Impact of the surface recombination on InGaN/GaN-based blue micro-light emitting diodes

JIANQUAN KOU,1,4 CHIH-CHIANG SHEN,2,4 HUA SHAO,1 JIAMANG CHE,1 XU HOU,1 CHUNSHUANG CHU,1 KANGKAI TIAN,1 YONGHUI ZHANG,1 ZI-HUI ZHANG,1,5 AND HAO-CHUNG KUO2,3,6

1School of Electronics and Information Engineering, Hebei University of Technology, Key Laboratory of Electronic Materials and Devices of Tianjin, 5340 Xiping Road, Beichen District, Tianjin 300401, China
2Department of Photonics and Institute of Electro-optical Engineering, National Chiao Tung University, Hsinchu 30010, Taiwan
3Department of Electrical Engineering and Computer Sciences and TBSI, University of California at Berkeley, Berkeley, CA 94720, USA
4Authors contributed equally to this work
5zh.zhang@hebut.edu.cn
6hckuo@faculty.nctu.edu.tw

Abstract: In this work, the size-dependent effect for InGaN/GaN-based blue micro-light emitting diodes (µLEDs) is numerically investigated. Our results show that the external quantum efficiency (EQE) and the optical power density drop drastically as the device size decreases when sidewall defects are induced. The observations are owing to the higher surface-to-volume ratio for small µLEDs, which makes the Shockley-Read-Hall (SRH) non-radiative recombination at the sidewall defects not negligible. The sidewall defects also severely affect the injection capability for electrons and holes, such that the electrons and holes are captured by sidewall defects for the SRH recombination. Thus, the poor carrier injection shall be deemed as a challenge for achieving high-brightness µLEDs. Our studies also indicate that the sidewall defects form current leakage channels, and this is reflected by the current density-voltage characteristics. However, the improved current spreading effect can be obtained when the chip size decreases. The better current spreading effect takes account for the reduced forward voltage.

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1. Introduction

Compared to organic light-emitting diodes (LEDs), III-nitride based light-emitting diodes have many advantages, including high brightness, low power consumption, long operating lifetime, and so on. Therefore, III-nitride based micro-level solid-state lighting is considered as the emerging display technology of the next generation [1,2]. Because of the high modulation bandwidth, micro-light emitting diodes (µLEDs)-based visible light communications (VLC) become increasingly popular and have achieved remarkable development progress [3]. Recently, mobile device displays such as smart watches, augmented reality, virtual reality, mobile phones and wearable appliances are also receiving extensive attention from semiconductor community [4–6]. As a result, devices featuring ultra-high resolution and low power consumption are strongly required at the current stage. Therefore, to meet the demands, the size for III-nitride based LEDs that serve as display pixels has to be reduced, i.e., µLEDs are proposed. However, the development for µLED display technology still encounters multiple challenges, e.g., high-accuracy mass transfer [7–9] and the size-dependent device efficiency [10]. Targeting at the technologies for one-time transferring µLED chips at the level of mass production, LuxVue and KIMM have
preliminarily proposed electrostatic pick-up array and roll-based multiple transfer technology after much effort, respectively [4]. Thus, the technical solution for the mass transfer of µLED chips can be expected in the near future.

In general, the reduced chip size helps to release the strain and improve the luminous efficiency [11], homogenize the current spreading [12], decrease the junction temperature [13] and enhance the light extraction efficiency [14]. In spite of the listed advantages for small size LED chips, the external quantum efficiency (EQE) for LEDs drops drastically as the chip size reaches micro-level, which is tentatively ascribed to Shockley-Read-Hall (SRH) non-radiative recombination taking place at the sidewall defects [15]. At present, sidewall passivation using dielectric materials has been verified as an effective approach to minimize the effect of sidewall defects for µLEDs. However, sidewall passivation that is performed by different methods has different impact on µLED photoelectric properties. Sidewall passivation is conventionally performed using plasma enhanced chemical vapor deposition (PECVD) method, which provides a rapid deposition rate, leading to the poor film quality [16,17]. On this basis, Tian et al. demonstrate that sidewall defects caused by dry etching can be partially recovered by increasing the thermal annealing time to 3 min at the temperature of 500 °C, and thereby the efficiency can be improved [18]. Most recently, Wong et al. have conducted a systematic experimental study on various sidewall passivation methods [19]. According to their report, by combining the atomic layer deposition (ALD) technique and the buffered hydrofluoric acid (HF) wet etch, the passivation layer for the fabricated µLEDs enables the lowest leakage current. Moreover, the light emission is uniform across the chips and the EQE is 33% at the current density of 40 A/cm². Hence, the currently developed techniques for fabricating the passivation layer have improved the µLEDs to some certain level. Nevertheless, the previously reports are more on the fabrication technology for µLEDs, we believe that, before maximizing the EQE, it is also essentially important to understand the carrier injection and the electron-hole recombination process for µLEDs, which however has been rarely discussed till now. For that reason, it is worth uncovering the physical mechanism regarding the impact of the sidewall defects on the carrier injection, since by doing so, the µLED structures can be fully optimized in a targeted manner. Hence, in this report, we numerically investigate the size-dependent efficiency for InGaN/GaN based blue µLEDs. Our results illustrate that, without considering sidewall defects, the µLEDs possess the enhanced EQE and optical power density when the chip size decreases, which is attributed to the improved current spreading. However, when the sidewall defects are considered in our models, we find that the EQE and optical power drop drastically as the device size decreases, which is consistent with the earlier experimental reports [2,15]. Very importantly, we also observe the poor carrier injection efficiency and the stronger current leakage when the chip size for µLEDs shrinks. Hence, our results suggest that, besides annihilating the sidewall defects during the chip fabrication, it is vitally important to enhance the carrier injection capability even for µLEDs.

2. Device structures and parameters

All the investigated InGaN/GaN based blue µLED devices comprise a 4 µm thick n-GaN layer with the Si doping concentration of $5 \times 10^{18}$ cm$^{-3}$. Next four-period In$_{0.15}$Ga$_{0.85}$N/GaN multiple quantum wells (MQWs) follow, which enable the peak emission wavelength of ~445 nm. The thicknesses for the quantum wells and the quantum barriers are 3 nm and 22 nm, respectively. On top of the active region, there is a 26 nm thick p-Al$_{0.15}$Ga$_{0.85}$N electron blocking layer (EBL) and a 120 nm thick p-GaN cap layer. The hole concentration levels for the p-EBL and the p-GaN cap layer are set to $3 \times 10^{17}$ cm$^{-3}$. Finally, a 20-nm thick heavily doped p-GaN layer is adopted for achieving the p-type ohmic contact. In order to probe the dependence of the performance on the chip size for blue µLEDs, three sets of µLEDs with the dimensions of 20 × 20 µm$^2$, 60 × 60 µm$^2$ and 100 × 100 µm$^2$ are designed, respectively. Here, we use two different models to study our µLEDs. In model 1, we do not incorporate any
surface defects for our devices, i.e., LEDs I, II and III with the dimensions of 100 × 100 µm², 60 × 60 µm² and 20 × 20 µm² are studied, respectively. In model 2, we consider the surface defects for our devices, i.e., LEDs A, B and C with the dimensions of 100 × 100 µm², 60 × 60 µm² and 20 × 20 µm² are studied, respectively. The depth for the damaged region is set to 4 µm wide [see Fig. 1], which is within the reasonable range from the point view of actual experiments.

The numerical calculations are performed by using APSYS simulator, which is able to solve current continuity equations, Poisson’s equations and Schrödinger equations with proper boundary conditions. For all our six µLEDs, the Auger recombination coefficient and the SRH lifetime are set to be 1 × 10⁻²⁰ cm³ s⁻¹ [20] and 1 × 10⁻⁷ s⁻¹ [20], respectively. The energy band offset ratio between the conduction band offset and the valence band offset of 70/30 is adopted for InGaN/GaN MQWs [21]. The light extraction efficiency for the studied blue µLEDs is 88.1% [2]. Specifically, for LEDs A, B and C, the electron trap level is set at 0.24 eV below the conduction band (i.e., E⁰ ≈ 0.24 eV) with the capture cross-section of 3.4 × 10⁻¹⁷ cm² and the density of 1 × 10¹⁵ cm⁻³ [22]. The hole trap level is set at 0.6 eV above the valence band (i.e., E⁺ ≈ 0.46 eV), for which the density is 1.6 × 10¹³ cm⁻³ and the capture cross-section is set to 2.1 × 10⁻¹⁵ cm² [23]. The other material parameters used in the numerical models can be found elsewhere [24].

![Fig. 1. Schematic structures for LEDs I, II and III without sidewall damages and LEDs A, B, C with sidewall damages. The usable area ratios for LEDs A, B and C are 85%, 75% and 36%, respectively.](Image)

3. Results and discussions

We firstly calculate and present the EQE and the optical power density in terms of the injection current density level for the investigated devices in Figs. 2(a) and 2(b), respectively. We firstly compare LEDs I, II and III, and we can get the EQE and the optical power density increase as the chip size decreases, which is tentatively attributed to the better current spreading effect [12]. However, if we compare LEDs I, II and III with LEDs A, B and C, we can get that the EQE and optical power decrease when the surface defects are considered for LEDs A, B and C. Further investigation into LEDs A, B and C shows that the EQE and the optical power density become worse when the chip size gets small, thus the opposite trend observed. Although the current spreading for small-dimension devices has been improved, the surface recombination plays a more dominant role. Hence, we attribute the observation for LEDs A, B and C to the very strong surface recombination when the chip size decreases.
Moreover, according to the report in [19], our findings by numerical calculations for LEDs A and C agree well with the experimental results [see the inset in Fig. 2(a)], such that the experimentally measured EQE for the 100 × 100 µm² µLED is significantly higher than that for the 20 × 20 µm² µLED and the efficiency droop for the 20 × 20 µm² µLED is not observed within the tested current density range. Both numerical and experimental results show that with the increase of the surface-to-volume ratio for µLEDs, the impact of sidewall defects on device performance cannot be ignored. Therefore, it is also worth emphasizing here that the surface defects have to be considered when modelling µLEDs.

Figure 2 shows the numerically calculated current density as a function of the applied bias for the six investigated µLEDs. The values of the forward operation voltages are 3.48 V, 3.37 V and 3.33 V, 3.47 V, 3.33 V and 3.23 V at the current density of 20 A/cm² for LEDs I, II and III, A, B and C, respectively. For both sets of LEDs, we can see that the forward operation voltage decreases when the chip size is reduced. The reduced forward operation voltage is ascribed to the reduced lateral spreading resistance when the chip size is decreased [2]. More discussions regarding the influence of the chip size on the current spreading will be made in the end of this work. If we compare the two sets of LEDs, e.g., LED III and LED C, we can find from Fig. 3 that the turn-on voltage for LED C is lower than that for LED III. Here, we define the voltage difference of ΔV for LED A/LED I, LED B/LED II and LED C/LED III, respectively. The values of ΔV are 0.01 V, 0.04 V, 0.1 V at the current density of 20 A/cm², respectively. It indicates that ΔV becomes large when the chip size becomes small. The inset figure in Fig. 3 presents the current-voltage characteristics in semi-log scale for LEDs III and C, we can see the very strong current leakage through the defects. Thus, the large ΔV reflects the current leakage paths through the sidewall defects for the µLEDs especially when the chip size further decreases.
In order to reveal the origin of the size-dependent efficiency for blue µLEDs, we also calculate and show the electron concentration profiles within the MQWs for all the studied devices in Fig. 4. It can be seen from Fig. 4(a) that the overall electron concentration in the MQWs for LEDs I, II and III increases as the device dimension decreases. The improved electron injection arises from the better current spreading effect when the chip size is reduced. On the contrary, the overall electron concentration in the quantum wells for LEDs A, B and C decreases with the decreasing device dimension according to Fig. 4(b). The improved current spreading enables the electrons to reach the mesa edge and most of the electron are finally captured by the sidewall defects, which therefore reduces the electron density in the MQWs when the chip size becomes small. This explanation is also supported by comparing Figs. 4(a) and 4(b), such that the electron concentration level in the MQWs in Fig. 4(b) is much lower than that in Fig. 4(a), e.g., LED A in Fig. 4(b) shows the lower electron concentration level in the MQWs than LED I in Fig. 4(a). Because of the SRH recombination taking place at the sidewall defects, the electron leakage level into the p-GaN layer becomes small, i.e., we can see that the leakage electrons for µLEDs in Fig. 5(b) have been significantly decreased when compared to the devices in Fig. 5(a). Moreover, if we compare LEDs A, B and C, we also find that LED C has the least leakage electrons in the p-type GaN layer. Note, LED C only possesses 36% of the total mesa area that can efficiently produce light, and hence most of the electrons are captured by the sidewall defects and recombine non-radiatively therein, leading to the lowest electron leakage.
We also investigate the hole transport for the six µLEDs in Figs. 6(a) and 6(b). Figure 6(a) demonstrates that, if the sidewall defects are not considered in our models, the hole concentration in the MQWs increases as the device size decreases, which is due to the better current spreading effect. Surprisingly, when we consider sidewall defects, we can see that the hole concentration in the MQWs decreases significantly as the µLED dimension diminishes as shown in Fig. 6(b). By comparing Fig. 4 with Fig. 6, we can find an interesting phenomenon that the impact of defects on hole injection is far greater than that on electrons, especially for very small device. The results can be understood from the following two aspects: on one hand, the hole traps have large capture cross-section and big trap density as compared to the electron traps according to [22,23], which leads to a bigger probability for holes to be captured by the defects. On the other hand, the hole mobility is much lower than that of electrons, and hence holes have small kinetic energy. As a result, when compared with
electrons, the holes are less likely to be emitted again once they are captured by the defects. Therefore, the hole injection is more challenging than the electron injection for µLEDs.

![Graph](image1)

Fig. 6. Numerically calculated hole concentration profiles in the MQW region for (a) LEDs I, II and III, (b) LEDs A, B and C, respectively. Data are calculated when the injection current is 100 A/cm². Inset figure shows the position along which the hole concentration profiles are captured.

Since the sidewall defects are located at the mesa edges, thus we shall present the lateral electron and hole distribution profile. For the purpose of demonstration, we compare the lateral carrier density for LEDs III and C in Figs. 7(a) and 7(b), respectively. It is found that the carrier distribution profiles in LEDs III and C are quite different. The observations in Fig. 7(a) agree well with the previously reports that the current crowding occurs under the p-electrode [25,26], and the carrier density level gradually decreases when far apart from the p-electrode. However, the carrier concentration at the mesa edge for LED C drops quickly [see Fig. 7(b)], which is due to the presence of sidewall defects. Therefore, care shall be taken to µLEDs that, once the carriers reach the mesa edge, they can be captured by the sidewall defects and the SRH recombination occurs. Note, we also discuss the lateral carrier concentration profiles for LEDs I, II, III, A, B and C subsequently.

![Graph](image2)

Fig. 7. Numerically calculated carrier concentration profiles in the first quantum well near the p-region for (a) LED III, and (b) LED C, respectively. Data are calculated when the injection current is 100 A/cm².
To further discuss the influence of the chip size on the current spreading effect, we calculate and show the lateral carrier concentration profiles in the first quantum well near the p-region for LEDs I, II and III in Figs. 8(a), 8(b) and 8(c). We can see that the hole and electron distributions in the last quantum well becomes more uniform as the chip size reduces, such that the droop levels at the mesa edge for electrons are 62.8%, 44.4% and 12.4% for LEDs I, II and III, respectively, while the droop levels for holes are 90.4%, 75.5% and 27.1% for LEDs I, II and III, respectively. This is attributed to the reduction of the spreading resistance as the device size decreases. Note, the electron distribution is more uniform than holes. Next, we calculate and show the lateral carrier concentration profiles in the first quantum well near the p-region for LEDs A, B and C in Figs. 9(a), 9(b) and 9(c). The same conclusion is obtained that the current spreading can be improved with the decreasing chip size. However, when the sidewall defects are considered in our calculations, the hole and electron significantly decreases at the defected regions for the mesa. The very low carrier concentration levels at the defected mesa regions are well attributed to the surface damages, which give rise to the carrier consumption by the way of SRH non-radiative recombination. The very strong SRH non-radiative recombination at the defected mesa edges for LEDs A, B and C explains the leakage current in Fig. 3.

Fig. 8. Numerically calculated carrier concentration profiles in the first quantum well near the p-region for LEDs I, II and III, respectively. Data are calculated when the injection current is 100 A/cm². Inset in Fig. 8(a) shows the position along which the carrier concentration profiles are captured for LEDs I, II and III.
4. Conclusions

To summarize, we have numerically investigated and demonstrated the impact of sidewall defects on EQE, optical power, operating voltage and carrier concentration profiles for blue μLEDs. If the sidewalls are perfectly fabricated, then the EQE for μLEDs increases as the chip size decreases. Moreover, a small chip size helps to homogenize the lateral current. Nevertheless, sidewall defects that are generated during the etching process cannot be completely avoided even if the passivation layer is deposited. As a result, when modeling μLEDs, the impact of the sidewall defects cannot be ignored. The sidewall defects serve as the current leakage paths (i.e., the carriers are capture by the sidewall defects and the SRH recombination takes places therein), which therefore degrades the carrier concentration in the MQWs especially when the chip size for the μLEDs further decreases. In particular, due to the large density and the capture cross-section for the hole traps, holes are more easily captured by the sidewall defects than electrons. Therefore, more attention ought to be paid to improve the hole injection for μLEDs, and we propose to incorporate a hole accelerator and/or a hole modulator during the epitaxial growth [27,28]. We strongly believe that this work provides the physical insight for the device physics and hence the findings in this work are very important for the community to further get μLEDs involved into micro-display pixel and multi-channel VLC systems.

Funding

Natural Science Foundation of Hebei Province (F2017202052); Natural Science Foundation of Tianjin City (16JCYYYB16220, 16JCQNJC0100); Program for Top 100 Innovative Talents in Colleges and Universities of Hebei Province (SLRC2017032); Program for 100-Talent-Plan of Hebei Province (E2016100010); Suzhou Institute of Nano-Tech and Nano-Bionics (SINANO) Research Fund (19ZS02) of Chinese Academy of Science.
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