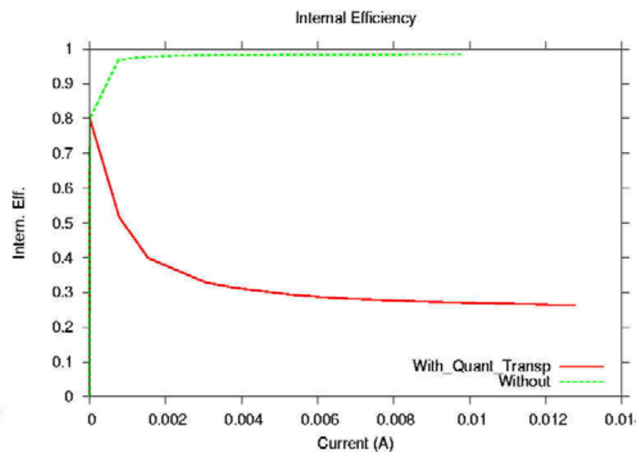


Figure 7(b) Internal efficiency as function of current

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