

# InGaN multiple quantum well based light-emitting diodes with indium composition gradient InGaN quantum barriers\*

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To improve the internal quantum efficiency (IQE) and light output power of InGaN light-emitting diodes (LEDs), we proposed an In-composition gradient increase and decrease InGaN quantum barrier structure. Through analysis of its *P-I* graph, carrier concentration, and energy band diagram, the results showed that when the current was 100 mA, the In-composition gradient decrease quantum barrier (QB) structure could effectively suppress electron leakage while improving hole injection efficiency, resulting in an increase in carrier concentration in the active region and an improvement in the effective recombination rate in the quantum well (QW). As a result, the IQE and output power of the LED were effectively improved.

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Light-emitting diodes (LEDs) are mostly used in general lighting, traffic lights, advertising, television, etc<sup>[1-5]</sup>. However, the internal quantum efficiency (IQE) of LEDs drops sharply at high currents. After analysis, the main reason for the decrease in efficiency is the low efficiency of electron leakage and hole injection, the mobility of electrons is much higher than that of holes, resulting in electron overflow, causing serious energy loss<sup>[6]</sup>, uneven carrier distribution, polarization field effects<sup>[7,8]</sup> and so on. In order to improve the problem of efficiency decline, researchers have proposed many solutions. In order to reduce the piezoelectric polarization field generated in the well layer due to the lattice-barrier mismatch, XU et al<sup>[9]</sup> proposed to use InGaN barriers with low In content and InGaN quantum wells (QWs) with relatively high In content, which reduces the lattice mismatch between the well layer and the barrier layer reduces the piezoelectric field. YEN et al<sup>[10]</sup> suggested using an n-type AlGaIn layer under the active region, and KUO et al<sup>[11]</sup> proposed to use an InGaN barrier instead of a tradi-

tional GaN barrier to reduce the efficiency drop of the LED. Recently, KUO et al<sup>[12]</sup> designed LED structures with GaN-InGaN-GaN multi-layer quantum barriers (QBs), such that electrons and holes have a uniform distribution in the multiple quantum wells (MQWs). In order to solve the problem of low hole injection efficiency, XIONG et al<sup>[13]</sup> designed an AlGaIn-based step-like barriers structure without an electron blocking layer, and improved the hole injection efficiency by removing the electron blocking layer. KARAN et al<sup>[14]</sup> increased the LED output power by introducing a gradient QW layer and adjusting the appropriate InGaN/GaN MQW base width. HENGSTELER et al<sup>[15]</sup> by introducing a compositionally step graded (CSG) InGaIn barriers to achieve a higher IQE. It is well known that most researchers use InGaIn/GaN based MQW to develop LEDs, and the quantum confinement Stark effect (QCSE) caused by strain-induced piezoelectric polarization of GaN-based LEDs is lower than that of InGaIn based LEDs, which indicates that GaN devices' electron-hole wave function

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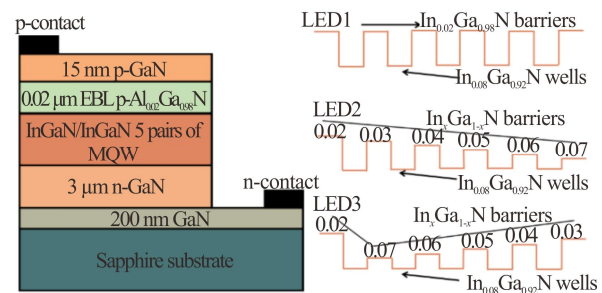
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overlap is higher than that of InGaN devices. The addition of Al to GaN further enhances this overlap, so InGaN/AlGaN based LEDs have higher photon confinement and emission power, but the GaN-based barrier reduces the electron-hole spatial separation when the wavelength exceeds 410 nm. For near-UV LEDs, AlGaN QB has higher advantages than GaN<sup>[16,17]</sup>. However, the Al composition does not contribute to the generation of excitons, which makes InGaN a suitable choice for near-UV LEDs<sup>[18]</sup>. To achieve high IQE and output power in LEDs, most of the recombination process must take place in the active region. Therefore, holes and electrons must be largely confined to the QW region. JIANG et al<sup>[19]</sup> used the InGaN quantum barrier with a gradient-increased structure to increase the luminous power of the LED, but the two pairs of gradient-decrease structures cannot make the holes pass through the active region and move closer to the n-layer QW. The distribution of carriers in the active region is uniform. In this paper, we use five pairs of In composition gradient subtracted barrier junctions to solve this problem, and in this study, we theoretically studied the influence of InGaN with gradient barrier structure on near-UV LEDs. The calculation results show that the barrier structure with reduced In composition gradient can weaken the energy band bending caused by the strong polarization problem, reduce the QCSE in the active region<sup>[20]</sup>, and increase the electronic barrier height. It is difficult for electrons to leak to the p-type region through the active region, and at the same time reduce the hole barrier height, so that holes can easily enter the active region, improving the hole injection efficiency, and a large number of carriers enter the active region for effective recombination, and the problem of device efficiency degradation is alleviated.

As shown in Fig.1, the basic LED structure consists of a sapphire substrate, which is followed by a 200 nm Si-doped GaN buffer layer, a 3- $\mu\text{m}$ -thick n-GaN layer, MQWs composed of five 4-nm-thick  $\text{In}_{0.08}\text{Ga}_{0.92}\text{N}$  wells (QWs) and six 10-nm-thick  $\text{In}_{0.02}\text{Ga}_{0.98}\text{N}$  barriers (QBs), a 20-nm-thick  $\text{Al}_{0.02}\text{Ga}_{0.98}\text{N}$  electron barrier layer, a 15 nm Mg-doped ( $3.0 \times 10^{18} \text{ cm}^{-3}$ ) GaN layer is used above the EBL, which is the underlying reference structure for LED1. On the basis of LED1 structure, we proposed to change six 10-nm-thick  $\text{In}_{0.02}\text{Ga}_{0.98}\text{N}$  barriers into In composition gradient (0.02, 0.03, 0.04, 0.05, 0.06, 0.07) LED2 structure and In composition gradient minus (0.02, 0.07, 0.06, 0.05, 0.04, 0.03) LED3 structure. The specific structure is shown in Fig.1.

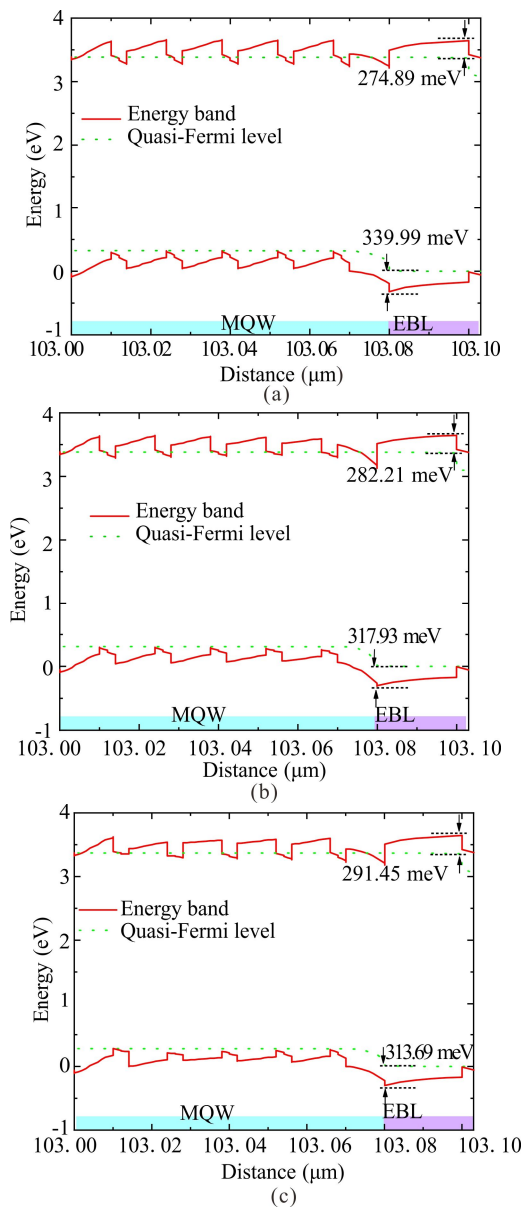
In this numerical study, device simulations were performed using the advanced physical modeling of semiconductor devices (APSYS) tool. APSYS software is used to calculate the electrical behaviour of all LEDs by solving the Poisson's equation and the current continuity equation for electrons and holes. In this study, the electrical and optical properties of the LED structure were

analyzed in detail<sup>[21]</sup>. Simulation parameters include energy band shift ratio, radiation recombination coefficient, Shockley-Read-hall (SRH) recombination lifetime, and Auger recombination coefficient is set to be 0.58,  $0.5 \times 10^{-16} \text{ m}^3/\text{s}$ , 100 ns, and  $1 \times 10^{-46} \text{ m}^6/\text{s}$ , respectively<sup>[22]</sup>. Other materials parameters of AlN and GaN, such as lattice constant, deformation potential, elastic constant, etc, are listed elsewhere<sup>[23]</sup>. The variation functions of electron and hole mobilities were calculated using the most commonly used Arora model<sup>[24]</sup>. All simulations are performed by assuming that the LED devices operate at room temperature.



**Fig.1 Schematics of the DUV-LED structure, and LED1, LED2, and LED3 structures**

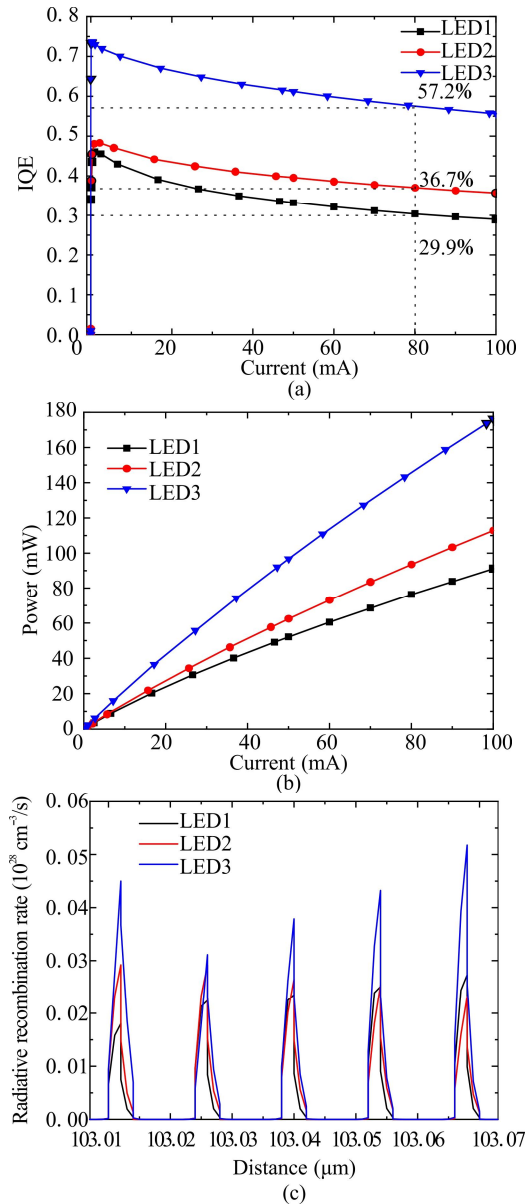
To investigate the performance of the proposed structure, the energy band diagrams of the three structures LED1, LED2, and LED3 are obtained by using well-calibrated APSYS, as shown in Fig.2. The principle of improving hole injection and electron leakage is to reduce the effective barrier height of the valence band and increase the effective barrier height of the conduction band. The effective barrier height is defined as the energy difference between an energy band and its corresponding quasi-Fermi level<sup>[25]</sup> and is a reliable parameter for evaluating the electron confinement ability and hole injection efficiency of a laser. Compared to the reference structure LED1, both LED2 and LED3 have increased effective electron barrier heights and decreased hole barrier heights. The structural change in LED3 is the most noticeable, as its electron barrier height increases to 291.45 meV from 274.89 meV in LED1, effectively preventing electron leakage from the active region to the p-type region. At the same time, the hole barrier heights of LED1, LED2, and LED3 are 339.99 meV, 317.93 meV, and 313.69 meV, respectively, and the hole barrier height of LED3 is lower than that of LED1, which increases the efficiency of holes entering the active region. This is mainly because for the gradient QB structure, the lattice mismatch between QW and QB is reduced, thus, this design generates less piezoelectric field, resulting in lower band bending. Therefore, the effective holes barrier height is reduced to improve hole injection efficiency, while the effective electrons barrier height is increased to reduce electron leakage.



**Fig.2 Energy band diagrams and quasi-Fermi levels of (a) LED1, (b) LED2, and (c) LED3**

To further explore the performance of LEDs, we studied the output optical power and IQE of the three structures. Due to the strong electron confinement in the MQW, at the same time, a large number of holes can be injected into the active region. Therefore, the IQE of the designed LED3 is higher than that of conventional LEDs, reaching 57.2% at a current density of 80 mA, as shown in Fig.3(a). Compared with the conventionally structured LED, the IQE decrease rate of the designed LED3 becomes slower with the increase of injected current, indicating that the designed LED3 has higher radiative recombination within the MQW. As shown in Fig.3(b), our conclusion is verified. With the increase of the current, when the current reaches 100 mA, the power of LED3 reaches 176.2 mW compared with LED1 (91.3 mW), an increase of 92.9%. Therefore, the de-

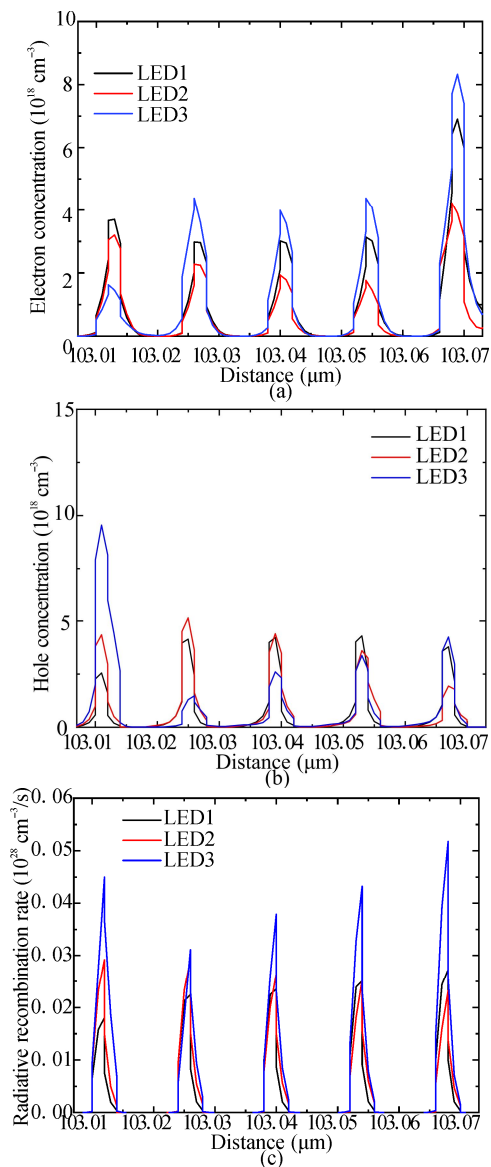
signed LED3 can effectively solve the problem of efficiency drop caused by carrier overflow when large current is injected<sup>[26]</sup>.



**Fig.3 (a) IQEs, (b) output power, and (c) radiative recombination rates of three structures**

Next, we studied the carrier concentration and radiative recombination efficiency of the three LED structures, as shown in Fig.4. To achieve high IQE and output power in LEDs, most of the recombination process must take place in the active region. Due to the large effective mass and low mobility of the holes, it is difficult for the holes to reach the QW close to the n-layer. Therefore, the distribution of holes in the active region is not uniform compared to electrons. In the optimized LED3 structure, the concentration of electrons in the last QW near the p-side layer increases, the concentration of holes in the first QW near the n-side layer increases, and the

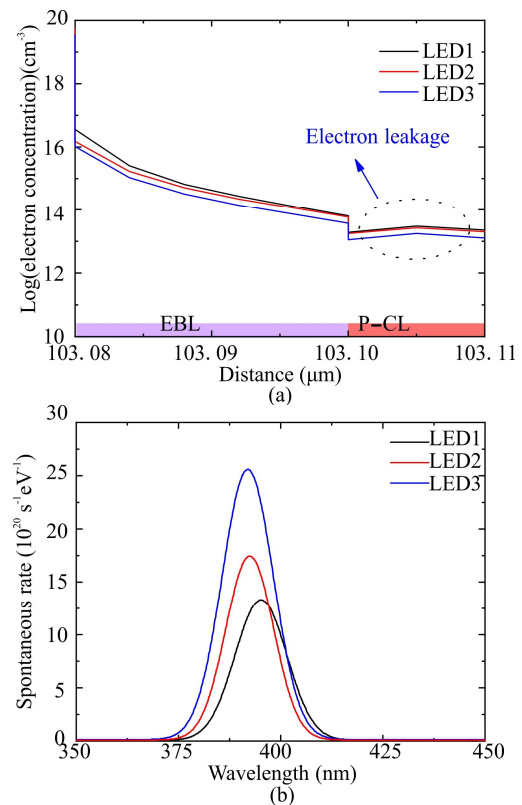
distribution of holes and electrons in the LED3 structure is more uniform than that of LED1, as shown in Fig.4(a) and (b). As shown in Fig.4(c), the radiative recombination rate is more uniform in the QW of the optimized LED3, because the electron and hole concentrations are more, the distribution is uniform, and the electron and hole overlap is larger for the optimized LED3 structure.



**Fig.4 (a) Electron concentrations in the MQWs, (b) hole concentrations in the MQWs, and (c) stimulated recombination rates in the MQWs for LED1, LED2 and LED3**

To further verify the ability of LED3 to suppress electron leakage, we performed a numerical study on the electron concentration in the p-region. Fig.5(a) shows the electron concentrations in the p-region for the three structures. The electron concentration of LED3 is significantly lower than that of LED2 and LED1, which is enough to prove that the gradient reduction quantum

barrier structure of In composition enhances the ability of LED to suppress electron leakage. Finally, we explored the spontaneous emission rate of LED1, LED2 and LED3 at 100 mA injection current as shown in Fig.5(b). It can be seen that as the gradient quantum barrier structure replaces the traditional structure, the peak emission wavelength of InGaN MQW moves from 394 nm to 390 nm, which is caused by the unequal radiative recombination rate and carrier injection efficiency. This investigation also provides insights for further research on LEDs in the near-UV region.



**Fig.5 (a) Electron leakage in the p-type region and (b) spontaneous emission rate at 100 mA injection current for three structures**

In this experiment, we proposed a quantum barrier structure with gradient subtraction of In composition to improve the IQE and output power of InGaN-based LEDs. The hole transport and carrier concentration of the LED are improved by tuning the barrier structure in the MQW. The comparison found that the electrons effective barrier height increased from 274.89 meV to 291.45 meV by 6.02%, and the holes effective barrier height decreased from 339.99 meV to 313.69 meV by 7.73%. The designed quantum barrier structure with gradient reduction of In composition, the well/barrier interface lattice mismatch is reduced, so this design generates less built-in electric field, which improves IQE. Compared with the traditional structure LED1, the output power of the LED3 is increased from 91.3 mW to 176.2 mW, an increase of 92.9%. This design has solved the problem of low efficiency of the device very well.

## Ethics declarations

## Conflicts of interest

The authors declare no conflict of interest.

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