

Performance Improvement of InGaN-Based Red Light-Emitting Diodes via Ultrathin InN Insertion Layer

Qianxi Zhou, Peng Du, Lang Shi, Yuechang Sun and Shengjun Zhou * 

Center for Photonics and Semiconductors, School of Power and Mechanical Engineering, Wuhan University, Wuhan 430072, China

* Correspondence: zhousj@whu.edu.cn; Tel.: +86-027-5085-3293

Abstract: The serious separation of electron–hole wavefunctions, which is caused by the built-in electric field, prevents electron–hole radiative recombination in quantum wells (QWs) in high-In-content InGaN-based red light-emitting diodes (LEDs). Here, we propose a staggered structure that inserts an ultrathin InN layer in the single quantum well (SQW) to reduce the piezoelectric polarization and suppress the quantum confined Stark effect (QCSE). We have numerically simulated the effects of SQW with the InN insertion layer (IL) on the energy band structure and electron–hole wavefunctions of the red LED. Owing to alleviated piezoelectric polarization and improved overlaps of electron–hole wavefunctions, the simulation results have revealed that the internal quantum well (IQE) of the red LED with InN IL exhibits 42% higher than that of the red LED with a square-shaped QW (SSQW) at 60 A/cm², and the efficiency droop ratio of red LED with InN IL is 48% lower than that of red LEDs with SSQW. Furthermore, we have found that the position of InN IL can affect the energy states of carriers, which has a great influence on the IQE and peak emission wavelength of red LEDs.

Keywords: InN insertion layer; piezoelectric polarization; electron–hole wavefunction; internal quantum efficiency; efficiency droop



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1. Introduction

Micro light-emitting diodes (μ LEDs) based on self-emissive inorganic III-nitrides can cover a wide spectral range from ultraviolet to near-infrared, which are considered as an ideal light source for next-generation displays and visual systems due to their high efficiency and robust durability, such as augmented reality and virtual reality [1–5]. In recent decades, InGaN-based blue and green LEDs have been widely investigated and achieved high external quantum efficiency (EQE) [6]. However, the research on InGaN-based red LEDs is still insufficient, especially for red μ LEDs, which impedes the monolithic integration for full-color μ LED displays [7]. Moreover, the common AlGaInP-based red LEDs suffer from severe efficiency droop as size decreases and are sensitive to operation temperature [8,9]. Consequently, it is crucial to further study InGaN-based red μ LEDs.

GaN, InN, and InGaN grown on (0001) sapphire are wurtzite crystal structures that are non-centrosymmetric and can induce polarization along the (0001) axis [10,11]. Due to the large lattice mismatch between GaN and InN, there are strong built-in electric fields in heterostructures arising from spontaneous and piezoelectric polarizations [12]. The built-in electric field causes energy band bending, leading to spatial separation of electron–hole wavefunctions and reduction of the internal quantum well (IQE), which is described as the quantum confined Stark effect (QCSE) [13]. Another difficult issue is that the IQE of LEDs drastically drops under a high injection current, which is caused by Auger recombination [14,15]. To alleviate the strong QCSE and efficiency droop, energy band engineering strategies are extensively proposed, including the quantum dots [16], the semi- or non-polar structures of InGaN [17–19], the graded electron block layer (EBL) [20,21], the

staggered quantum wells (QWs) [22–26], the strain compensation layer on QW [27], and other QWs structures [28–30]. However, these strategies are rarely used in InGaN-based red LEDs and the corresponding mechanism needs to be further investigated.

It is difficult to realize the growth of device-quality In-rich InGaN or InN QW due to the high vapor pressure of nitrogen and low dissociation temperature of InN [31,32]. Moreover, the poor crystalline quality of In-rich InGaN or InN is attributed to high-density dislocations caused by the large lattice mismatch (~16%) between InN and GaN. However, in recent years, the high quality of InN/InGaN [33,34] and InN/GaN [35] QWs has been reported through the implementation of radio-frequency plasma-assisted molecular-beam epitaxy (RF-MBE) for epitaxial growth. Experimental study has indicated that one-monolayer InN can grow on a GaN template with high crystal quality and uniformity.

In this work, we propose a staggered single quantum well (SQW) structure that embeds an ultrathin InN layer into the SQW. Compared with the conventional three-layer staggered structure using thick and high In content InGaN insertion layer (IL) as an intermediate layer, our proposed InN IL can serve as a strain compensation layer and confine the distribution of carriers within a narrow region. We have numerically simulated the effect of red LED with InN IL. The overlaps of electron–hole wavefunctions are significantly increased due to the suppressed QCSE, leading to a higher IQE. Additionally, we have found that the position of InN IL can change the carrier distribution and the recombination energy, which affects the IQE and peak emission wavelengths of red LEDs.

2. Device Structures and Simulation Parameters

Figure 1 shows the schematic of red LED epitaxial structures with a square-shaped QW (SSQW) (labeled as LED A) and with an InN IL in SQW (labeled as LED B). The LED A serving as the reference device structure mainly consists of the following parts: a 2 μm thick n-GaN (Si-doping = $1 \times 10^{18} \text{ cm}^{-3}$), an $\text{In}_{0.45}\text{Ga}_{0.55}\text{N}$ (2.5 nm)/GaN (10 nm) SQW, a 20 nm thick p- $\text{Al}_{0.1}\text{Ga}_{0.9}\text{N}$ (Mg-doping = $5 \times 10^{18} \text{ cm}^{-3}$), and a 300 nm thick p-GaN (Mg-doping = $1 \times 10^{19} \text{ cm}^{-3}$) [36,37]. It has been reported that a thickness of 1–2 monolayers of the InN IL is sufficient to suppress the QCSE, while a thicker InN IL will remarkably degrade the crystal quality of the QW [38]. We selected an InN IL thickness of 0.5 nm based on the trade-off between suppressing the QCSE and maintaining high crystal quality in the QW. The two sides $\text{In}_x\text{Ga}_{1-x}\text{N}$ of the InN IL were 1 nm thick, where x represents the In content. We used the following equation to calculate the average In content ($\bar{x}$) in QW:

$$\bar{x} = \frac{x_1 \cdot L_1 + x_2 \cdot L_2 + x_3 \cdot L_3}{L_1 + L_2 + L_3} \quad (1)$$

where L is the length of different parts in QW. For LED B ($x_1 = x_3, x_2 = 1$), the L_1, L_2 , and L_3 were 1, 0.5, and 1 nm. To ensure the average In content ($\bar{x}$) in QW of LED B was equal to that of LED A, both the x_1 and x_3 were set to be 0.3.

SiLENSe 5.14 software was used to investigate the performance of the proposed LED structures. The software uses drift–diffusion equations, Poisson equations, and Schrödinger equations to obtain band structure diagrams, carrier concentrations, and overlaps of electro-hole wavefunctions in SQW [39]. In this simulation, the areas of all structures were set as $50 \times 50 \mu\text{m}^2$. The band offset ratio was 0.7/0.3 [40]. The mobility of electrons and holes was set to be 100 and $10 \text{ cm}^2 \cdot \text{V}^{-1} \cdot \text{s}^{-1}$, respectively [41]. The dislocation density of the epitaxial layer was set as $1 \times 10^9 \text{ cm}^{-2}$, which can be used to calculate the carrier lifetime. The Auger recombination coefficient was set as $2.5 \times 10^{-30} \text{ cm}^6 \text{ s}^{-1}$ and the operating temperature was 300 K. The degree of relaxation was set as 0.2. We used the quantum potential model in the software to precisely describe carrier transport and obtain more realistic simulation results. The electron and hole quantum potential correction factors were set as 0.7 and 1, respectively. Other parameters were default and can be found elsewhere [7,42].

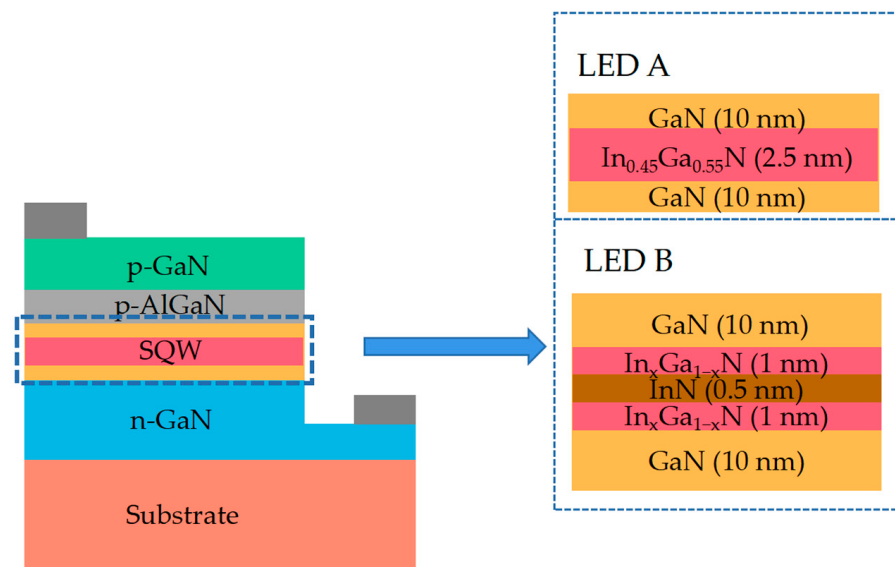


Figure 1. Schematic structure of conventional LED A and InN embedded in LED B.

3. Results and Discussion

The unstrained lattice constants of InN and GaN are about 0.354 and 0.311 nm, and the lattice constant $\text{In}_x\text{Ga}_{1-x}\text{N}$ layer can be calculated by the following equation [10]:

$$a_{\text{InGaIn}} = a_{\text{InN}} \cdot x + a_{\text{GaN}} \cdot (1 - x), \quad (2)$$

where x is the proportion of In content. The lattice constant of $\text{In}_{0.3}\text{Ga}_{0.7}\text{N}$ is 0.324 nm, which is 8.47% smaller than that of InN. Hence, the InN layer provides tensile stress for the adjacent InGaIn layers in SQW, which compensates the compressive stress caused by the mismatches between SQW and quantum barriers (QBs). Figure 2a,b show the energy band structure and quasi-Fermi levels of LED A and LED B at 60 A/cm², respectively. It can be observed that the energy band profiles of the SQW in LED A and adjacent QBs are apparently bent due to the piezoelectric polarization. For the LED B, there is a slender pit in the middle of the energy band in SQW caused by InN IL. Figure 2c,d show the enlarged energy band diagrams near the SQW region of LEDs A and B, respectively. To quantitatively describe the degrees of band bending, the energy differences (labeled as ΔE) between the top and bottom energies of the SQW conduction band are shown in Figure 2c,d. As for LED A, the value of ΔE is equal to 0.763 eV, attributed to the piezoelectric polarization occurring between the SQW and QBs. Regarding LED B, the region of SQW can be divided into three parts. The energy differences of the conduction band between the three parts were labeled ΔE_1 , ΔE_2 , and ΔE_3 (from n-side QB to p-side QB). The values of ΔE_1 , ΔE_2 , and ΔE_3 were 0.235 eV, 0.228 eV, and 0.135 eV, respectively. The sum of ΔE_1 , ΔE_2 , and ΔE_3 was 0.598 eV. Compared with LED A, the degrees of band bending in the SQW of LED B are apparently mitigated by InN IL. In addition, to precisely reflect the degrees of band bending in SQW, we calculated the value of energy difference per nanometer, which can be expressed as:

$$\Delta \bar{E} = \frac{\Delta E}{L}, \quad (3)$$

where L is the length of the different regions in SQW. Through calculation, the $\Delta \bar{E}$ of LED A was determined to be 0.305 eV/nm. The $\Delta \bar{E}_1$, $\Delta \bar{E}_2$, and $\Delta \bar{E}_3$ of LED B were 0.235 eV/nm, 0.456 eV/nm, and 0.135 eV/nm, respectively. It is obvious that the band bending of InGaIn in the SQW of LED B is alleviated. The energy band of InN IL is more tilting compared with that of the other parts in SQW.

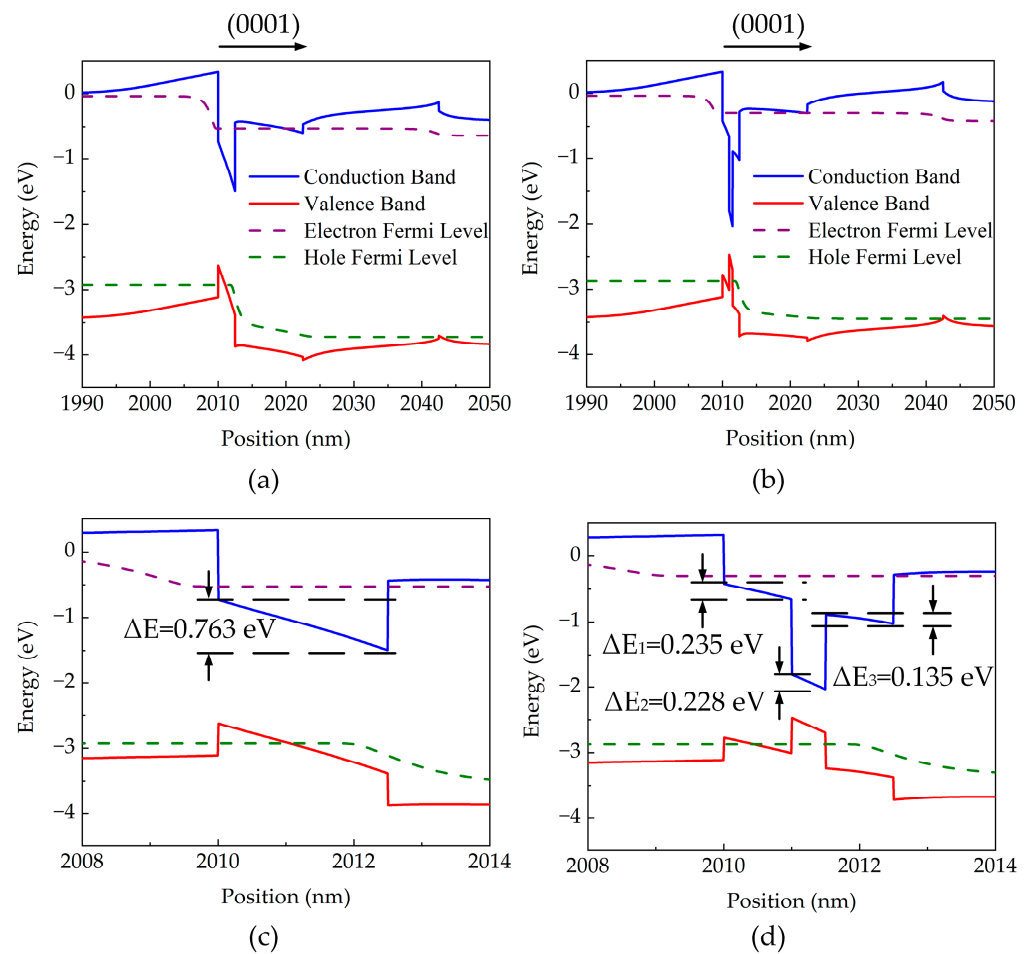


Figure 2. Energy band diagrams of (a) LED A and (b) LED B; magnified energy band diagrams around the SQW of (c) LED A and (d) LED B. All energy band diagrams were calculated at 60 A/cm².

We have numerically simulated the polarization fields of LED A and LED B to investigate the effects of InN IL, and the results are plotted in Figure 3. For Ga-polar wurtzite hexagonal InGa_N/Ga_N, the polar axis (0001) is parallel to the normal direction of epitaxy layers. Unlike a spontaneous electric field with a fixed direction, the orientation of a piezoelectric polarization field depends on the built-in strain in materials. Moreover, the orientation of spontaneous polarization is opposite to the piezoelectric polarization caused by compressive stress. Due to the large lattice mismatch between Ga_N and In_N, the polarization field of an InGa_N-based red LED is dominated by piezoelectric polarization. These conclusions above can be confirmed well by the polarization curves in Figure 3a,b. The InN IL induces a strong polarization field in SQW, which contributes to substantial polarization charges accumulated at the interface between the InN IL and InGa_N layers. These polarization charges can compensate for the built-in electric fields in two side InGa_N layers. Therefore, the right InGa_N layer in the SQW is nearly free from the piezoelectric field. The flattened energy band in SQW can greatly alleviate the QCSE and increase the overlap of electron–hole wavefunctions.

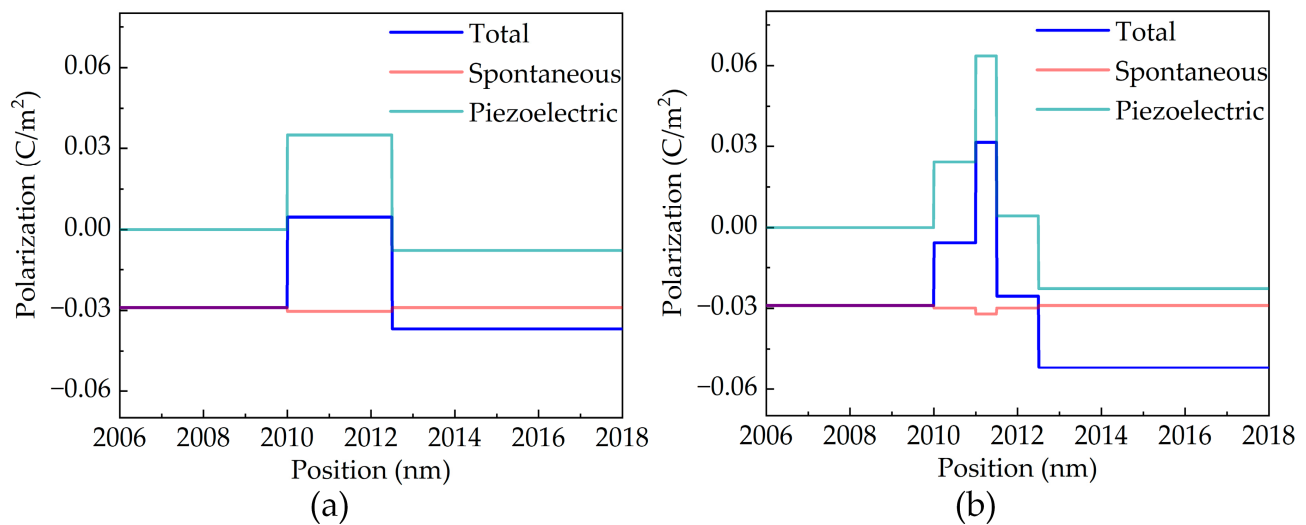


Figure 3. Polarization electric fields of (a) LED A and (b) LED B at 60 A/cm².

Figure 4 shows the simulated energy band diagrams, carrier wavefunction curves, and carrier concentration distribution of LED A and LED B at 60 A/cm². In Figure 4a, it can be apparently observed that the wavefunctions of the e1 ground state and hh1 ground state are spatially separated by built-in electric fields. The $\langle e1 | hh1 \rangle$ carrier wavefunction overlap in LED A is 0.22321. For LED B, the $\langle e1 | hh1 \rangle$ carrier wavefunction overlap is 0.76750. The enhancement of $\langle e1 | hh1 \rangle$ wavefunction overlap in LED B is attributed to the alleviated built-in electric field in InGaN layers caused by InN IL. In addition, the wavefunctions of the e1 state and h1 state are confined in the InN IL region due to the large polarization field, as shown in Figure 4b. Figure 4c,d show the carrier concentration distribution in LED A and LED B, respectively. As can be seen in Figure 4c, electrons and holes accumulate at the two sides of SQW due to the polarization fields. This is unwanted, because a large amount of carriers recombine through the nonradiative Auger process. In contrast, both the electrons and holes of LED B are concentrated towards the InN IL region, which indicates that a higher radiative recombination is expected in comparison with LED A. However, the hole concentration in the SQW of LED B is one order of magnitude lower than that of LED A, which could explain why the increase in IQE is not as significant as the increase in carrier wavefunction overlap.

The calculated I-V characteristics and IQE under various current densities for LED A and LED B are plotted in Figure 5. As shown in Figure 5a, the forward voltages of LED A and LED B are about 3.69 V and 3.42 V at 60 A/cm², respectively. The forward voltage of LED B is lower than that of LED A, indicating a lower sheet resistance of SQW with InN IL. Due to the strong polarization-induced sheet charge caused by the InN IL, which compensates for the built-in electric field in SQW, the energy band in the SQW of LED B becomes flatter than that of LED A. Therefore, the potential barriers for electrons and holes through SQW in LED B are reduced, which results in lower sheet resistance of SQW with the InN IL. In Figure 5b, the IQEs of LED A and LED B are 21.2% and 30.2% at 60 A/cm², and 17.4% and 27.4% at 200 A/cm², respectively. The IQE of LED B is 42% higher than that of LED A at 60 A/cm². At 200 A/cm², the IQE of LED B is 57% higher than that of LED A. Moreover, the efficiency droop ratio of LED B is 9.3%, which is much lower than that of LED A (17.9%). From the above discussion, we can conclude that the InN IL in QW not only decreases the forward voltage, but also significantly improves the IQE and thus reduces the efficiency droop.

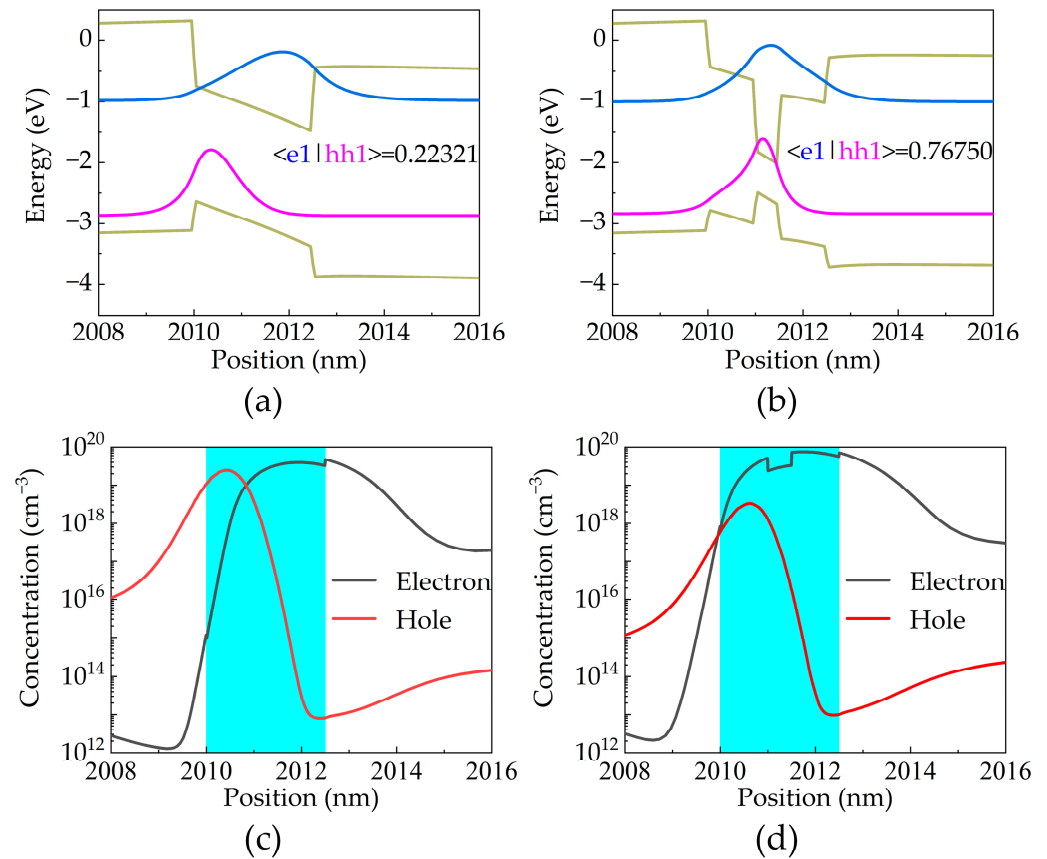


Figure 4. Simulated energy band diagrams and electron–hole wavefunctions of (a) LED A and (b) LED B; carrier concentration of (c) LED A and (d) LED B at 60 A/cm². The blue regions represent SQW.

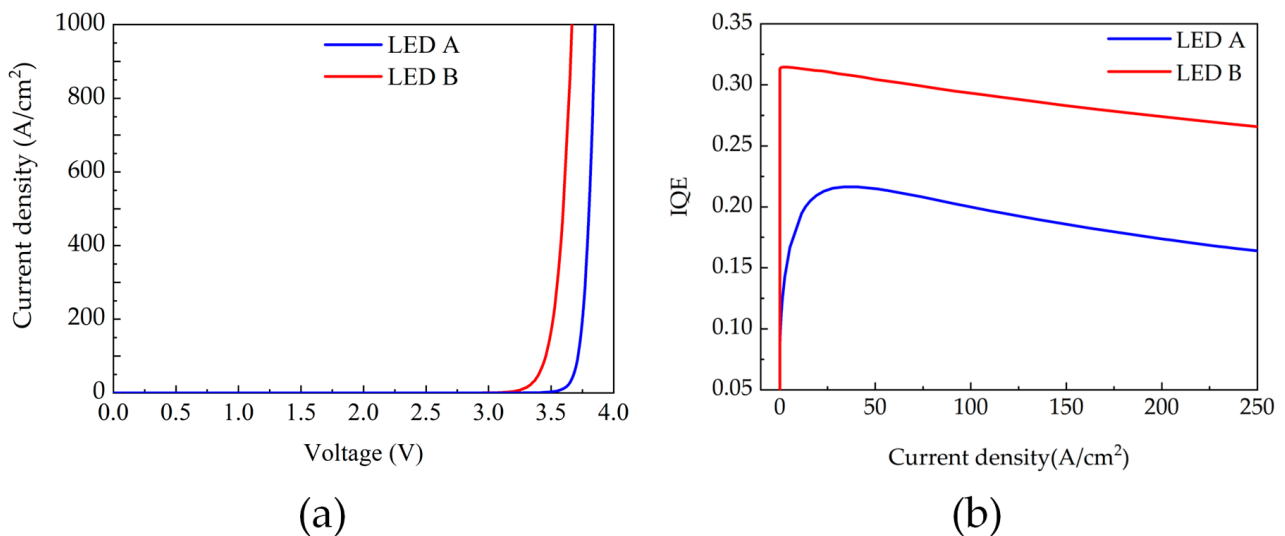


Figure 5. (a) I–V curves of LED A and LED B, respectively; (b) IQE versus current density curves of LED A and LED B.

Additionally, we have further investigated the effect of the InN IL position on the IQE and emission wavelength of red LEDs. Figure 6 shows the IQE and peak emission wavelength of red LEDs as a function of InN IL position at 60 A/cm². When the InN position shifts from n-side QB to p-side QB, both the peak emission wavelength and IQE of red LED increase first and then decrease. The IQE of red LED reaches a maximum value

of 32.2% as the distance between InN IL and n-side QB is 1.5 nm, and the maximum peak emission wavelength is observed when the distance between InN IL and n-side QB is 1 nm. However, there is a significant difference in the peak emission wavelength and the IQE among the red LEDs with different positions of the InN IL.

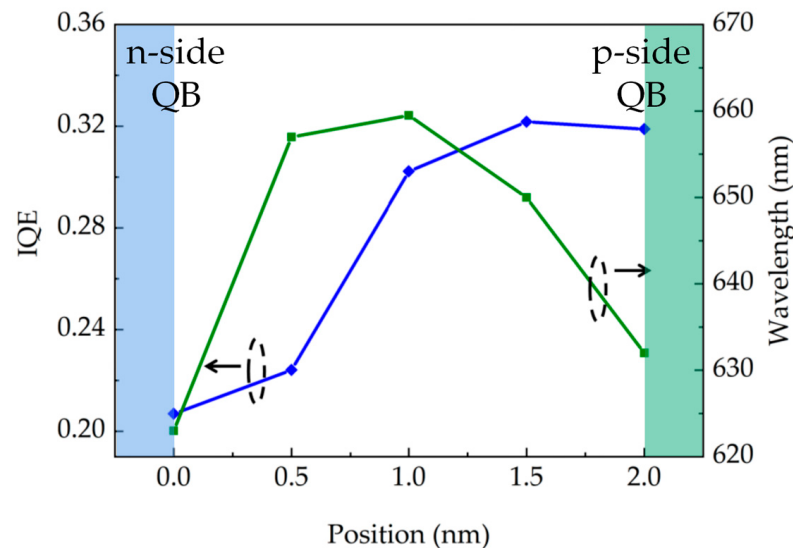


Figure 6. The curves of IQE and peak emission wavelength as a function of InN position at 60 A/cm².

To explain this phenomenon, we numerically simulated the electron–hole wavefunctions of red LEDs with different InN IL positions and the results are presented in Figure 7a–d. When the distance between the InN IL and n-side QB is 0, 0.5, 1.0, 1.5, and 2.0 nm, the carrier wavefunction overlaps of $\langle e1 | h1 \rangle$ are 0.54674, 0.70567, 0.7675, 0.62687, and 0.07505, respectively. As the InN IL approaches the middle of the SQW from the n-side, the carrier wavefunction overlap gradually increases, leading to an enhancement of the radiative recombination and the IQE. However, when the distance between the InN IL and the n-side QB is 2 nm, although the carrier wavefunction overlap is less than 10%, the IQE is still higher than 30%. Therefore, we have investigated the carrier distributions in the SQW for different positions of the InN IL at 60 A/cm², as shown in Figure 7e–h. The IQE depends not only on the carrier wavefunction overlaps but also on the carrier density. Moreover, the carrier wavefunction overlap (Γ_{eh}) changes the carrier density (n) at a given current density (J) through the relation [42]:

$$J = qd \cdot (\Gamma_{eh}An + \Gamma_{eh}Bn^2 + \Gamma_{eh}Cn^3). \quad (4)$$

where q is the elementary charge, d is the QW thickness, and A , B , and C are the Shockley–Read–Hall, radiative, and Auger recombination coefficient, respectively. It can be noted from Equation (4) that as the carrier wavefunction overlap decreases, the carrier density increases instead, and this conclusion is confirmed in Figure 7h. When the distance between n-side QB and InN IL is 2 nm, a higher concentration of holes is observed compared to the other SQW with different positions of the InN IL. Hence, despite the reduced carrier wavefunction overlap, the presence of high hole concentration can still result in a considerable enhancement of the IQE. In addition, apart from the hh1 sub-band, other sub-bands may also have an impact on the radiative recombination in the SQW. For instance, the $\langle e1 | hh2 \rangle$ wavefunction overlap is up to 0.75135, as shown in Figure 7d.

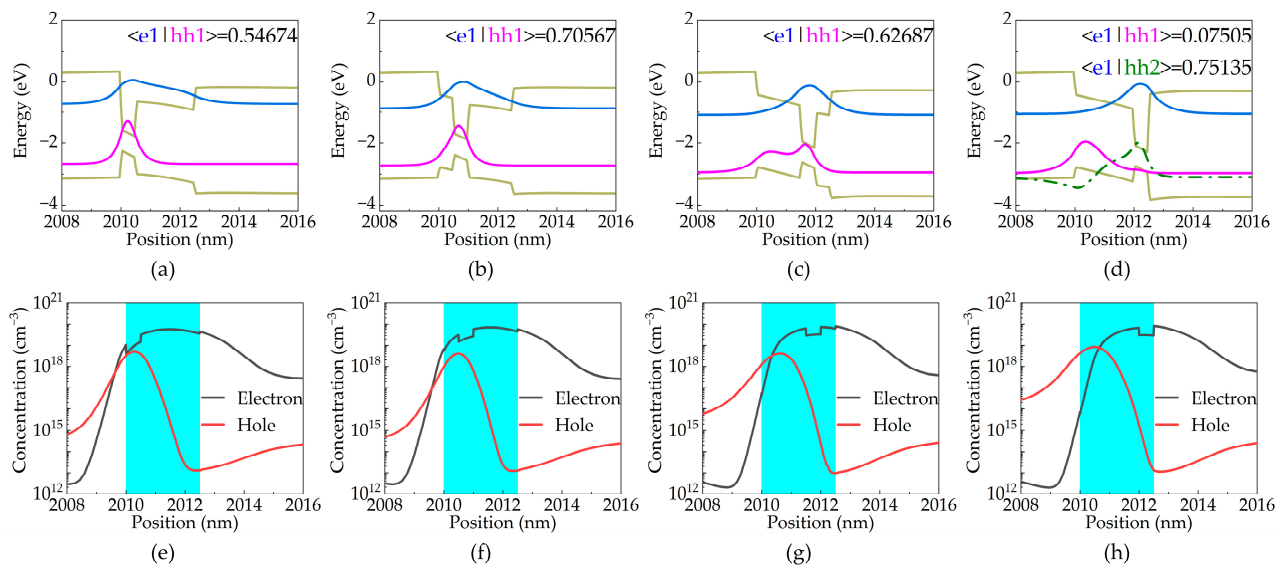


Figure 7. Schematic of electron–hole wavefunctions and carrier concentrations of red LEDs with different InN IL positions: (a) 0 nm, (b) 0.5 nm, (c) 1.5 nm, and (d) 2 nm at 60 A/cm²; diagrams of carrier concentration of red LEDs with different InN positions: (e) 0 nm, (f) 0.5 nm, (g) 1.5 nm, and (h) 2 nm at 60 A/cm².

An apparent blue-shift in the emission wavelength of the red LED is observed when the InN IL is on either the n-side or the p-side. To explain this, we investigated the energies of the e1 sub-band (E_{e1}) and hh1 sub-band (E_{hh1}) with different InN IL positions. The values of E_{e1} , E_{hh1} , and $E_{e1} - E_{hh1}$ are listed in Table 1. The $E_{e1} - E_{hh1}$ can represent the transition energy of the recombined electrons. It can be observed from Table 1 that the values of E_{e1} and E_{hh1} gradually decrease as the position of InN IL shifts from the n-side to the p-side. The $E_{e1} - E_{hh1}$ value reaches the maximum when the InN IL is on the n-side. This phenomenon is attributed to the large lattice mismatch between InN and GaN, resulting in a large polarization-induced electric field that increases the $E_{e1} - E_{hh1}$. Therefore, the electrons have higher transition energy as the InN IL is on either the n-side or the p-side, compared to the other positions of InN IL, leading to the emission wavelength blue-shift.

Table 1. E_{e1} , E_{hh1} , and $E_{e1} - E_{hh1}$ of red LEDs with different InN IL positions at 60 A/cm².

Distance (nm)	0	0.5	1.0	1.5	2.0
E_{e1} (eV)	−0.725	−0.879	−1.001	−1.083	−1.052
E_{hh1} (eV)	−2.674	−2.725	−2.838	−2.947	−2.971
$E_{e1} - E_{hh1}$ (eV)	1.949	1.846	1.837	1.864	1.919

4. Conclusions

In summary, we have proposed a staggered SQW structure with InN IL and numerically investigated the effects of this structure. The built-in electric field caused by the lattice mismatch between the InN IL and InGaN can localize the distribution of carriers around InN IL, which can remarkably improve the carrier wavefunction overlap and the IQE of red LEDs. The IQE of red LEDs with InN IL is improved by 42% at 60 A/cm² compared to red LED with SSQW. We believe that the staggered structure with InN IL can provide a promising method for realizing high-efficiency InGaN-based red LEDs.

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