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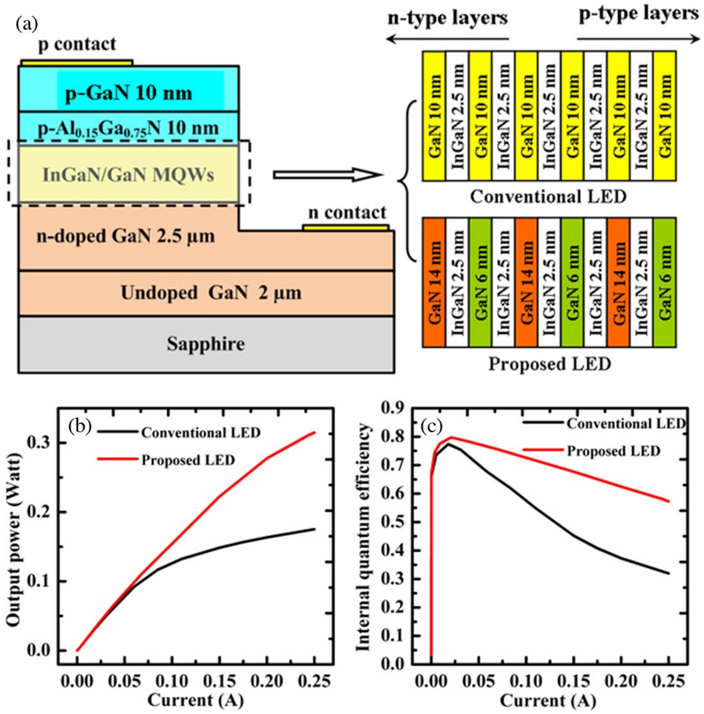

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Abstract: The advantages of blue InGaN light-emitting diodes (LEDs) with thickness-chirped barriers in the active region have been investigated by using the Crosslight APSYS programs. The results show that the output power of the proposed LED is increased 80% and the efficiency droop is decreased from 59% in conventional LED to 28% at the current of 250 mA. Based on the analysis of electrical and optical characteristics, these improvements are mainly attributed to the change of electrostatic field in the active region by using thickness-chirped barriers. In the even-numbered barriers, the fields are increased, which gets rid of more seriously bended valence band and results in decreased barrier heights for hole transport in the active region. Furthermore, the direction of electrostatic field in the last barrier is reversed to along the drift direction of holes, which not only can lead to upbended conduction band to rise the barrier height for electron escape but also can accelerate holes to increase the hole injection current. As a result, electrons blocking and holes injection are enhanced, and in turn, the performance of the proposed LED is improved.

Index Terms: InGaN light-emitting diode (LED), thickness-chirped barriers, efficiency droop, Crosslight.

1. Introduction

In the past decades, InGaN/GaN light-emitting diodes (LEDs) have made tremendous progress, and they are now regarded as the new-generation light-emitting sources to replace the traditional lamps [1]–[3] due to the advantages of wide spectrum coverage, low power consumption, compact size, and long lifetime [4]–[7]. However, the problem of current injection efficiency quenching still needs to be solved [8]–[10], which is a challenge to the improvement of efficiency, confining their high power applications, such as solid-state lighting and display. The origins of current injection efficiency quenching in InGaN-based LEDs [8], [9], [11]–[14] have previously been clarified, which relates to the carrier transport (limited by hole transport), thermionic carrier escape processes, recombinations in both quantum wells (QWs) and barrier layers. The findings are consistent with the recent experimental works that show the importance of thermionic electron escape processes [15]–[17] in affecting the current injection process in blue InGaN-based LEDs at high current injection level. Some factors cause the thermionic electron escape processes to happen. Firstly, the barrier height for electron escape is small, which is hard to prevent all electrons from spilling over to p-side [18], [19]. Secondly, the radiative recombination rate is lowered due to the electron-hole wavefunction envelop is reduced by the polarization field, which results in fewer carriers recombined in the active regions [20]. Then the chance of spilling over the active region is increased. Thirdly, the low hole injection efficiency is also an important factor contributing to the electron overflow and efficiency droop [21], [22]. Due to the large effective mass and low mobility, holes usually distribute in the quantum wells near the p-type layers or near the interface of electron blocking layer (EBL), which can not only reduce the radiative recombination rate but also attract electrons to flow over the EBL [13], [23], aggravating the efficiency droop. On the other hand, several works have also shown the importance of interband Auger process as limiting factors in InGaN-based LEDs [24]–[26], and recent works have also shown the dilute-As GaNAs as new material with negligible interband Auger recombination [26], which is also an important way to improve the efficiency of blue LEDs. Therefore, to enhance the quantum efficiency and suppress the current injection quenching of InGaN LEDs, it is important to design a new structure which has high efficiency of electron blocking and hole injection.

Several researches about improving the recombination efficiency and suppressing the electron escape have been pursued by novel barrier design in nitride-based LEDs, specifically by using large bandgap AlInN [9], [16], AlInGaN [27] or AlGaN barrier materials [28], gradual barrier design [13], and staggered quantum wells structure [29]–[32], to decrease the electron overflow. Moreover, non-polar/semi-polar QWs are used to mitigate the band bending and increase the electron-hole wavefunction envelop to improve the internal quantum efficiency (IQE) [33]–[35]. Furthermore, the structure with thickness-varied quantum wells has been designed to improve the uniform distributions of electrons and holes [36]. In addition, some other approaches have been proposed to improve the hole injection efficiency via optimizing the EBL, such as grading barrier design for the EBL [37], using polarization matched AlInGaN EBL [38], special designed AlGaN/GaN superlattice EBL [39], and polarization manipulated LED [40]. These approaches can modify the profile of potential to increase the barrier height for electron escape but add to the difficulties to the realization in the metal–organic chemical vapor deposition (MOCVD) process. Therefore, a simple but efficient structure should be developed to enhance the efficiency of electron blocking and hole injection simultaneously.

In this work, the structure with thickness chirped barriers in the active region is proposed to overcome those drawbacks in the current InGaN LEDs design. The optical and electrical properties of the structure are investigated by Crosslight APSYS (Advance Physical Model of Semiconductor Devices) programs with non-local QW transport model. In order to probe the origins of the performance improvement, the energy band, field and carrier distributions are studied by solving the Schrödinger equation, Poisson's equation, the carrier transport equations, and the current continuity equation self-consistently [41], [42].

2. Structure and Parameter

As shown in Fig. 1, the conventional and proposed LED are designed to be grown on a *c*-plane sapphire substrate, followed by a 2-μm-thick undoped GaN layer, and a 2.5-μm-thick n-type GaN layer (n doping $= 5 \times 10^{18}$ cm^{-3}). The active region of the conventional LED includes five 2.5-nm-thick $In_{0.21}Ga_{0.79}N$ QWs separated by six 10-nm-thick GaN barriers, while the barrier thickness of the proposed LED is chirped. To ensure the same active region thicknesses of these two structures, the widths of odd-numbered barriers of the proposed LED are set to be 14 nm and the even-numbered barriers are set to be 6 nm, and the thicknesses have been optimized. A 10-nm-thick p-type $Al_{0.15}Ga_{0.85}N$ EBL (p doping $= 8 \times 10^{18}$ cm^{-3}) is on top of the active region, followed by a 150-nm-thick p-type GaN contact layer (p doping $= 1 \times 10^{19}$ cm^{-3}). The active efficiency of p-doping is set to be 1% via modifying the active energies of Mg dopant in AlGaN materials according to the experiment report [43]. Three-dimension finite element analysis is used for the simulation, and the size of the electrons is set to be 200 μm $\times$ 200 μm. The main advantages of

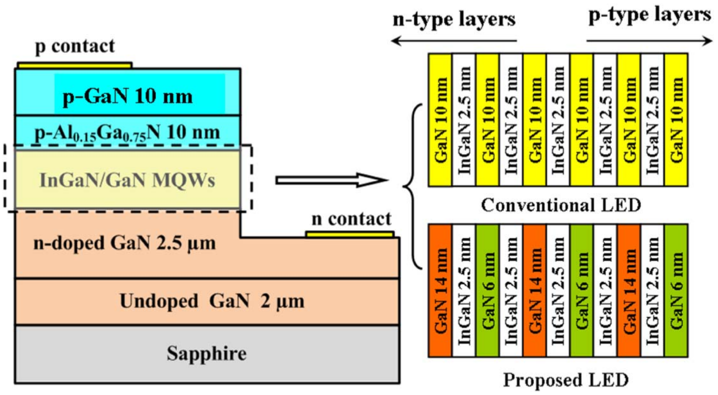

Fig. 1. Schematic diagrams of the conventional and proposed LED. In conventional LED the barriers of InGaN/GaN quantum wells are of uniform thickness, while in proposed LED the barrier thickness is chirped.

TABLE 1

Some important parameters of AlN, GaN, and InN used in the programs

Parameters	GaN	AlN	InN
a (Å)	3.189	3.112	3.545
c (Å)	5.185	4.982	5.703
$m_{//e}$	0.2	0.32	0.07
$m_{\perp e}$	0.2	0.3	0.07
C_{13} (GPa)	106	108	92
C_{33} (GPa)	398	373	224
e_{13} (C/m^2)	-0.35	-0.5	-0.57
e_{33} (C/m^2)	1.27	1.79	0.97
P_{sp} (C/m^2)	-0.034	-0.09	-0.042

the proposed sample are expected to not only mitigate the electron overflow, but also change the distribution of holes in each QW, and then to alleviate the current injection efficiency quenching. The Shockley–Read–Hall (SRH) recombination time is set to be 20 ns [32], [44], and the internal loss is 2000 m^{-1}. The Auger recombination coefficient is 5×10^{-34} cm^6/s [32].

In general, the band gap energies of InGaN and AlGaN are governed by the following formulas [37]:

$$E_g(\mathrm{In}_x\mathrm{Ga}_{1-x}\mathrm{N}) = xE_{g,\,\mathrm{InN}} + (1-x)E_{g,\,\mathrm{GaN}} - b_1 x(1-x)$$
$$E_g(\mathrm{Al}_x\mathrm{Ga}_{1-x}\mathrm{N}) = xE_{g,\,\mathrm{AlN}} + (1-x)E_{g,\,\mathrm{GaN}} - b_2 x(1-x)$$

where $E_{g,\mathrm{InN}}$, $E_{g,\mathrm{GaN}}$, and $E_{g,\mathrm{AlN}}$ are the bandgap energies of InN, GaN, and AlN, which equal to 0.77, 3.42, and 6.25 eV, respectively. The bowing parameters b_1 and b_2 of InGaN and AlGaN are 3 and 1 eV respectively, and the band-offset ratio is assumed to be 0.7/0.3 for InGaN and AlGaN materials. The fixed interface charge densities caused by the spontaneous and piezoelectric polarizations are calculated from the method proposed by Fiorentini *et al.* [45]. Taking into account the screening by defects, the surface charges densities are assumed to be 40% of the calculated values. Other material parameters of $\mathrm{In}_x\mathrm{Ga}_{1-x}\mathrm{N}$ ($\mathrm{Al}_x\mathrm{Ga}_{1-x}\mathrm{N}$) used in the simulation, such as lattice constants a and c, electron effective masses $m_{//e}$ and $m_{\perp e}$, piezoelectric constants C_{13} and C_{33}, elastic constants e_{13} and e_{33}, as well as spontaneous polarization, can be obtained by the linear interpolation between the physical properties of GaN and InN (AlN). Table 1 lists some important parameters of AlN, GaN and InN, which can be found in [46].

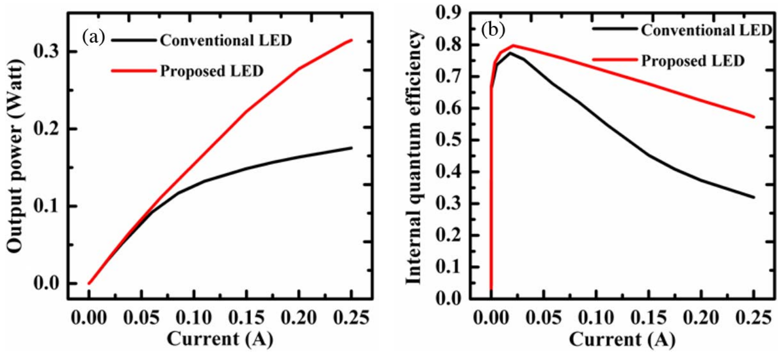

Fig. 2. (a) Output powers and (b) internal quantum efficiencies as a function of current for these two structures.

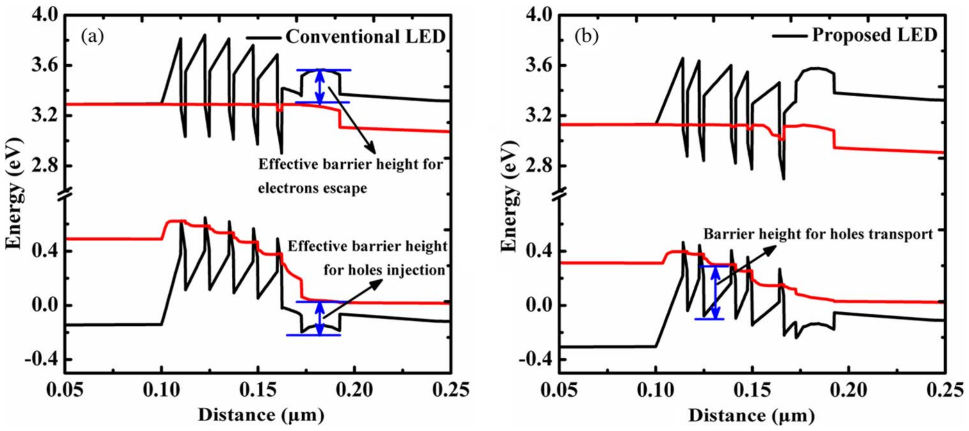

Fig. 3. Potential profiles of the conventional (a) and proposed LED (b) at 150 mA.

3. Simulation Results and Discussion

Regarding the advantages of using thickness-chirped barriers in the active region on the performance of InGaN-LED, we probe into the optical powers and IQEs of both structures. Fig. 2(a) shows the output powers as a function of current for both structures. Evidently, compared to the conventional LED, the optical performance of the proposed LED is much better, and the power of latter increases almost linearly with the current while it is a nonlinear increase for the conventional LED. Furthermore, when the current is 250 mA, the output power of proposed LED is 315 mW, about 80% larger than the conventional LED (175 mW), which means more carriers recombined in the proposed LED. This result is consistent with the internal quantum efficiency. As shown in Fig. 2(b), the IQEs of these two structures are almost the same at low current. However, when the current is increased to 250 mA, the efficiency droop appears and the difference is apparent. From this figure, the IQE of conventional structure decreases almost 59% when the current is increased to 250 mA, while the IQE of the proposed LED decreases only 28%. This demonstrates that the structure with thickness-chirped barriers in the active region can improve the efficiency droop significantly, which suggests that the proposed structure can mitigate the problem of current injection efficiency quenching efficiently.

In order to probe the reasons why the proposed structure with thickness-chirped barriers can improve the performance of InGaN-LED, the diagrams of energy band, electrostatic field, carrier concentrations and current densities are investigated. As shown in Fig. 3(a), the conduction band of conventional structure is bended downward near the interface of last barrier and the EBL due to the

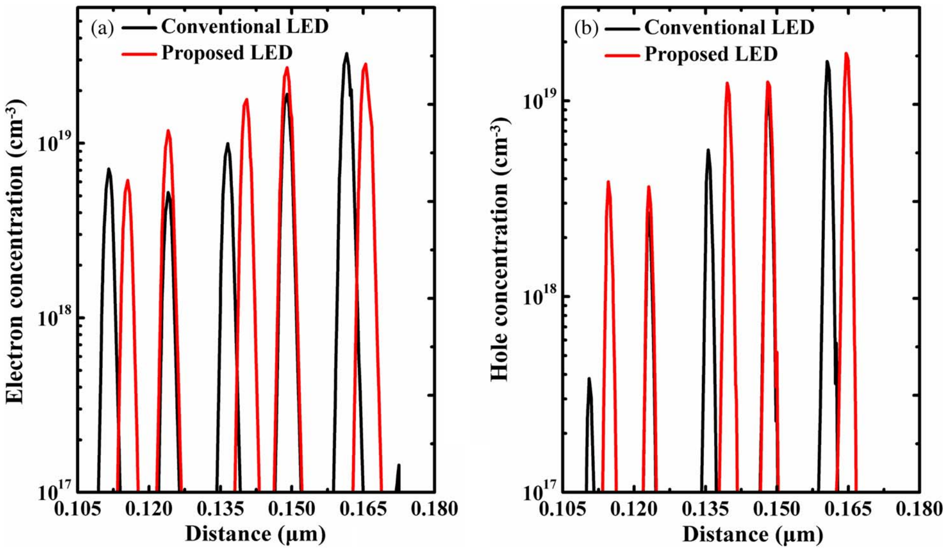

Fig. 4. Distributions of electrons (a) and holes (b) in the active regions of these two structures at 150 mA.

large electrostatic field caused by the big polarization field in AlGaN material, which gets rid to the shorted energy distance between the electron Quasi-Fermi level (red line shown in the figure) and conduction band near the EBL. As a result, the effective barrier height for electron escape is decreased, leading to a lot of electrons overflow, and in turn the problem of efficiency droop appears. Furthermore, because of this down-bended band, a paretic quantum well is formed and many electrons reside in this well, increasing the chance of overflow. However, the conduction band of the last barrier in the proposed LED is up-bended as shown in Fig. 3(b), and the energy space of conduction band and the Quasi-Fermi level near the EBL is enlarged, resulting in increased effective barrier height for electron escape. According to Fig. 3, the barrier height for electron escape is increased from 290 meV (conventional LED) to 458 meV (proposed LED). Therefore, electrons spilling over to p-side can be mitigated efficiently, and more holes can be injected into the active region. In addition, the distance of valence band and hole Quasi-Fermi level in the active region of the conventional LED is increased from p-side to n-side, which means that the barrier height for holes transport in the active region is increased monotonously. Then few holes can transport to the quantum wells near n-side layers. However, when the barrier thickness is chirped in the proposed LED, the barrier height for holes transport in the active region is decreased, as shown in Table 1, resulting in more holes being transported to the wells near the n-type layers.

As shown in Fig. 4(a), compared to the conventional structure, the overall density of electrons in the active region with the thickness-chirped barriers is increased, which means that this structure can enhance the confinement of electrons. This agrees with the energy band shown in Fig. 3. In addition, the hole concentrations in each well of the proposed LED are increased apparently, which may result from the decreased barrier height in the active region for holes transport when the barrier thickness is chirped as show in Table 2. Furthermore, because the barrier heights for holes transporting into the first and third wells are decreased more obviously, it can be seen that the hole concentrations in those odd-numbered wells are increased significantly, especially in the first and third wells (numbered from n-side to p-side). Although the barrier height for holes injecting into the fifth well is increased, the distance for holes injection is decreased, which may contribute to the increase of hole concentration in the last well [47]. However, this is not the only reason for the improved hole injection. The electrostatic field in the last barrier may also pay an important role, which will be analyzed below.

Because of the increased barrier height for electrons escape, as shown in Fig. 5(a), the electron current density of proposed LED in the p-side layer is almost 0 while it is still as large as 478 A/cm^2 for the conventional LED, which suggests a higher electron blocking efficiency of the proposed

TABLE 2

Barrier height for holes injecting into each quantum well (numbered from n-side to p-side)

	Quantum barrier 1	Quantum barrier 2	Quantum barrier 3	Quantum barrier 4	Quantum barrier 5
Conventional LED	492 meV	449 meV	406 meV	351 meV	323 meV
Proposed LED	420meV	421 meV	347 meV	329 meV	358 meV
Energy Difference	72meV	28 meV	59 meV	22 meV	-35 meV

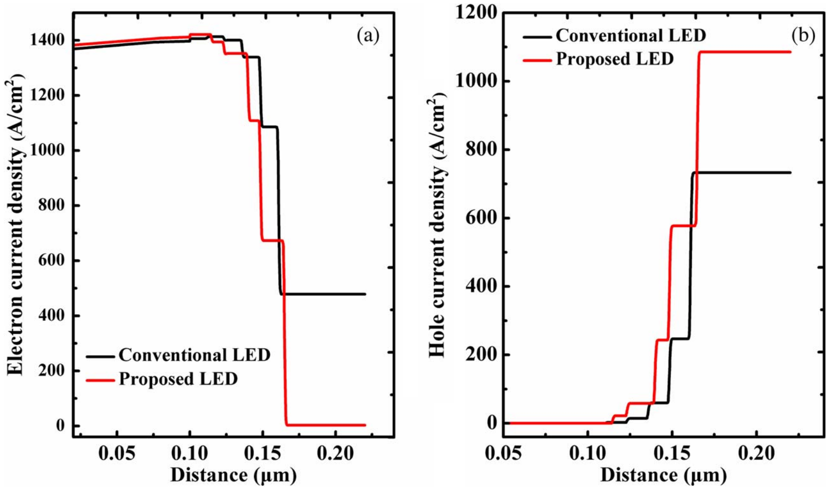

Fig. 5. Electron current densities (a) and hole current densities (b) of conventional (the black line) and proposed LED (the red line) at 150 mA.

LED. In the meantime, due to the decreased barrier height for holes injection, the hole current density of proposed LED in the p-side layer is larger than that of the conventional LED, which means that hole injection is enhanced. Therefore, the hole concentration in the active region is increased. As a result, the droop of IQE is mitigated and the output power is improved.

As discussed above, the electron blocking and hole injection can be enhanced via adopting thickness-chirped barriers, and this effect can be deduced from the changing of the potential profile directly. However, the original reason for the variation of potential profile still needs to be studied. To shed light on the mechanism responsible for this, the electrostatic field is studied. As shown in Fig. 6, the electrostatic fields in these barriers change apparently. When the barrier thickness is reduced, the field is enhanced, resulting in the more seriously bended valence band. Then the valence band covers more with the Quasi-Fermi level, leading to the reduced barrier height for holes transport. Furthermore, in comparison with the conventional LED, the electrostatic field in the last barrier of the proposed structure is changed from -1.6×10^5 V/cm to 7.6×10^4 V/cm, which leads to a big difference in the potential profile. The positive field results in up-bended potential of the last barrier, which leads to the disappearance of the parasitic QW [37]. As a result, few electrons are resided at the interface of last barrier/EBL, and the chance for spill-over is reduced. What is more, the direction of the field in the last barrier of proposed LED is from p-side to n-side, along the drift direction of holes. Therefore, holes can be accelerated in this layer and more holes inject into the active region, which can increase the hole injection current. In addition, the fields in the InGaN quantum wells of the proposed LED are weaker than these of the conventional LED, which means that the quantum-confined Stark effect is mitigated. As a result, the wavelength is blue shift and the wavefunction envelop is increased for the proposed LED. Fig. 7(a) shows the spontaneous radiative rates of those two structures, which indicates the peak emission wavelength is blue shifted

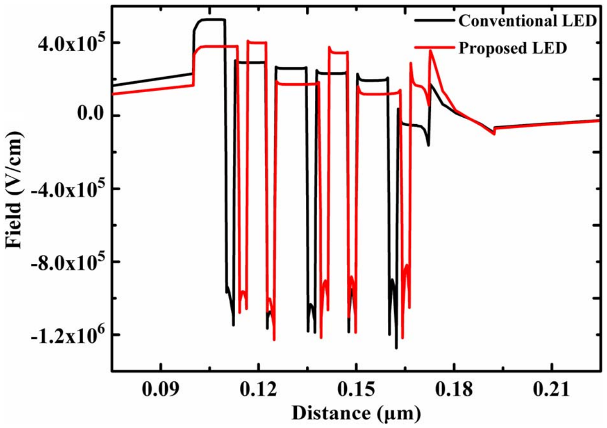

Fig. 6. Electrostatic fields in conventional structure (the black line) and proposed structure (the red line) at 150 mA.

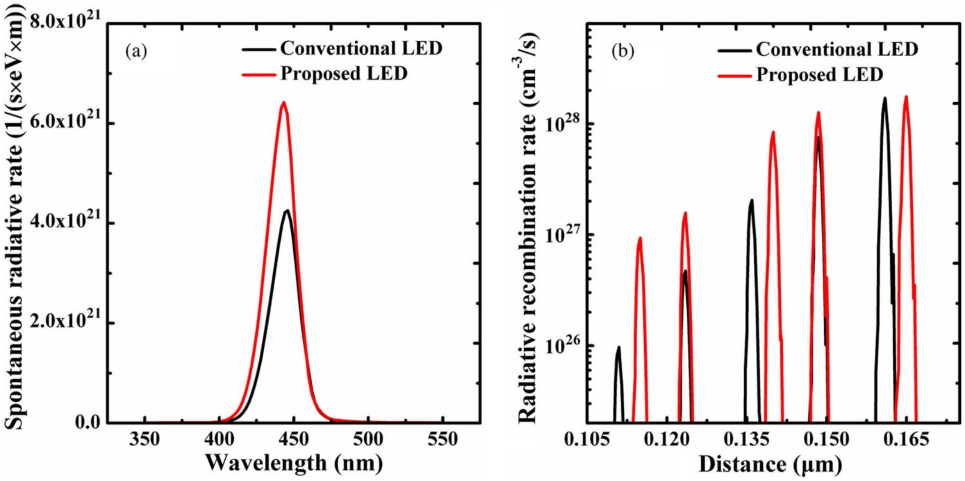

Fig. 7. Spontaneous radiative rates (a) and radiative recombination rates (b) of conventional (the black line) and proposed LED (the red line) at 150 mA.

from 446 nm (the conventional LED) to 443 nm for the proposed one. Moreover, the spontaneous recombination rate is also increased, which means that the recombination efficiency is improved. This can also be proved by the radiative recombination rates of these two structures shown in Fig. 7(b), which indicates the advantage of thickness-chirped barriers on the improvement of radiative recombination.

From the above discussion, it is clear that the proposed LED performs better than the conventional one in both optical and electrical aspects. The design of thickness-chirped barriers in the active region is preferable for high power and high efficiency blue and white lighting applications, which also can be applied to other III-nitrides light-emitting diodes.

4. Conclusion

In summary, the effects of thickness-chirped barriers on the performance of InGaN LED structure are studied by designing a sample with the active region including thickness chirped barriers. The simulation results show that, when the GaN barrier thickness is chirped, the electrostatic fields in the even-numbered barriers are enhanced, getting rid of the modified potential profile. Then the barrier height for electron escape is increased while barrier height for hole transport is decreased.

Furthermore, compared to the conventional structure, the direction of electrostatic field in the last barrier is reversed to along the drift direction of holes in the proposed LED, which not only leads to the up-bended band but also increases the speed of holes. Then the hole injection and electron blocking are enhanced. Therefore, more holes inject and transport into the active region and fewer electrons overflow to the p-side layers. As a result, compared to the conventional LED, the light output power of the designed LED is increased 80%, and the IQE droop is reduced from 59% to 28% at the current of 250 mA, which is promising for the high efficiency solid-state-lighting and other optoelectronic applications. However, this approach requires further growth optimization to realize the potential advantages of this proposed structure.

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