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PAPER

Effects of polarized-induced doping and graded composition in an advanced multiple quantum well InGaN/GaN UV-LED for enhanced light technology

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Abstract

In this paper, a light-emitting diode in the ultra-violet range (UV-LED) with multiple-quantum wells (MQWs) of InGaN/GaN is designed and analyzed through Technology Computer-Aided Design (TCAD) simulations. The polarization effects in III-nitride heterojunction and the effects of graded composition in the electron blocking layer (EBL) are exploited to enhance the performance of the proposed UV-LED. It is observed that the effect of graded composition in the EBL helps to enhance the electrical and optical performance of the LED, thereby enabling the achievement of some promising results. The simulation-based results demonstrated that superior internal efficiency and an inferior leakage current are achieved by using a graded Al composition in the EBL rather than a uniform composition. The reported results also confirm the remarkable improvement of the light output power by 17% at ∼100 mA when using the graded composition and also show a reduction in series resistance leading to more current. Graded Al composition in the EBL results in the enhancement of electroluminescence spectra (i.e., an increase in the peak of the spectral density).

1. Introduction

From the last few years, the group III-nitride materials have revolutionized the light intensity, leading to the improvement of light emitting diodes (LEDs) with high efficiency and high brightness [1–6]. Because of the poor power consumption, densely packed size, and long life-span; LEDs have great advantages over the conventional light devices [7]. Group III-nitrides have numerous applications such as lighting, displays, sensing recording data at a very large density, ultra-violet (UV) curing, authentication of document, phototherapy, various medical and pharmaceutical applications, and many others because of their wide range of tunable bandwidths [7]. III-nitrides like gallium nitride (GaN), indium nitride (InN), aluminium nitride (AlN) and their alloys have energies ranging from 0.7 eV (InN) through 3.4 eV (GaN) to 6.2 eV (AlN), making them uniquely suitable for visible and ultra-violet LEDs [8]. The most well-known example is GaN and its alloy-based blue light emitting diodes which have revolutionized modern light technology [9]. Nitride semiconductors have been identified as one of the most favorable materials in order to realize optical devices in the UV as well as infrared (IR) visible regions. Also being the most electro-negative and smallest sized element of group V, there exists a metal-N bond with quite better iconicity compared to other III–V bonds [9].

Because of the real breakthrough in the emission of bright and efficient light by the Nobel Prize winners in 2014 in the blue to UV spectral range; it was easy to later on produce white LEDs [10, 11]. In 1927, the Russian scientist Oleg Losev, invented the first LED and, few years later in 1962, the American engineer Nick Holonyak Jr invented the first visible LED emitting red light [12]. In 1969, H P Maruska and J J Tietjen discovered that GaN has a direct transition band structure having a band gap energy of about 3.39 eV [13]. This encouraged a lot of researchers to study the domain of GaN, thereby leading to many publications over the years. In 1971, R Dingle *et al* demonstrated GaN crystal which optically pumped UV stimulated emission at a low temperature of 2 K [14]. In the same year, J Pankove announced the first blue LED having a metal–insulator–semiconductor (MIS) structure and the patent was issued in 1972 [15]. In 1972, J I Pankove and E A Miller went on to produce a blue GaN numeric display based on zinc (Zn)-doped GaN [15]. During 1990, D L Barton *et al* investigated the degradation of GaN-based blue LED devices and showed that the reduction of light output reduced mainly due to the yellowing of epoxy [16]. In 2001, N Narendran *et al* observed that the indicator-style white-LED packages degraded rapidly with the LEDs reaching 50% light output levels [17].

In 1994, a novel light-emitting device based on the hot-electron related operation was proposed by N Balkan also known as Hot Electron Light-Emitting and Lasing in Semiconductor Heterostructures (HELLISH) [18]. One of the unique features of HELLISH is that the operation of conventional semiconductor light emitters is based on the vertical transport of charge carriers in a forward-biased p-n junction. The quantum wells are incorporated in the active regions of the conventional LED providing superior photon and carrier confinement thus amplifying their efficiency. The contact structure of HELLISH was modified latter on as separate p- and n-channels with a longer p and a shorter n-channel known as TH-HELLISH which acts as multifunctional device being as an absorber and emitter together [19, 20] and also as a vertical-cavity semiconductor optical amplifier [21, 22].

InGaN and AlGaN alloys are promising candidates in the realization of efficient LEDs because of their wide range of bandwidths. Al-rich AlGaN serves as magnesium (Mg)-doped electron blocking layer (EBL), which plays a vital role in the LED performance. During the tunneling of high energy electrons along the active region, EBL blocks and then restricts them inside this region [23]. Consequently, by suppressing the overflow of electrons, the efficiency of the device is enhanced [24]; its primary advantage is to lower the efficiency droop when current injections are high. By balancing the concentration of aluminum in the p-type AlGaN EBL, we can obtain efficient injection resulting in trapping of charge carriers, which will ultimately lead to an improvement in the device's efficiency. In the present work, a multi-quantum well (MQW) UV-LED is designed to exploit the polarization effects in III-nitride heterojunction. The effects of graded composition in the EBL are studied, which eventually improve the performance of proposed device. The use of the graded composition in the EBL enhances the device's electrical and optical performance, increases internal injection efficiency, and lowers leakage current when compared to the conventional LED having uniform composition in the EBL.

The remainder of this article is organized as follows: section 2 is aimed at the description of the polarization-induced doping method and graded composition, section 3 is focused on the description of the physical structure of the developed LED, section 4 is devoted to the discussion of the achieved results, and section 5 is dedicated to the conclusions of this study.

2. Polarization-induced doping and graded composition

Sometimes the growth of LEDs based on nitride materials is restricted by the poor electrical conductivity of p-doped material. The deep nature of the Mg acceptor activation energy somewhere between 125 and 215 meV in p-AlGaN results in ineffective acceptor activation, low hole concentration, and low p-type conductivity [25]. Various methods, such as Mg-delta doping [26] and short period super lattice (SL) [27], are used to improve the activation efficiency of Mg-dopants. The injection of hole into the active region in deep-ultra-violet (DUV) LED will be of low efficiency for low conductivity of p-type Al-rich AlGaN alloy as EBL [28]. Also because of the light effective mass of electrons than that of holes in nitride semiconductors, there is a tendency of electrons to escape from the active region [28]; this overflow of electrons results in reduction of emission efficiency [28]. Leaked electrons accumulate in the EBL interface can produce radiative recombination with holes resulting in unanticipated emission in shorter wavelength [28]. This situation was improved later on by L Zhang *et al* [29] and others by using the polarization-induced doping method, proposed by J Simon *et al* which enhanced the internal quantum efficiency [30].

In between the remarkable success of GaN-based LEDs, there is an obstacle when the wavelength extends to a longer range in correspondence to the maximum sensitivity of human eyes. The emitting efficiency of the MQWs starts dropping abruptly, known as green-gap, because of the increasing non-radiative recombination rates [31, 32]. This non-radiative recombination rates are caused by deteriorative material quality [33], quantum confinement stark effect (QCSE) [34] and Auger effect [35]. It was reported that InGaN under layers can reduce potential point defects and boost MQWs efficiency [36, 37]. In order to minimize the efficiency droop in InGaN-based LEDs, various possible methods have been adapted, such as carrier leakage and current injection quenching [38–40], non-uniform distribution of holes [41–43], carrier delocalization [44], and polarization field [27, 45], high performance GaAs-based RCLED using dilute nitride GaInNAs active layers having barrier materials causing high differences between the energy band offsets [46]. To minimize this, non-polar or semi-polar GaN substrates techniques are used to control QCSE by decreasing the built-in polarization [47–49], blue MQWs were used to strain modulation layers to improve material quality[50]; thus reducing the carrier overflow. Some works have been done by focusing on expanding electron-hole wave function overlap by solving the issue related to charge separation within the active region using staggered InGaN quantum well [51, 52]. Many scientists have employed the conventional AlGaN/GaN SL to get better optical performance. However, L Zhang *et al* noticed its limitations, owing to the acute band bending of the EBL that is created due to strong electrostatic field initiated by lattice mismatch between AlGaN and GaN interface [53]. Thus, to overcome this issue, graded composition EBL (GEBL) has been employed and it shows some promising results. Studies showed that graded composition in the EBL improve the transport of holes in the active region leading to the reduction in efficiency droop [52].

Group III-nitrides experience both piezoelectric as well as spontaneous polarization. Due to wurtzite structure in GaN based and its devices, mostly spontaneous polarization due to low symmetry is observed [54]. III-nitride materials, also known as polar materials, acquire spontaneous polarization even without the presence of external electric field with an orientation along [0001] axis and can be influenced only by reversing the polarity of GaN. Due to the divergence from an ideal tetrahedral coordination across [0001] direction and the dissimilarities in the electro negativities of respective two elements generating a bond, the spontaneous polarization occurs in III-nitride materials. However, this polarization effect is detrimental to the quantum effect of MQW optoelectronic devices [54]. When the materials experience any kind of strain, there will be a distortion in the crystal lattice aggravating further deviation from ideal bonding and (c/a) ratio. This results in the presence of another kind of polarization known as piezoelectric polarization which plays a vital role as most of the films of wurtzite materials are grown heteroepitaxially. Because of the hetero-structure device, there are in-plane lattice constant mismatch leading to contraction or expansion of the devices. In this study, we have designed a MQW LED structure and examined the phenomenon of polarization-induced doping technique by implementing a graded Al composition in the EBL and then compared with a conventional LED based on a uniform Al composition EBL. This is done so as to attain a LED with enhanced and better efficiency and reduced droop.

3. Device structure and physics

The aim of this paper is to investigate the effects of polarization-induced doping in the electron blocking layer and the device's optical performance. AlGaN alloys are very promising materials in the realization of deep-ultra-violet LEDs as Al-rich AlGaN serves as an Mg-doped EBL and InGaN as the active region.

Here, we have designed an UV-LED device with multi-quantum well structure based on InGaN/GaN hetero-structure using Silvaco Atlas TCAD as shown in figure 1. The structure consists of five light emitting quantum well layers of InGaN inserted between GaN barriers within its active region. The width of the InGaN and GaN layers are 2.5 nm and 10 nm, respectively. The device is embedded between p-type and n-type of AlGaN coating layers. The details of the sequential layers, initiating from the base, are as given: 80 μm thick n-type GaN layer that acts as a substrate followed by 1.5 μm thick n-type AlGaN layer with 12% aluminium content. Above that there is the active region, which consists of alternate layers of five 2.5 nm thick InGaN quantum wells and four 10 nm thick GaN barriers. Above that there is a 20 nm thick electron blocking layer (EBL) of p-type AlGaN with 20% aluminium content (either graded or uniform Al composition). Finally, on the top of the EBL lies 150 nm thick p-type AlGaN layer with11% Al content followed by a 60 nm thick p-type GaN layer.

The p-type and n-type regions used in the device have their respective doping concentrations as 4.5×10^{17} cm^{-3} and 2×10^{17} cm^{-3}, respectively. However, there lies a problem with the doping of p-type GaN that the superficial acceptors have not being located yet. The best material used to dope p-type GaN is Mg. In GaN, a sufficient amount of Mg is doped; its ionization energy is quite low in order to produce some free holes [25]. Also, the acceptor impurities in Mg are proficiently passivated primarily by nitrogen vacancies and hydrogen [25]. To remove the carrier localization, mixing of In into GaN is essential but it results in a shift towards the red light in the output spectrum. In order to minimize this effect and maintain the output wavelength in the range of 480–510 nm, 1% of Al is added to the quantum well. Therefore, Al and In contents are stabilized at 1% all throughout simulation.

The energy band gaps of the GaN, InN, and AlN used in the simulations are taken as 3.42 eV, 0.77 eV, and 6.2 eV, respectively [55, 56]. The respective radiative recombination rate of coefficient (COPT) is 2×10^{-10}, 1.1×10^{-8}, and 1.1×10^{-10}cm^3 s^{-1}. The values of lattice constants of GaN, InN, and AlN are 0.3189 nm, 0.3548 nm, and 0.3112 nm, respectively. The Auger coefficient and carrier lifetime have their default values as 1×10^{-34}cm^6 s^{-1} and 1×10^{-9} s, respectively. The band gaps of AlGaN and InGaN semiconductors are

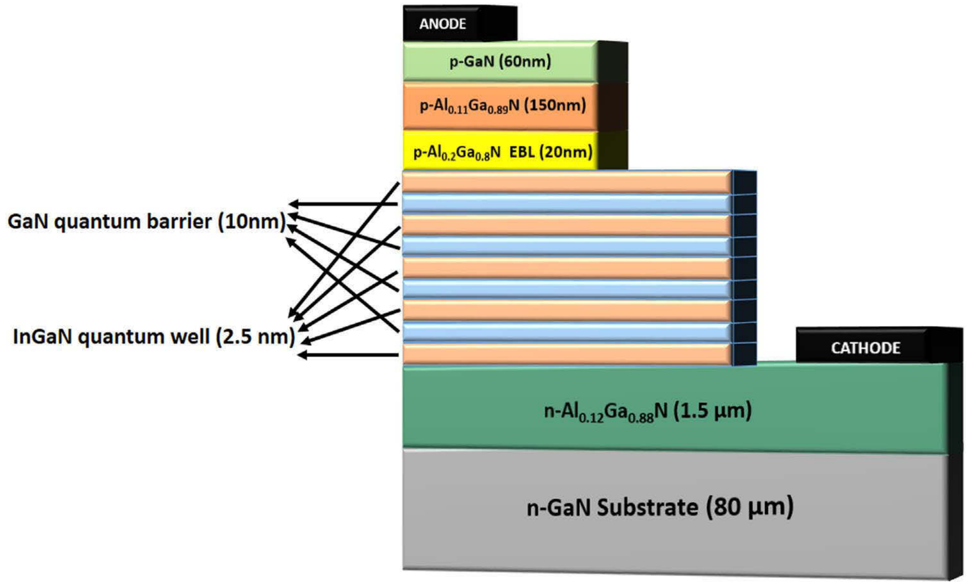


Figure 1. Schematic diagram of the UV-LED using InGaN/GaN multiple-quantum well structures.

calculated as follows:

$$E_g(Al_xGa_{1-x}N) = E_g(AlN)x + E_g(GaN)(1-x) - 1.3x(1-x) \tag{1}$$

$$E_g(In_xGa_{1-x}N) = E_g(InN)x + E_g(GaN)(1-x) - 3.8x(1-x) \tag{2}$$

4. Results and discussion

The device simulation is carried out in the Silvaco Atlas TCAD. The simulation process undergoes mainly in two steps: design of the device structure followed by device simulation. The developed model consists of material properties, contact description, choice of defects, physical models, and mathematical methods used by the simulator [57].

To study the reliability of the simulation, comparison has been done between InGaN/GaN device with uniform and graded composition of aluminum in the EBL.

4.1. Current-voltage characteristics

Figure 2 shows the I–V characteristics consisting of the anode current versus anode voltage for the UV-LED when considering uniform (LED_1) and graded (LED_2) Al composition in the EBL. The thickness of the layer as well as the quantum well structures is fixed in both the situations. From the graph, when graded Al composition is used in the EBL, a reduction in the series resistance is noticed compared to that in case of uniform Al composition in the EBL i.e. higher current density may be obtained for the same forward voltage in the case of LED_2 compared to LED_1. With graded composition in the EBL there occurs a reduction in the threshold voltage because of which the resistance drastically decreases allowing a great deal of current to flow through. The forward voltage at 60 mA of LED_1 and LED_2 are 4.4 V and 4.25 V, respectively. This reduction in the forward voltage is attributed to the betterment of the hole injection by decreased polarization field of graded Al composition in the AlGaN EBL [58]. The forward voltage reduction for LED_2 is because of the conversion of the two-dimensional hole gas (2DHG) into a three-dimensional hole gas (3DHG) as uniform Al composition in the EBL is replaced by graded Al composition [54]. In other words, when the EBL consists of graded composition of Al, a larger current density may be attained for the identical forward voltage in the LED.

4.2. Luminous power

Figure 3 displays the luminous output power versus anode current for the UV-LED when considering uniform (LED_1) and graded (LED_2) Al composition in the EBL. It is observed that the InGaN/GaN LED device has the finest performance (in terms of optical power) when we consider graded Al composition in the EBL over the

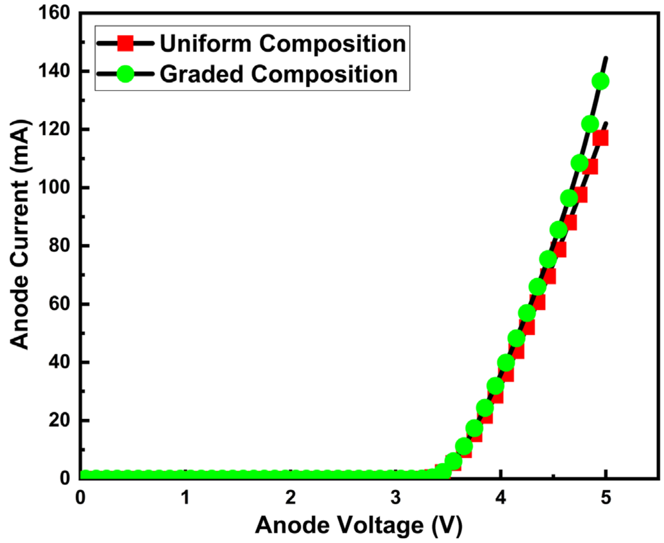


Figure 2. Behavior of the anode current versus anode voltage for UV-LED with uniform (LED_1) and graded (LED_2) Al composition in the EBL.

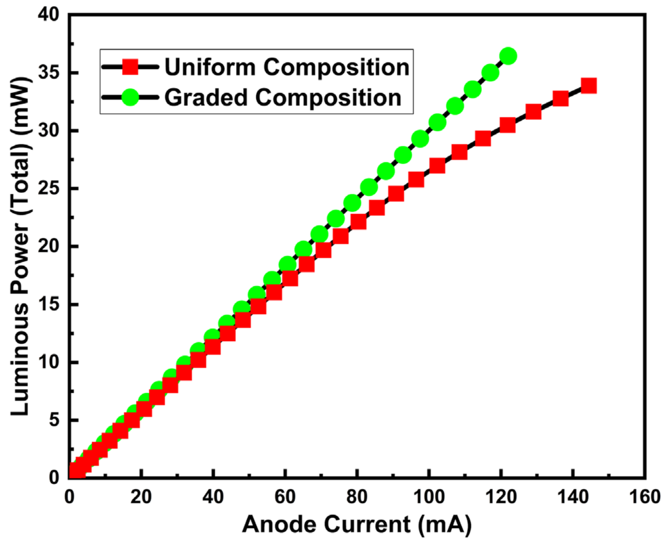


Figure 3. Behavior of the luminous power versus anode current for UV-LED with uniform (LED_1) and graded (LED_2) Al composition in the EBL.

whole injection current range. The light power of LED_2 is observed to be amplified by 17% at 115 mA. LED_2 has the highest light output power, with graded Al composition, because this structure benefits from superior electron confinement capability and larger hole injection efficiency. The superior optical properties of LED_2 compared to LED_1 are also attributed to the decrease in polarization field in the multiple quantum wells [27]. This improved light power means that more carriers radiating will recombine in the quantum wells of LED_2 and graded Al composition in the EBL can effectively improve light efficiency of InGaN/GaN LED. It can be observed that the current through the blue LED and the light intensity are directly proportional to current of less than 130 mA in case of LED_1. Saturation effect of P_{out} is referred to the current overflowing the quantum wells. The less current overflowing the QWs takes place in strong carrier localization inside the QW sample i.e. in case of graded LED hence it takes more time to enter the saturation region. For LED_1, in the injection current region of $I < 80$ mA, light output increases linearly. However, with rise in injection current, L–I curve shows a sub-linear behavior and a tendency to saturate at $I \sim 130$ mA. However, in case of LED_2, light output starts saturating at a large current (beyond ~150 mA). An increase in the current hardly contributes to the increase in light output, which means, only a small portion of injected carriers result in radiative recombination.

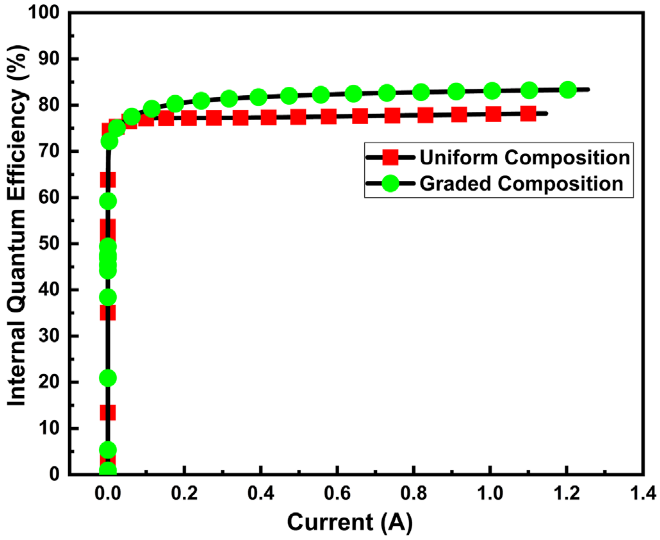


Figure 4. Behavior of the internal quantum efficiency versus anode current for UV-LED with uniform (LED_1) and graded (LED_2) Al composition in the EBL.

4.3. Internal quantum efficiency

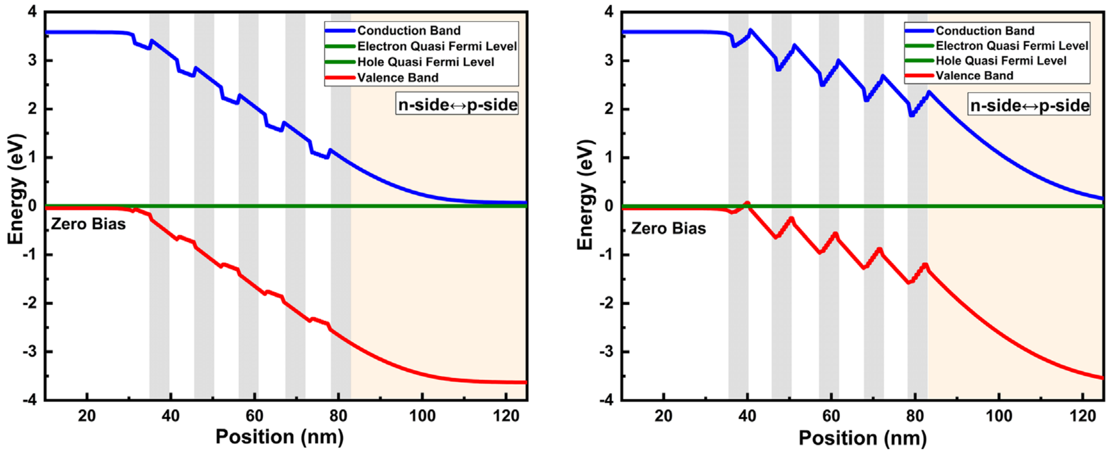
In figure 4, the internal quantum efficiency (IQE) for the designed LED is shown with respect to the current density. When a high brightness LED is operated at a current of nearly 1 A, the nonlinearity in the optical output power increases with increasing current [54]. This is then reflected as the droop of efficiency in the graph of the IQE versus current density, also called 'efficiency droop'. Generally, the efficiency droop occurs because of two reasons: (i) crossover of carriers at larger injection levels which is why the EBL is required [59]; (ii) Auger recombination occurring due to large concentration of carriers in quantum wells [35]. From figure 4, the IQE of LED_2 (with graded Al composition) is increased by 11.5% at a current of 0.4 A compared to LED_1 (with uniform Al composition). Efficiency droop $(n_{peak} - n_{0.4A})/n_{peak}$ is weakened from 24.8% to 13.3% because of the improvement of hole injection as well as electron confinement, thus indicating the development of radiative recombination rate because of efficient hole injection and distribution [58].

4.4. Energy band structures

The cause of superiority of LED_2 is the joint effect of the efficient injection and uniform distribution of holes. In order to elaborate the above phenomenon, the band structures along with their quasi-Fermi levels for uniform (LED_1) as well as graded (LED_2) are shown in figure 5 (zero bias) and figure 6 (forward bias of 4 V). Both conduction and valence bands have a downward slope from n towards the p-side leading to the separation of electron and hole wave function thus causing the carrier leakage at high injection level. The grey lines in the figures indicate quantum wells and the cream portion represents the EBL. The energy structures of LED_1 i.e. conventional LED display highly tilted structure in the active region as well as in the EBL compared to the graded (LED_2) LED. This indicates that the reason for increase of potential difference in the energy band between quantum wells and barriers is the potential induced internal field. Hence, there will be a reduction of recombination rate and IQE because of poor overlap between electron and hole wave functions. For grade EBL (LED_2) structure as shown in figure 6(b), the slope of valence band is alleviated because of relatively small band bending induced by reduced internal field in the active regions.

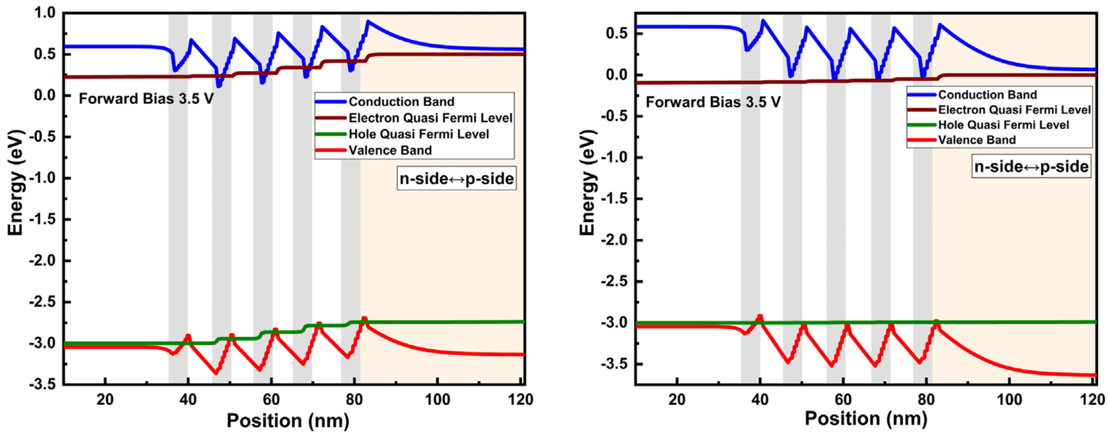
4.5. Electron and hole concentration

From figures 7(a) and (b), the carrier concentration profile is illustrated for uniform (LED_1) as well as for graded Al composition (LED_2) in the EBL. The grey lines in the figures indicate quantum wells. For p-AlGaN EBL with uniform Al composition, the electron and hole concentrations in the active regions are smaller than that of the EBL with graded Al composition. The hole concentration, as shown in figure 7(b), exhibits a uniform distribution in the graded p-type layer, due to polarization induced 3DHG. So the primary source of series resistance in InGaN/GaN based LEDs can be credited to the p-doped region, because the resistivity of p-GaN is larger than that of n-GaN [54].



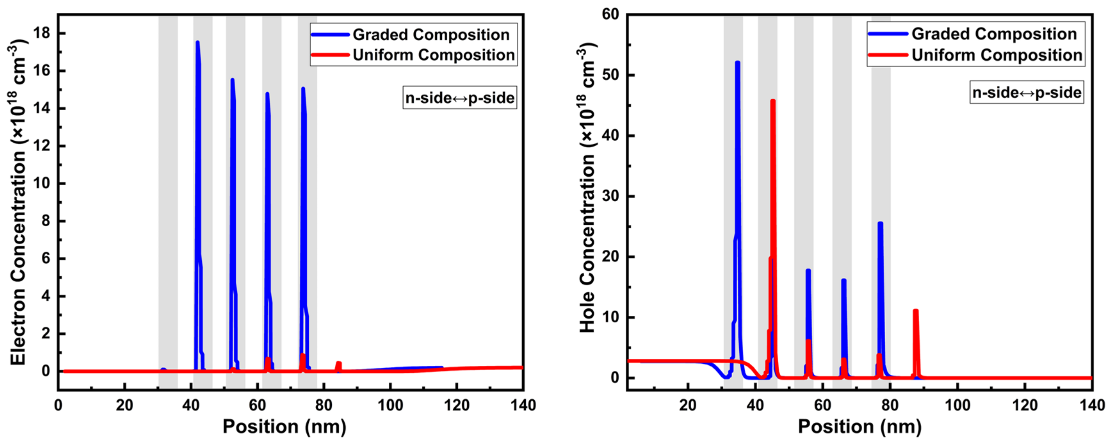
(a) (b)

Figure 5. Energy Band Diagrams for InGaN/GaN UV-LED for zero bias (a) Uniform (LED_1) and (b) Graded (LED_2).



(a) (b)

Figure 6. (a) Energy Band Diagrams for InGaN/GaN UV-LED for forward bias (a) Uniform (LED_1) and (b) Graded (LED_2).



(a) (b)

Figure 7. (a) Electron and (b) Hole concentration for InGaN/GaN UV-LED considering uniform (LED_1) and graded (LED_2) Al composition in the EBL.

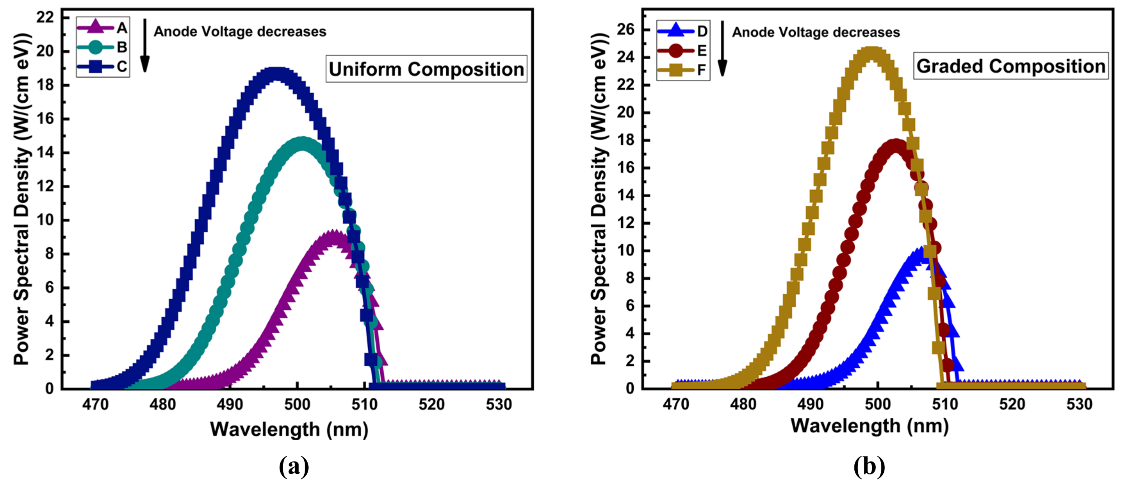


Figure 8. Normalized power spectral density versus wavelength for different anode current when considering the UV-LED with (a) uniform and (b) graded Al composition in the EBL.

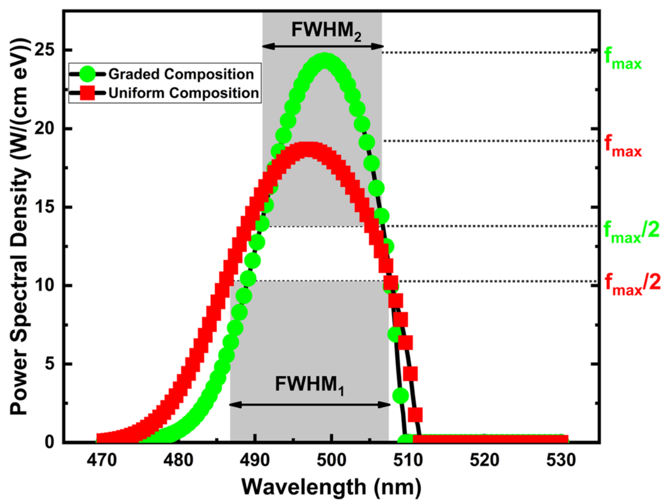


Figure 9. Normalized power spectral densities versus wavelength for UV-LED with uniform (LED_1) having $FWHM_1$ and graded (LED_2) Al composition in the EBL having $FWHM_2$.

4.6. Normalized power spectral density

The plot of the normalized power spectral density versus wavelength for UV-LED with uniform Al composition is shown in figure 8(a). Its variation with the change in the applied anode voltage is studied. The anode voltage has been varied in ascending order i.e. increased from 3.5 V, 4 V to 5.5 V (represented by structures A, B and C respectively). By varying the anode voltage, the change in the peak of power spectral density is observed which increases with a rise in the applied anode voltage. With the same steps, the normalized power spectral density of the device considering graded Al composition in the EBL is plotted in figure 8(b). Similarly the applied voltage of the device is increased from 3.5 V, 4 V to 5.5 V (represented by structure D, E and F respectively) and the same change is observed here i.e., the peak increases with increase in the anode voltage.

In figure 9, a comparison graph of the electroluminescence spectra (EL) is plotted for the UV-LED by considering uniform and graded Al composition in the EBL. It is depicted from the figure that the LED with graded Al composition in the EBL (LED_2) shows better performance i.e., higher peak than that achieved by considering uniform Al composition in the EBL. The peak wavelength of LED_2 is 500 nm, which is larger than the one of LED_1 (i.e., 494 nm). This shift is ascribed to the relieved electric field in the quantum wells and it increases with the increase in current which is due to carrier screening [60]. However, a small shift refers to the better polarization electric field mitigation [60]. Therefore, the wavelength shift in LED_2 confirms the importance of graded Al composition resulting in the reduction of polarization field.

The full width at half maximum (FWHM) of each spectrum were determined by peak fitting as shown in figure 9. The EL intensity of the graded LED is around 36.84% superior to that of the uniform LED. The cause for the superiority can be attributed to the combined effects of the improved capability of graded electron blocking and larger efficient hole injection in the EBL. Because of strong electron confinement in the QW of LED_2, it radiates a relatively sharp and narrow beam of light. As a result it has a narrow spectral width and FWHM. In contrast, uniform composed LEDs (LED_1) have much wider radiation patterns (beam width) and thus shows broader FWHM with large spectral widths.

Thus, in respect to all the aforesaid factors, the major advantage of graded Al composition in the EBL consists of reducing series resistance and thus enhancing the luminous intensity and quantum efficiency of the LED device.

5. Conclusion

A high efficiency multiple-quantum well UV-LED with InGaN/GaN layers was designed and analyzed through TCAD simulations. The performance of polarization induced doping in III-Nitrides was demonstrated by incorporating EBL with graded Al composition. When conventional EBL with uniform Al composition is replaced by the graded composition with Al increasing from 0 to 15%, the hole injection efficiency into the active region is improved and electron leakage current is decreased, leading to better electrical and optical characteristics. Also, it results in the reduction of series resistance thus lowering the forward bias voltage. Graded Al composition in the EBL shows an enhancement in the internal quantum efficiency and electroluminescence spectra of the device. This highlights the great potential of accomplishing high luminance LED for light technology.

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Data availability statement

All data that support the findings of this study are included within the article (and any supplementary files).

Ethics approval

The manuscript is ethically approved.

Consent to participate

All authors have given consent to participate.

Consent for publication

All authors have given consent for publication.

Availability of data and materials

No supplementary materials are available.

Competing interests

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Authors' contributions

All authors equally contributed for the preparation of the manuscript.

Disclosure of potential conflicts of interest

The authors declare that they have no conflict of interest.

Declarations

This article does not contain any study on human beings or animals.

Informed consent

Not applicable

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