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RESEARCH ARTICLE

Effect of p-GaN layer and High-k material in InGaN/GaN LED for optical performance enhancement

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Abstract

The p-GaN layer adjacent to the quantum well is proposed for InGaN/GaN Light Emitting Diode (LED), it enhances the output optical power and internal quantum efficiency. The physical simulator Technology Computer-Aided Design (TCAD) is used to analyze the performance of the proposed LED. In the simulation, physics-based models are used to obtain optical properties such as luminous power and recombination rate. The suggested InGaN/GaN LED outperformed conventional LEDs in terms of internal quantum efficiency and luminous power. At the injection current of 700 mA, the output luminous power and internal quantum efficiency in the proposed LED are improved by 24% and 18%, respectively. Furthermore, the suggested InGaN/GaN LED has a smaller Auger recombination than conventional LEDs. Thus, the proposed p-GaN layer technique in GaN LED is a promising one for future solid-state lighting applications due to its high internal quantum efficiency of 90% at 100 mA injection current.

Keywords p-GaN · Quantum-well · GaN · InGaN · LED · Efficiency

Abbreviations

R	Recombination rate
R_{SRH}	SRH recombination
R_{rad}	Radiative recombination
R_{aug}	Auger recombination
d	Recombination region thickness
P_T	Total polarization
P_{sp}	Spontaneous polarization
P_{pz}	Piezo-electric polarization
J	Current density
p	Hole concentration
n	Electron concentration
E	Electric field
q	Electric charge
μ_n	Electron Mobility
μ_p	Hole Mobility

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Introduction

GaN is an outstanding material for light-emitting diodes as it has a wide band gap, higher thermal conductivity, and higher electron mobility [1–3]. It is mainly used in optoelectronic, high-power, and high-temperature electronic devices because they feature a variety of appealing electrical, optical, and thermal properties. Our understanding of III-V nitride light-emitting diodes (LEDs) and laser diodes (LDs) has recently made tremendous strides [4, 5]. Despite the enormous progress made, a few significant obstacles still stand in the way of the further development of high-brightness LEDs for general lighting, including green gap and efficiency droop. Efficiency-droop phenomenon is the phenomenon where the efficiency of InGaN quantum well (QW) LEDs drastically decreases at high current density $J >= 10–70\ A/cm^2$. In InGaN QW LEDs, the

efficiency-droop problem worsens when the emission wavelength is pushed into a longer spectrum range. It is necessary to operate LEDs at J > 200 A/cm^2 for general illumination, highlighting the need to solve the efficiency droop problem [6, 7].

Current overflow, ineffective current injection, polarisation fields, junction heating, the quantum confinement stark effect (QCSE), electron leakage, Auger recombination, and a lack of hole injection are the factors causing this degradation in InGaN/GaN MQW LEDs. Auger effects, current overflow (or current spillover), and polarisation effects are three of these nonradiative recombination processes that may be the primary driving forces behind the observed efficiency decline. Even though LED has good material properties, there has been a lot of progress in GaN LED architectures and surface modification to boost the efficiency of both internal and external. The advancement is briefly discussed as follows. First, the insulating sapphire substrate of these diodes often necessitates the use of a lateral carrier injection type. However, a lateral injection-type application may experience an issue with uneven current spreading when the device is in use. Recently, Eliashevich et al. [8] reported that uniform current spreading is significantly impacted by the conductivity of an n-type GaN layer. It was demonstrated that the current crowding in a specific area of the device caused by non-uniform current spreading might considerably reduce the attributes of LED performance.

Secondly, the Ni particles, ZnO, and Al_2O_3 are used on the surface of the LED to improve extraction efficiency [1, 9, 10]. LED combination technique is used to obtain the white light [11]. Further, the extraction efficiency is improved using AlGaAs, ITO, and GaP [12–14]. This is due to the semiconducting properties of these materials. Current crowding at the p-contact is another significant barrier to overcome in order to improve efficiency [15–17], particularly for traditional devices grown on insulating substrates (e.g., sapphire) [18]. Because driven current with lower resistivity tends to pass along the channel, current crowding at the p-contact of these InGaN/GaN LEDs occurs. Because of the current crowding effect, highly localized carrier density and heat are generated beneath the p-electrode, resulting in non-uniform light emission from InGaN/GaN LEDs [19]. Thirdly, a resistive layer is typically added to the LED layout to increase current spreading [20, 21]. Foreseeing the boundaries that Threading Dislocations may impose on obtaining higher Internal Quantum Efficiency (IQE) depends on determining the effectiveness of such localization mechanisms under key conditions, such as high current densities, high temperatures, and higher indium compositions.

Finally, the efficiency and thermal stability of LED devices is increased to a greater extent by the employment of multiple quantum well structures. Although a lot of advancement has been made in GaN-based LED, the efficiency of LED is still suffering from threading dislocation and self-heating [22, 23]. Therefore, alternative or innovative techniques are still invited to improve internal and external efficiency.

Theoretically, the p-GaN layer impacts the current spreading effect, causing the current to be crowded locally [24–26]. It also provides high threshold voltage and less leakage current. By considering the above issues, this paper introduces a p-GaN layer adjacent to the multiple quantum well. To the best of the author's knowledge, the p-GaN layer in the devices described in the literature was created to be compatible with high-power applications while demonstrating low static power dissipation, which increases the output luminous power and efficiency. The performance of the proposed technique is analysed using TCAD physical simulator. Improvement in LED performance is achieved using the proposed technique, which provides the best solution for leakage current and efficiency droop. Physics-based models are used in the simulation to obtain optical properties of the device.

Design specification

The LED device is proposed with four InGaN/GaN-based quantum well. Figure 1(a) & 1(b) shows the conventional and proposed InGaN/GaN LED. In comparison to typical LEDs, the suggested LED has a p-GaN layer. The p-GaN layer has the potential to significantly impair internal quantum efficiency (IQE), which will impede the advancement of External Quantum Efficiency (EQE). In this work, we discover that using a current spreading layer for an LED with a p-GaN layer can enhance the current spreading effect, which in turn improves the efficiency and luminous power of the LED. The substrate used is sapphire, which has less lattice mismatch compared to the silicon substrate. The n-type GaN and p-type GaN layers are used since it is a GaN LED and the n and p doping are 1×10^{18} cm^{-3} and 1×10^{19} cm^{-3} respectively to increase the conduction.

AlGaN Electron Blocking Layer is included in the LED to diminish the carrier leakage; thus, the radiative recombination is improved. Multiple quantum wells (InGaN/GaN) are used to enhance the recombination rate of the device. The quantity of quantum wells employed in the active zone is another crucial factor; it may vary depending on the applications. Numerous experts contend that a single quantum well is superior to multiple quantum wells in terms of efficiency. One of the key concepts in a single quantum well is carrier leakage is a drawback. The usage of several quantum wells prevents carrier leakage. Efficiency declines with an increase in the number of quantum wells. To attain the

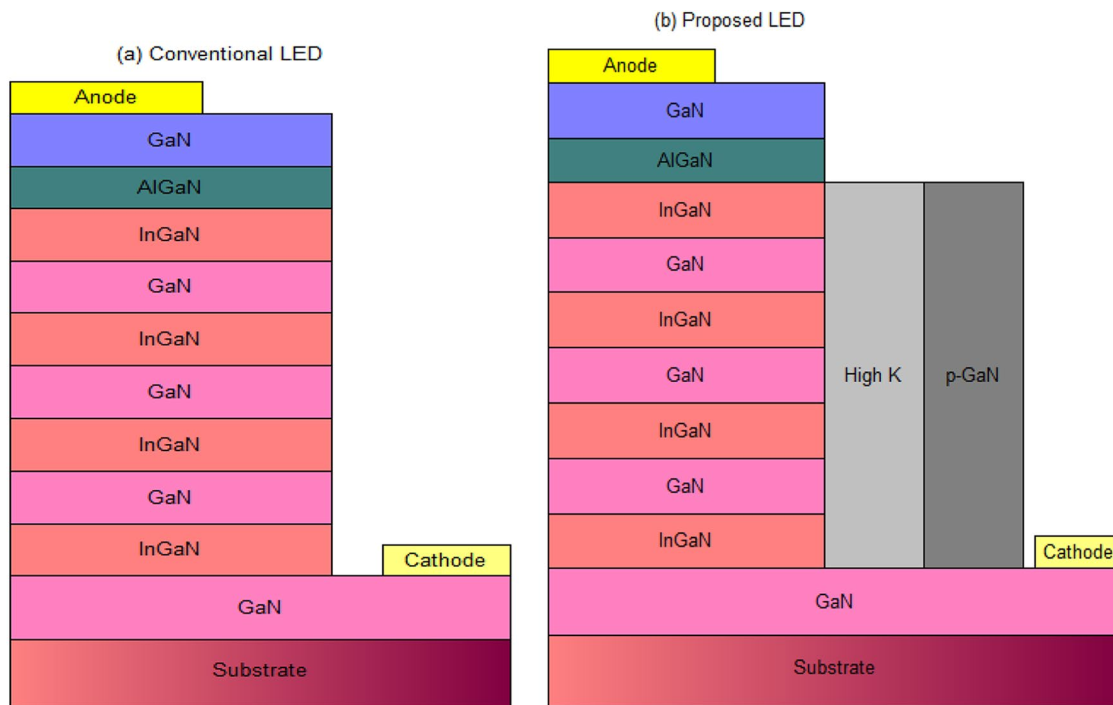


Fig. 1 (**a**) Conventional LED of InGaN/GaN LED. (**b**) Proposed LED of InGaN/GaN LED

intended results, appropriate trade-offs need to be made and it is widely considered from the standard LED gadget with three pairs of multiple quantum wells (InGaN/GaN).

In nanometer scale device, leakage current is the serious issue. In order to overcome, high-k material with larger permittivity and bandgap are used to enhance the device parameters [27–29]. Among several high-k dielectric material such as Al_2O_3, SiO_2, HfO_2, Si_3N_4, ZrO_2, TiO_2, Y_2O_3, Ta_2O_5, and LaZrO, HfO_2 is used as a high-k material because of its unique feature as suppressed leakage current, and it is placed between the p-GaN layer and quantum wells. The HfO_2 modifies the electric field surrounding the quantum well, to increase carrier concentration and recombination in the well by reducing the interface trap density. Lower interface traps help fewer defects and imperfections at the boundary between two materials, resulting in better charge carrier confinement and improving the recombination efficiency. The introduction of p-GaN effectively suppresses the leakage of electrons through the sidewalls and improves the forward breakdown of the device. It provides high threshold voltage and low leakage current which in turn improves the recombination rate of the device. In summary, the HfO_2 layer helps to enhance carrier injection and improves the overall performance of the device, leading to more efficient and long-lasting light emission. The details of dimension are reported elsewhere [30].

Materials and methods

Drift and diffusion models are used to govern the carrier transport in the simulation. In the simulation, the K.P. model is used to facilitate the energy state and wave function physics of electrons in a potential well. The recombination process in a light-emitting diode is obtained by the ABC recombination model. The first-order process (the trapping of electrons or holes) and the second-order kinetic processes (the radiation-free (NR) recombination of the trapped electrons and free holes) and the third order such as NR Auger recombination are considered in this model.

The ratio of the radiative to the total recombination rates is then used to define the devices' internal quantum efficiency and is expressed as

$$IQE = \frac{R_{rad}}{R} = \frac{R_{rad}}{R_{rad} + R_{SRH} + R_{aug}} \tag{1}$$

Where R is the total recombination and it is equal to the summation of Shockley–Read–Hall (SRH) (R_{SRH}), Auger recombination (R_{aug}), and radiative recombination (R_{rad}). All these recombination processes are enabled by using the respective recombination models. SRH non-radiative recombination is a first-order recombination processing in which electron and hole recombine via a trap state or recombination centres. The Shockley–Read–Hall (SRH) and

Table 1 Dimension of GaN LED

Layer	Thickness
Anode side GaN	500 nm
AlGaN EBL	100 nm
InGaN well	3 nm
GaN barrier	5 nm
Cathode side **GaN**	3.375 µm
High – k	27 nm
p-GaN	27 nm
Sapphire	6 µm

Auger recombination models are used to model the carrier generation and recombination process.

To calculate the simplified and well-known form for the current density J through the LED that corresponds to the ABC model is given as follows:

$$J = qd(An + Bn^2 + Cn^3) \tag{2}$$

Where q is the charge, d is the thickness of the active or recombination region, n is the electron density in the active region and A, B, and C are the SRH, radiative and auger recombination parameters of the ABC model, respectively.

As III-nitride is a polarized semiconductor, the polarization model is enabled in the simulation. The ATLAS TCAD determines the total polarization (P_T) using

$$P_T = P_{SP} + P_{PZ} \tag{3}$$

where, P_{SP} and P_{PZ} spontaneous and piezo-electric polarization. The piezoelectric polarization is determined by

$$P_{PZ} = 2\frac{a_1 - a_0}{a_0}\left(\in_{31} - \frac{c_{13}}{c_{33}}\in_{33}\right) \tag{4}$$

where, a_0 and a_1 are lattice constant and average lattice constant, respectively. The c_{13} and c_{33} are elastic constants. The $\in_{31}$ and $\in_{33}$ are piezoelectric constants. To extract the energy profile, radiative recombination rate, and Auger recombination rate, the corresponding extraction deck-build commands are enabled in the output statement. The Anode and cathode are fixed as ohmic contact using a metal work function.

The materials and dimensions of the various layers used in the Proposed LED structure are surveyed from various research articles and listed in Table 1.

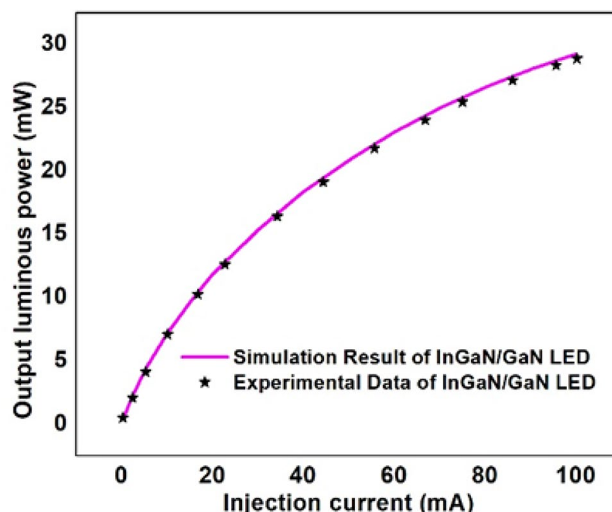


Fig. 2 Simulated and experimental output luminous power of InGaN/GaN LED

Results and discussion

Study on the effect of luminous power

In any numerical-based simulation, validation of the simulation with the experimental result is essential as it ensures the correctness of the simulation. Therefore, the experimentally reported InGaN/GaN LED structure in [19] is simulated in TCAD physical simulator. The simulated and experimental output light power in [23] is shown in Fig. 2. It is verified that the simulated results fit well with experimental data. Therefore, the simulation is calibrated well and realistic. To examine the electrical properties of the device, the numerical simulation makes use of the current continuity, Poisson, carrier transport, and heat transfer equations. The optical gain parameters of the device are examined using the Schrodinger and quantum mechanical wave equations. Once the simulation calibrated, the same simulation setting is used to analyse the proposed and conventional LED in this paper.

The experimental data is reported in [19]. The quantum behavior of the carriers in the sub-band energy levels mainly depends on the formation of the quantum well and its thickness. Therefore, it is essential to verify whether the quantum well is formed in the simulated structure or not. Figure 3 shows that the quantum well is formed for both proposed and conventional devices. The valence band of the proposed LED is shifted upwards when compared to conventional LED due to quantum confinement and photon excitation, in which more holes are available for the recombination process tends to have high luminous power. This ensures that the simulation is realistic.

The anode voltage of GaN LED is swept and luminous power is observed. Figure 4(a) shows the luminous power

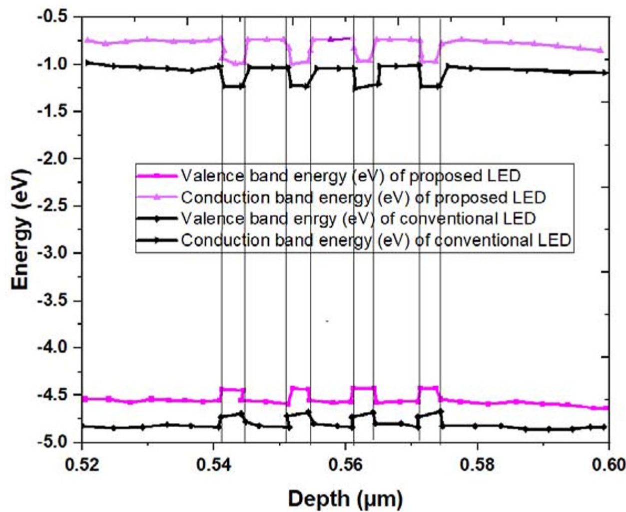


Fig. 3 Conduction and valance energy profile of proposed and conventional LED

over the anode voltage. It observed that the InGaN light emitting diode works at a large bias voltage of 3.3 V, which is consistent with the bias voltage reported in [31–35]. This large bias does not allow the band to be flat. Rather, the band edges are tilted by the polarization-induced electric field. Furthermore, approaching the threshold voltage, the optical power of the proposed InGaN/GaN LED and the standard InGaN/GaN LED is the same. The luminous power of the proposed device is higher than that of the conventional device at higher bias (a little beyond threshold voltage). Figure 4(b) shows the electrical performance of GaN LED. In the conventional LED, the increase in the forward voltage increases exponentially the current through the LED. Whereas in the proposed device, the introduction of HfO_2 layer alters the voltage characteristics. The below graph shows the increased forward voltage of 2.9 V at 30 mA current.

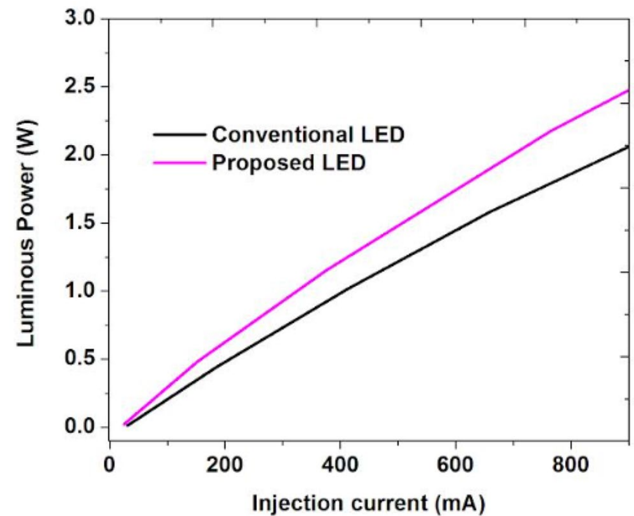
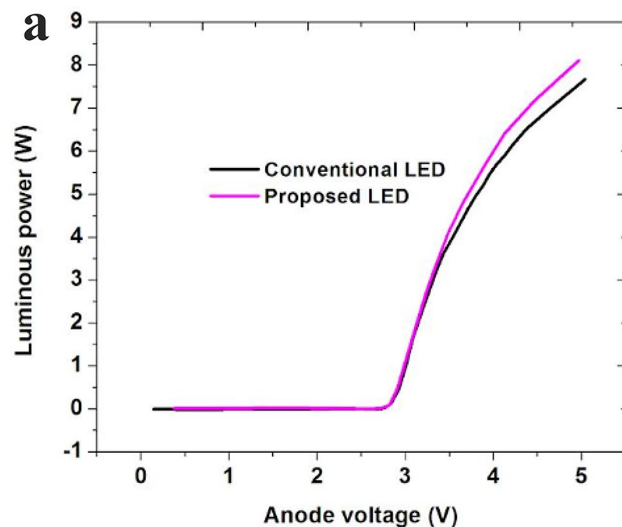


Fig. 5 Luminous power versus injection current

The luminous power as a function of injection current is calculated and shown in Fig. 5. When compared to LEDs without a p-GaN cap layer, the suggested InGaN/GaN LED with a p-GaN cap layer has a higher luminous power. It is attributed to the proposed device's increased radiative rate, which is discussed in the subsequent section.

Study on the effect of recombination rate

The key mechanism in the light-emitting diode is recombination process. More specifically, the radiative recombination process. As shown in Fig. 6, the radiative rates of the proposed and conventional InGaN/GaN LEDs are compared. The proposed device's radiative rate is found to be



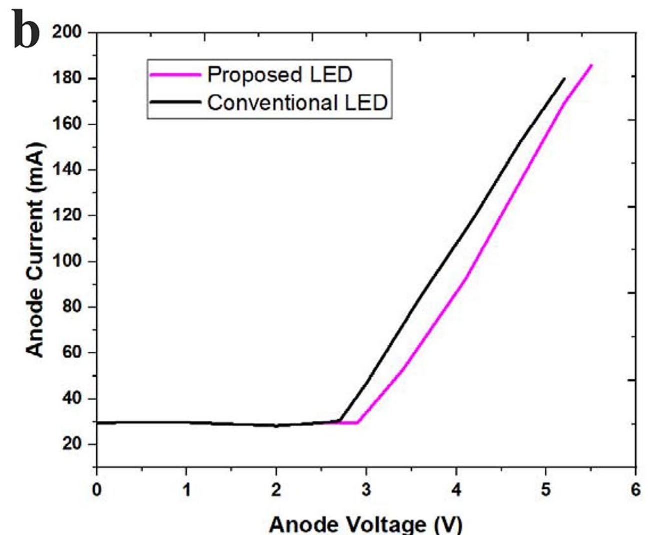


Fig. 4 (**a**) Luminous power versus anode voltage GaN LED. (**b**) Anode Voltage versus Anode Current of GaN LED

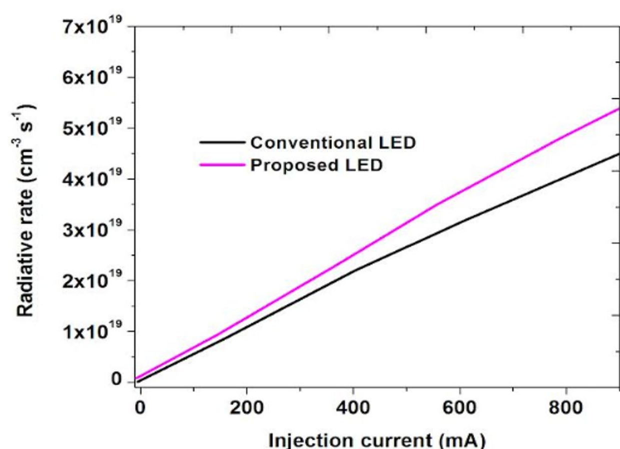


Fig. 6 InGaN/GaN LEDs' radiation rate Vs injection current for conventional and proposed

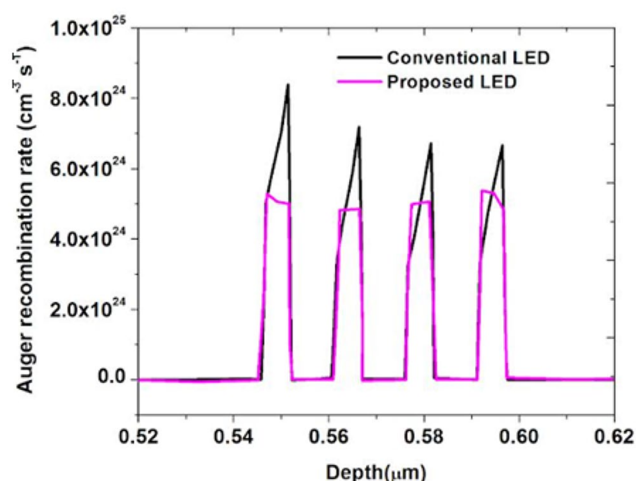


Fig. 7 Auger recombination of proposed InGaN/GaN and conventional InGaN/GaN LED

improved. It is due to the presence of GaN layer closer to the quantum well. p-GaN effectively suppresses the leakage of electrons through the sidewalls and improves the forward breakdown of the device. It provides high threshold voltage and low leakage current which in turn improves the recombination rate of the device.

The radiative recombination process is desirable for a light-emitting diode. The SRH and Auger recombination processes, on the other hand, are unfavourable for LEDs. Because the SRH and Auger recombination processes produce phonons rather than photons, phonons are produced. The LED's Auger recombination process is depicted in Fig. 7. It is found that Auger recombination rate in the proposed device is lower. It is a welcome feature for the proposed device.

The comparison analysis of radiative recombination is made for the conventional and the proposed InGaN/GaN

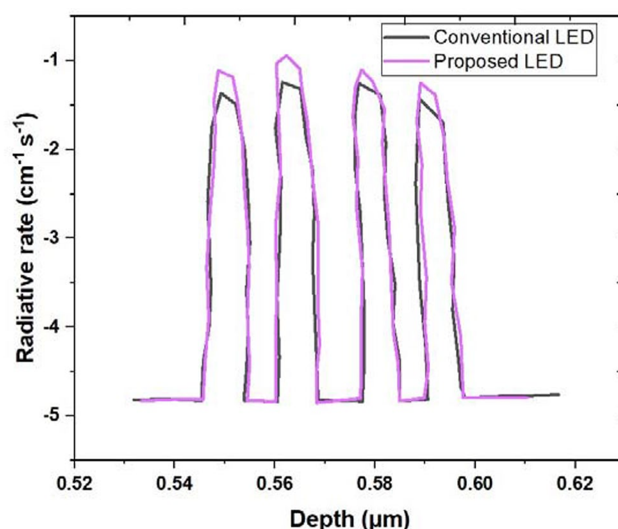


Fig. 8 Radiative rate of proposed InGaN/GaN and conventional InGaN/GaN LED

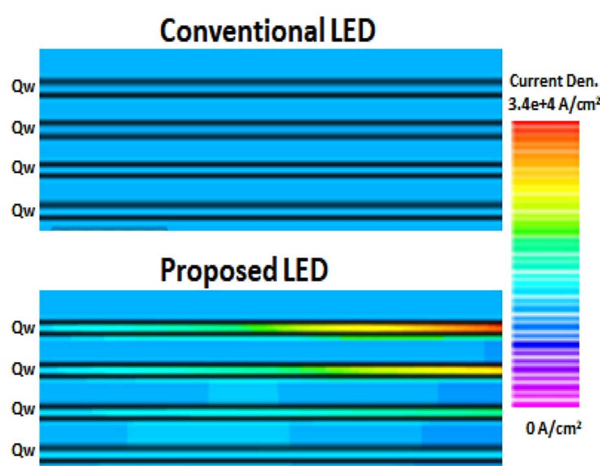


Fig. 9 Current density Comparison of proposed and conventional LED in the quantum well

LED is shown in the Fig. 8. It is evident that the recombination rate is increased with the effect of depth of the quantum wells.

Study on the effect of current densities in multiple Quantum Wells

The injection of electrons and holes could be analysed using the current density in LED. Figure 9 depicts the current density in the simulated LED. The current density is higher in the well region. It's related to the well region's localization of holes and electrons. Furthermore, the proposed LED has a higher current density due to the presence of HfO_2 layer. The HfO_2 layer reduces the interface trap densities, resulting in more carrier confinement in that region leading to

high current density. Therefore, the radiative recombination rate of the proposed is enhanced, which is shown in the above Fig. 8. This clearly shows that the proposed device's carrier injection efficiency is higher than that of ordinary conventional LEDs. The color difference in Figs. 9 and 10 shows the current density and potential is changed by HfO_2 and p-GaN.

The potential spread of the proposed and conventional light-emitting diode is shown in Fig. 10. It is evident that the use of the GaN layer adjacent to the quantum well changes the potential spread. Consequently, the electric field is affected by the potential distribution. The effect in the electric field impacts the drift current density (J).

$$J = nq\mu_n E + pq\mu_p E \quad \text{(x1)}$$

where, n and p are electron and hole concentrations, respectively. The μ_p and μ_n are hole and electron mobility, respectively. The q and E are the electronic charge and electric field respectively. From Eq. x1, it is clear that the change in the potential or electric field is responsible for the change in current density. This change in current density is shown in Fig. 9.

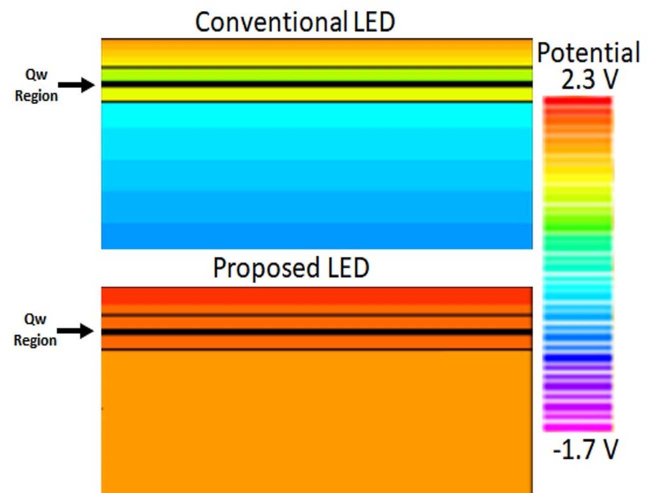


Fig. 10 Potential spread of conventional and proposed InGaN/GaN LED

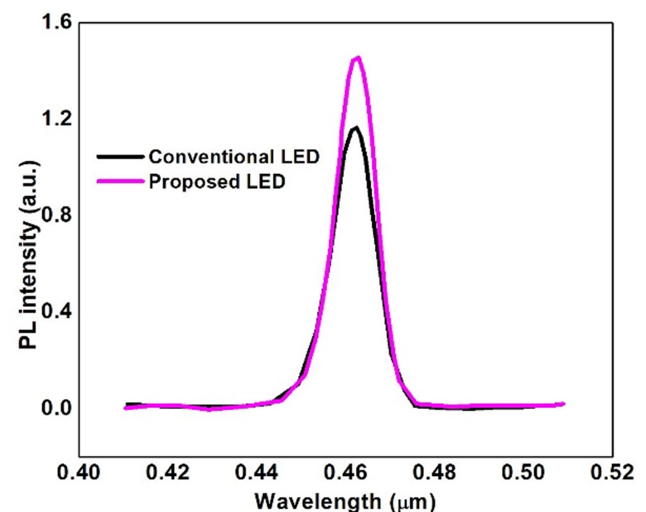


Fig. 11 Photoluminescence (PL) intensity versus wavelength

Study on the effect of photoluminescence

Figure 11 shows the photoluminescence (PL) intensity of conventional and proposed InGaN/GaN LED. The trend of PL intensity is consistent with reported data in [22]. Both conventional and proposed LED peaks at 460 nm. Further, at the wavelength of 460 nm, the peak intensity of conventional and proposed LED are 1.16 and 1.45, respectively. The PL indensity in propsed LED is improved by 20% compared to the convention LED. It is due to more number of injection of carriers in the proposed LED.

Study on the Effect of Internal Quantum Efficiency

One of the most essential figures to consider when evaluating LED performance is internal quantum efficiency. The amount of radiative recombination occurring inside the quantum well divided by the overall number of carriers pumped into the LED is known as internal quantum efficiency. In any case, the ABC model often explains it as the percentage of injected current that transforms into photon production in the active zone. As a result, the internal quantum efficiency is analyzed. This is extracted using radiative, SRH and Auger recombination rate. For this, the extraction statement is used in TCAD simulator. The extracted IQE of the proposed and conventional InGaN/GaNLED is depicted in Fig. 12. It is observed that the IQE of the proposed InGaN/GaN LED is higher than that of conventional InGaN/GaN LED. It is due to the lower Auger recombination rate in the proposed LED as shown in Fig. 7.

Further, in order to show the improvement in the proposed device, the performance metrics are contrasted with the conventional InGaN/GaN LED in Table 2. As can be seen, the proposed device shows improved output luminous power, radiative rate, and internal quantum efficiency at the injection current of 700 mA. Therefore, the proposed InGaN/GaN LED device is suitable for solid-state lightingapplications. The Performance comparision of conventional and proposed InGaN/GaNLED is highlighted in Table 2.

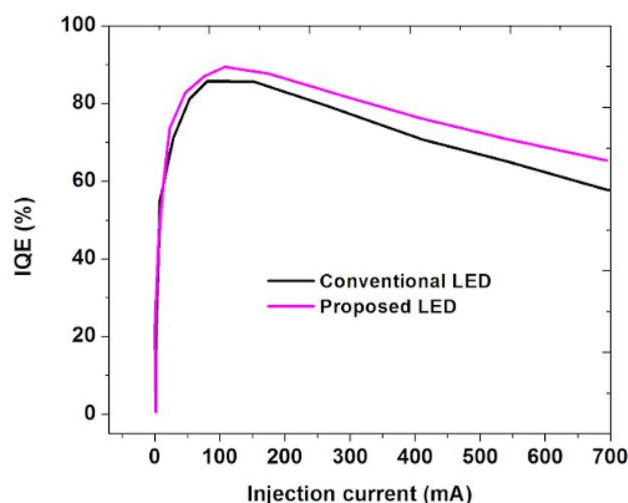


Fig. 12 Internal quantum efficiency of the proposed and conventional LED

Table 2 Performance comparison of conventional and proposed LED

Parameters	Conventional LED	Proposed LED
Radiative rate (cm^{-3} s^{-1})	3.51×10^{19}	4.42×10^{19}
Luminous output power (W)	1.6	2.1
Internal quantum efficiency (%)	56	68

Conclusion

This paper investigates the GaN LED with the proposed p-GaN layer. The performance of an InGaN/GaN LED diode was investigated using TCAD simulation. Using TCAD simulation various performance such as radiative rate, Auger recombination, output luminous power, and efficiency is analyzed. The projected GaN LED's performance is compared to that of traditional LEDs. When compared to ordinary LEDs, the suggested LED has a higher internal quantum efficiency and output luminous power. The improvement in luminous power and IQE for the proposed LED is 24% and 18%, respectively. This is attributed to a lower Auger recombination rate and higher radiative rate in the proposed GaN-LED.

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Author contributions All authors contributed to the study conception and design. Material preparation and simulation were performed by [Saranya G], [Siva Mangai N M], [R Babuji] & [Kalaivani C T]. The first draft of the manuscript was written by [Saranya G] and all authors commented on previous versions of the manuscript. All authors read and approved the final manuscript.

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Data availability Not applicable.

Declarations

Ethical approval Not applicable.

Consent to participate Not applicable.

Consent for publication Not applicable.

Informed consent Not applicable.

Research involving human participants or animals Not applicable.

Conflict of interest Not applicable.

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