Enhancement of Luminous Power and Efficiency in InGaN/GaN–Light Emitting Diode using high-k dielectric material

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Abstract
A novel high-k dielectric material is proposed for InGaN/GaN–LED to improve the performance. The proposed LED is analyzed and benchmarked with conventional LED using Technological Computer Aided Design (TCAD). The qualitative consistency of the optical characteristics of LED in this work has been observed that validate the TCAD simulation. Further, it is observed that proposed LED recorded higher luminous power and internal quantum efficiency (IQE) than that of conventional LED. At the injection current of 600 mA, the proposed and conventional LED yielded luminous power of 1600 mW and 1400 mW, respectively. Further, IQE of the proposed LED is higher than that of conventional LED by 12%. The improvement in the optical performance is attribute to high-k dielectric material induced additional electric field and radiative recombination rate. Thus, the proposed LED with high-k dielectric material is an outstanding device in lightning application.

Keywords LED · GaN · High-k dielectric · InGaN · IQE · HfO₂

List of symbols

| Symbol | Description |
|--------|-------------|
| $n_i$  | Intrinsic carrier concentration |
| $p$    | Hole concentration |
| $n$    | Electron concentration |
| $q$    | Electronic charge |
| $J_n$  | Electron current density |
| $J_h$  | Hole current density |
| $\mu_p$ | Hole mobility |
| $\mu_n$ | Electron mobility |
| $\psi$ | Quasi Fermi potential |
| $\epsilon$ | Permittivity |
| $\phi$ | Electrostatic potential |
| $R_{RAD}$ | Radiative recombination rate |
| $R_{AUGER}$ | Auger recombination rate |
| $R_{SRH}$ | Shockley–Read–Hall recombination rate |

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1 Introduction

In the past few decades, the research in GaN based LED has demonstrated impressive advancements. It is due to the excellent material property. Further, these properties facilitate GaN based LED to perform well in color display, automobile/home interior-lighting and running light. The performance of the LED in these applications depends on active layer, body thickness and crystal plane (Meneghini et al. 2009; Nishat et al. 2018; Gupta et al. 2020; Roelkens et al. 2010; Thomson et al. 2016). The active layer consists of barrier and potential well. LED with multiple well tend to have higher Internal Quantum Efficiency (IQE) and luminous power (Zhang et al. 2015; Li et al. 2014; Chang et al. 2012). The well thickness lower than 10 nm allow electrons to exist at discrete energy levels and better confinement. This leads to the enhancement of quantum efficiency. However, increasing number of quantum well more than 10 is not desirable since additional fabrication steps and its growth related defects. On the other hand, ultra-thin body based LED received impressive attention in inter/intra-chip interconnects (Gupta et al. 2020; Roelkens et al. 2010; Thomson et al. 2016). Further, the M-plane also enhances the IQE compared to c-plane (Nishat et al. 2018). In addition to aforementioned advancement, Electron Blocking Layer (EBL) also improve the efficiency as a result of reduced carrier over-flow. However, a lot of research have been carried out on barrier design to improve the LED performance (Shen et al. 2015; Cheng et al. 2012; Cheng and Wu 2014; Yang et al. 2015; Chang et al. 2010; Xia et al. 2011). Furthermore, analyzing and improving efficiency droop in light emitting diode also received a great attention in the last few decades (Zhu et al. 2013; Sun et al. 2014; Xu and Wang 2013; Cho et al. 2013; Schubert et al. 2007). Although, GaN–LED has shown improvements in efficiency and output power, it is still suffering from higher temperature, carrier-leakage, Auger recombination, micro-cracks and poor hole injection.

The elevated temperature due to recombination process has aging effect and reduces the device reliability for long life-time application. In addition, the higher temperature and material intrinsic defects induces micro-cracks which is physical damage (Egawa et al. 2002; Pinnington et al. 2008). The defects or micro-cracks is originating from lattice mismatch at nitride/substrate interface. Silicon (Si) and Sapphire substrate induce more dislocation and defects at Nitride/substrate interface. SiC emerged as an alternative substrate to Si and Sap as the manifestation of lower lattice mismatch and its corresponding lower micro-cracks or defects at Nitride/SiC interface. Thus, it is important to selected substrate and mitigate crack/defects as it is a serious concern in recombination process and efficiency droop. Micro-cracks enhance SRH non-radiative recombination through trap centers. The larger non-radiative recombination results in lower radiative recombination which is not desirable. Further, non-radiative recombination generates more phonons rather than photon and thereby increases the device self-heating and degrades the device reliability. Thus, the performance of the LED degraded as the manifestation of reduced radiative recombination and device self-heating. Hence, it is prime importance to enhance luminous power and quantum efficiency in LED. In this paper,
novel high-k dielectric material technique is introduced in the GaN LED to enhance the performance. Impact of dielectric material on the performance is analyzed using Technology Computer Aided Design (TCAD) simulation. Optical characteristics trend shows a qualitative consistency with reported works that ensure the validation of the simulation. Impact of dielectric material on luminous power, electric field and quantum efficiency is also analyzed.

2 Device description

The conventional and proposed GaN LED is shown in Fig. 1a, b, respectively. The GaN LED consists of 500-nm-thick GaN, 100-nm-thick AlGaN electron blocking layer, four 3-nm-thick InGaN well, three 5-nm-thick GaN well, 3.375-µm-thick GaN Buffer. Sapphire material is used as a substrate with thickness of 6 µm. Compared to conventional LED, the proposed LED has additional HfO₂ layer to enhance optical performance.

The role of HfO₂ is to modify the electric field around quantum well such that carrier concentration and recombination are enhanced in the well. The HfO₂ layer is defined in the simulation using region statement in ATLAS TCAD deckbuild. Band-gap and dielectric constant of HfO₂ are 6 eV and 22, respectively. The HfO₂ length is 25 µm and thickness is 1.5 µm. The field modulation and enhancement of recombination could be done by HfO₂ material. Further, in fabrication, HfO₂ needs deposition method rather than growth method. Deposition is simple process compared to the growth process. The difference between low K and high K material is dielectric constant. The variation in the dielectric constant results in variation of electric field across it. Therefore, the low K and high K material tend to have variation in electric field. The electron blocking layer is used to reduce the electron leakage. For n-GaN and p-GaN, the n and p doping are $1 \times 10^{18}$ cm$^{-3}$ and $1 \times 10^{19}$ cm$^{-3}$, respectively. The mole fraction (Aluminium composition) used in the EBL layer is 20%. Multiple quantum well is used to enhance the recombination. Thick GaN buffer is used to reduce defect propagation from substrate/ buffer interface.

![Fig. 1 Conventional and proposed GaN LED](image-url)
3 Simulation physics

Simulation of the conventional and proposed device are carried out using ATLAS TCAD. Various physical models are used to account recombination process and polarization effect in the simulation. The carrier transport in the LED is governed using Drift–Diffusion (DD) model in the simulation. In the DD model, the electron \( J_e \) and hole \( J_h \) current density are expressed as

\[ J_e = pq\mu_e \nabla \theta \quad (1) \]
\[ J_h = nq\mu_h \nabla \theta \quad (2) \]

The description of all model parameters used in the simulation is given in above nomenclature section.

On the other hand, the Poisson model is facilitated in the simulation to account the effect of carrier distribution over the space, which is denoted as

\[ \nabla (\varepsilon \nabla \varphi) = -\rho \quad (3) \]

However, the Poisson model is not enough since the GaN LED is more relevant to quantum effect. Thus, the Schrodinger model is augmented with Poisson model to account the electron/hole quantum behavior. Apart from fundamental models, Shockley–Read–Hall (SRH), Auger, and radiative models are used to govern carrier generation and recombination process in potential quantum well. The radiative \( R_{RAD} \), Auger \( R_{AUGER} \) and SRH \( R_{SRH} \) models are expressed as

\[ R_{RAD} = A(np - n_i^2) \quad (4) \]
\[ R_{AUGER} = (A_n n + A_p p)(np - n_i^2) \quad (5) \]
\[ R_{SRH} = \frac{np - n_i^2}{\tau_n \left( p + n_i \exp \left( \frac{-E_c}{kT} \right) \right) + \tau_p \left( n + n_i \exp \left( \frac{E_c}{kT} \right) \right)} \quad (6) \]

Polarization models are used in the simulation to account the piezoelectric and spontaneous polarization effect. Further, the carrier statistics also included using Fermi–Dirac model.

4 Result and discussion

On investigating the LED using physical TCAD simulator, first, it is mandatory to validate the simulation. Therefore, simulation is carried out to extract the current densities across the active layers of the device. The extracted current densities across the four quantum-well is shown in Fig. 2. Even, the extraction is done in vector component of the current densities rather than its magnitude. It is due to that vectors quantities expose a lot of and interesting intangible physics in the device. As it can be seen in Fig. 2, the following interesting facts has been observed such as: (1) current densities at barrier-well interface is higher, (2) the
current distribution is not uniform over the entire well-thickness and (3) the current densities gradually increase from 4th well down to 1st well. The gradual increase in the current densities with respect to well numbers is consistent with the reported data in Calciati et al. (2014). Thus, from this consistency, it could be stated that the simulation is valid one.

Electric field of the LED is analyzed as it is significantly relative to proposed high-k dielectric technique in the LED. Figure 3 contrasts the electric field vector of the conventional and proposed LED. It is observed that the electric field converge towards the InGaN/GaN interface and diverge at GaN/InGaN interface. It is due to the polarized negative charge at InGaN/GaN interface and positive charge at GaN/GaN interface. Therefore, the performed
simulation obeys the Gauss law. Furthermore, in contrast to conventional LED, an interesting field modulation is observed in proposed device which is high-lighted using a circle in Fig. 3. In between 1st and 2nd quantum-well of the conventional device, the electric field is in vertical direction. On the other hand, the field in the encircled region of the proposed LED from vertical direction to horizontal direction. It is due to the incorporation of high-k material in the proposed LED. This electric field deflection is important since it has great influence on generation and recombination of the carriers.

The radiative recombination rate across quantum well of proposed and conventional LED is contrasted in Fig. 4. It is observed that recombination rate is higher in well-region. It is due to higher electron/hole concentration in the quantum-well. In other words, recombination rate in the quantum well is proportional to the product of hole and electron concentration. Further, it is observed that the recombination is higher towards the P-GaN and it is due to higher hole injection in the quantum well which is closer to P-GaN layer. In addition, it is interesting to note that the recombination rate is higher in two well of proposed LED than that of conventional LED. It is a welcome feature and desirable in the proposed LED as it enhances the quantum efficiency and luminous power.

The current–voltage (I–V) characteristic a basis for any diode based device to describe its behaviors. Thus, the anode current is observed over Anode voltage, which is shown in Fig. 5. The anode voltage is swept in forward bias region and anode current is observed. The observation shows that the I–V characteristics trend of devices in this paper shows a qualitative consistency with I–V data reported in Antuña-Presa (2016). From Fig. 5, it has been seen that current of proposed device is same that of conventional device for all bias regime. However, a small discrepancy in current at the anode voltage of 3.0 V. The discrepancy could be used to relate the intrinsic series resistance of the device. In contrast to conventional device, a slight improvement in current for proposed device at 3 V results from lower series resistance.

The luminous power over injection current for proposed device and conventional device is depicted in Fig. 6. For both device, the same size of $1 \text{ mm} \times 1 \text{ mm}$ is considered in the simulation to provide quantitative comparison. Proposed and conventional LED exhibited 1600 mW and 1400 mW at the injection current of 600 mA, respectively. It is interesting
to note that the luminous power of proposed device is higher than conventional device by 200 mW. This substantial improvement in the light output power for the proposed device is attributed to dielectric material induced recombination.

Internal Quantum Efficiency is one of the important figure of merit to know-how of the device fit for specific application. Thus, the IQE is extracted for both conventional and proposed LED. It is extracted using the method that radiative recombination rate divided by all recombination rate, which is expressed as

$$IQE = \frac{Bn^2}{An + Bn^2 + Cn^3}$$ (7)

where A, B and C are SRH, radiative and Auger recombination coefficients, respectively. The extracted IQE against injection current is shown in Fig. 7. At lower injection current, both device exhibits the same efficiency. And it peaks up at the injection current of
100 mA. Beyond 100 mA, a droop in internal quantum efficiency is observed. The Augur recombination process at higher injection current is responsible for droop or degradation in efficiency. Although the droop occurs, the IQE of the both device is still comparable. At the higher injection current of 600 mA, the IQE of the proposed LED is higher than that of conventional device by 12%. The observed substantial improvement in IQE for the proposed device is due to high-k dielectric material induced higher electric field and recombination process around the quantum well. The improved IQE enable the device to yield higher luminous power with reduced power consumption.

In a fabricated real device, physical parameters such as well-thickness and well-depth are not necessary as expected all time. Hence, there might be inhomogeneity in the physical parameters and composition too. The Photoluminous (PL) intensity over a range of wavelength reflects the well-thickness, composition and well-depth. Further, the energy band profile and trap activation energy could be extracted from PL spectra. The device technologist in industry also fine-tune the fabrication process from PL spectra to obtain high-fidelity quantum-wells. Thus, analyzing PL spectra is of prime importance. Figure 8
shows the PL intensity versus wavelength. It is found that both proposed and conventional device peaks at 0.45 µm or 450 nm. The peak at 450 nm implies that both device has blue emission. Additionally, it is found that the peak value of proposed device is higher than the conventional device. It is due to higher injection current in the device.

In order to provide a better clarity on the performance of the LEDs, the proposed LED is contrasted with conventional LED in Table 1. The luminous power and IQE in the table is extracted at the injection current of 600 mA. It is clear that the luminous power and IQE of the proposed LED is superior than that of conventional LED.

### Table 1 Performance metrics of the LED AT 600 mA

| Device       | Luminous power (mW) | IQE (%) |
|--------------|---------------------|---------|
| Conventional LED | 1400                | 53      |
| Proposed LED  | 1600                | 60      |

#### 5 Conclusion

GaN–LED with a novel high-k dielectric technique is proposed and investigated using TCAD physical simulator. Radiative/non-radiative recombination, mobility and carrier statistics models are used to carry out the simulation. The high-k dielectric technique in proposed LED has the advantage of electric field modulation and enhanced recombination rate in the quantum-well compared to conventional LED. Further, the luminous power, IQE, PL intensity over wavelength, current densities and radiative recombination rate are extracted and a qualitatively consistency with reported data has been observed. In contrast to conventional LED, enhancement of luminous power and IQE in proposed LED is achieved.

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