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Simulation of AlGaN-based DUV-LED with The Variation of Step Al-graded QWs Configuration

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ABSTRACT

Analysis of aluminum composition grading is presented to enhance the efficiency of AlGaN-based deep ultraviolet light emitting diodes (DUV-LEDs). The optical performance of LEDs with varying quantum well (QW) thickness and aluminum composition grading were examined through drift-diffusion simulations. All LEDs featured step-graded QWs from 0.43 to 0.45 aluminum composition and have a total QW thickness of 3 nm, with thickness variations occurring at different aluminum composition gradings. Compared to LEDs with 0.5 nm and 1 nm QW thickness at an aluminum composition grading of 0.43, the LED with 1.5 nm demonstrated a high internal quantum efficiency (IQE) of 53.06%. The LED emitted at 283.327 nm. This design mitigated polarization effects, enhanced carrier injection efficiency, and improved carrier transport within QWs. This, in turn, increased the radiative recombination rates and luminescence intensity of the LEDs.

INTRODUCTION

In recent years, aluminium gallium nitride (AlGaN) based deep ultraviolet light emitting diode (DUV-LED) has received enormous attention due to their potential in advancing various areas of applications, such as medical treatment, communication, and water purification [1-5], including as a tool to eradicate SARS-COV 2 viruses which leads to COVID-19 diseases [6-8]. However, the performance of AlGaN-based DUV LEDs is limited due to AlGaN materials, which always introduce a built-in polarization electric field as a result of the lattice mismatch between the substrate and the epilayer [9] and between wells and barriers [10]. This electric field can reduce radiative recombination and ultimately cause efficiency droop in the DUV-LED [11].

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In general, efficiency droop refers to reducing efficiency with increasing current after the maxima peak of efficiency is reached [12]. So far, many factors have contributed to the drop in efficiency. One of them is associated with the carrier leakage from the multiquantum well (MQW) active region of the LED towards the p-regions, adversely reducing the number of carriers for radiative recombination and triggering the Auger recombination process [13]. Moreover, an unoptimized MQW separates electron and hole wavefunction, which would lower the radiative recombination efficiency [14]. In this study, radiative recombination refers to the recombination of electrons from the conduction band with the hole in the valence band, which produces photons [15]. Therefore, the MQW carriers must be well-confined to improve the radiative recombination rate [16]. A thinner MQW tends to result in poor carrier confinement, causing the electron to accumulate primarily in the last quantum well (QW) and impede hole injection from the opposite direction into the active region [17].

Furthermore, the electron and hole wavefunction separation aggravates as the energy band tilts due to the piezoelectric polarization caused by the lattice mismatch between the layer of QW and the quantum barrier (QB) [18]. The radiative recombination will be reduced, and the performance of the DUV-LED will be degraded. To realize a highly efficient DUV-LED with high radiative recombination, the thickness of the MQW should be thin enough, and the material composition needs to be optimal to increase the overlapping of electron and hole wavefunction, enhance the radiative recombination rates and improve the internal quantum efficiency (IQE) of the DUV-LED. At this point, the external quantum efficiency (EQE) for most of the reported DUV-LEDs remains below 10% [19-22]. However, a high IQE of DUV-LEDs has been reported to be between 30-40% by introducing linearly grading and asymmetrically step-grading the aluminium (Al) composition in the QWs [10,23,24]. The results indicate that optimizing the Al-graded composition in the QWs can reduce the polarization effect and increase the carrier confinement within the QW.

This work proposes a simulation work using a drift-diffusion approach to directly investigate the impact of Al-graded composition in AlGaN QWs of AlGaN-based LEDs with the variation of QW thickness for improving the optical properties of the LEDs. The energy band, electroluminescence (EL) properties, and IQE of three LEDs are considered in the calculation. Comparing the QW with uniform thickness for each graded Al composition, the higher thickness at 0.43 graded Al composition is anticipated to improve the carrier distribution within each QW and enhance radiative recombination efficiency.

METHODOLOGY

The simulated AlGaN-based DUV-LED heterostructure is schematically illustrated in Fig. 1. The LED heterostructure consists of a 2 μm-thick substrate, a 1 μm-thick n-GaN buffer layer, and a 2 μm-thick n-$Al_{0.55}Ga_{0.45}N$ cladding layer. Meanwhile, the MQW active region includes 3 nm-thick Al-graded AlGaN QWs (from $X_{Al} = 0.43$ to $X_{Al} =0.45$), 10 nm-thick $Al_{0.50}Ga_{0.50}N$ QBs with 5 periods. The subsequent layers are a 25 nm-thick $Al_{0.60}Ga_{0.40}N$ electron blocking layer (EBL), 300 nm thick p-AlGaN, and p-GaN. The doping concentration is set to 5.0×10^{18} cm-3 for Si-doped n-GaN and n-AlGaN, 1.2×10^{18} cm-3 for Mg-doped p-AlGaN, 3.0×10^{18} cm-3 for p-GaN and 1.9×10^{-10} cm-3 for undoped AlGaN QWs and QBs. The Auger and radiative recombination coefficients are set to be 2×10^{-11} and 2×10^{-31}, respectively, while the piezoelectric and spontaneous polarization-induced charge density are set at 100%.

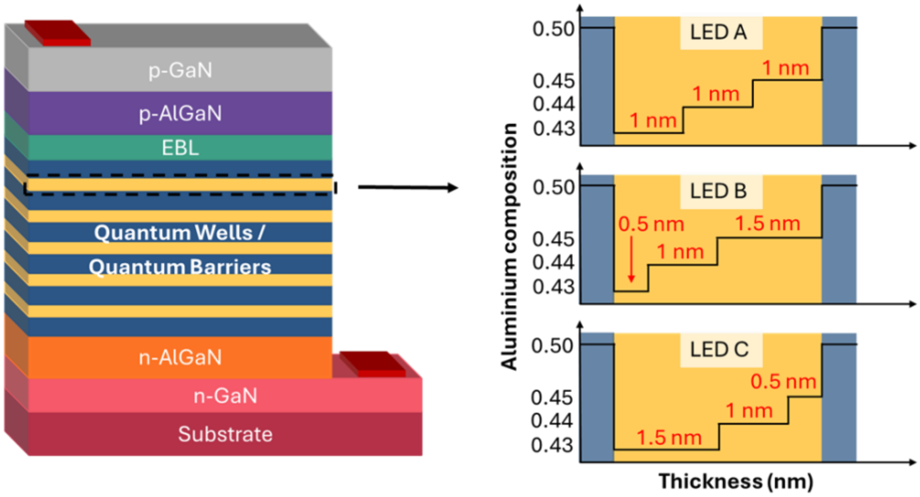

Fig. 1. Schematic diagram of the DUV-LED and the quantum well (QW) structure of LED A, B and C.

Table 1. The configuration parameters of step-graded QWs for LED A, LED B, and LED C

	QW Thickness (nm)		
Al Composition (X_{Al})	LED A	LED B	LED C
0.43	1.0	0.5	1.5
0.44	1.0	1.0	1.0
0.45	1.0	1.5	0.5

The details of different configurations of step-graded QW can be seen in Table 1: (1) For LED A, the aluminum (Al) composition in the QWs is step-graded from 0.43 to 0.45 with a uniform thickness of 1 nm for each Al composition; (2) For LED B, the thickness of the QWs varies with the Al composition, being 0.5 nm at X_{Al}=0.43, 1 nm at X_{Al}=0.44, and 1.5 nm at X_{Al}=0.45; (3) For LED C, the thickness of the QWs varies in a different order, being 1.5 nm at X_{Al}=0.43, 1 nm at X_{Al}=0.44, and 0.5 nm at X_{Al}=0.45. The simulation was performed using the One-Dimensional Drift-Diffusion Charge Control (1D-DDCC) simulator developed by Yuh Renn-Wu [25]. 1D-DDCC is a carrier transport simulation based on the semi-classical drift-diffusion model.

RESULTS AND DISCUSSION

The energy band diagram, carrier concentration, radiative recombination rate, and IQE for all the structures were analyzed at 13.15 V, where LED C achieved its highest IQE. The energy band diagrams for all LEDs are demonstrated in Fig. 2. The dotted black lines represent the quasi-Fermi level. In all structures, the bending of the energy band reduces due to the presence of step Al-graded QWs. Such structure decreases the energy band bending as the induced polarization bulk charges between QW and QB screened out part of the induced electric field [26].

However, significant differences in the energy band for all LEDs influence their optoelectronics performances regarding the carrier concentration and radiative recombination rates. Based on Fig. 2, the energy band for the QWs in LED C shows a higher potential barrier height ($\Delta\Phi_{CB}$ and $\Delta\Phi_{VB}$) and depth ($\Delta\Psi_{C}$ and $\Delta\Psi_{v}$) compared to LED A and LED B, which allows more electrons and holes to be confined and recombined radiatively [27,28]. The quasi-Fermi level for LED C also shows the highest overlap with the

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conduction band, indicating a high electron probability density [29]. Due to these energy band characteristics, LED C is uniform and has the highest carrier concentration density among the three structures. It can be inferred that this effect is influenced by setting the highest thickness of 1.5 nm at the Al composition of 0.43.

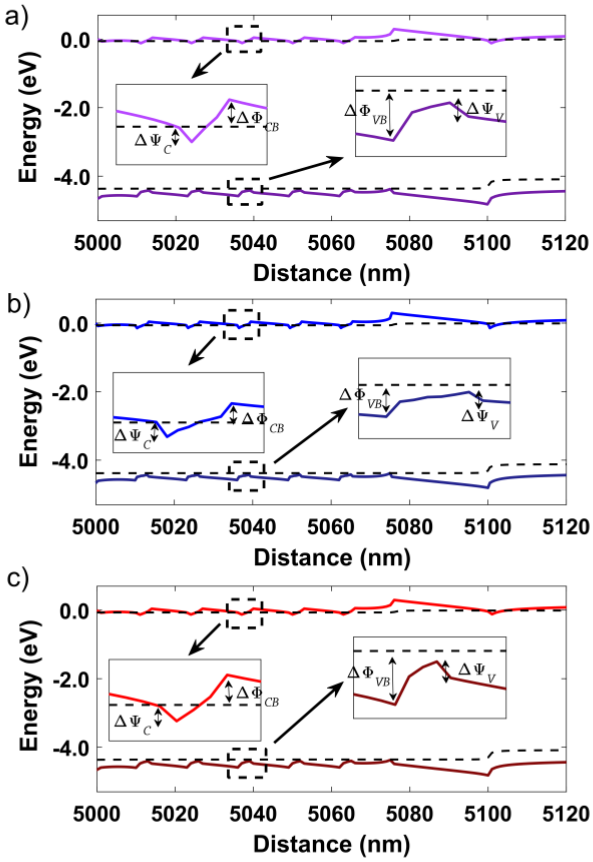

Fig. 2. Energy band diagrams and the magnification of conduction band and valence band of (a) LED A, (b) LED B, and (c) LED C. The dotted black lines across the active region represent the quasi-Fermi level.

Contrarily, LED B shows a lower overlap between the quasi-Fermi level and the conduction band. As mentioned above, LED B has the opposite design compared to LED C. As for LED A, the overlapping of the conduction band is slightly lower compared to LED C but higher QWs depth of the valence band than LED B. Fig. 2(b) shows that LED B has a lower potential barrier height, which limits the carrier confinement for more radiative recombination between electron and hole [30]. Moreover, the QWs structure of LED B aggravates hole accumulation at the last QW near the p-side while the electron gathered near the n-side, implying poor uniformity of carrier transport and low injection efficiency.

Furthermore, the band bending effect is due to the high difference in Al composition between QB (X_{Al} =0.50) and QW (X_{Al} =0.43), as depicted in Fig. 1. This difference causes negative polarization-induced charges at the heterojunction of QB and QW, which generate an electric field, resulting in the energy band bending upwards [31]. In LED C, the difference between the Al composition in QW and QB is accompanied by the QW thickness of 1.5 nm. Compared to LED A and LED B, the thickness of 1.5 nm in LED C, as shown in Fig. 1, leads to less bend bending since the induced electric field is distributed to larger space [32]. This allows higher electron injection and promotes carrier transport across the MQW active region. Correspondingly, the position of the highest thickness Al composition grading in graded QWs does play a role in alleviating the polarization effect in the active region of DUV-LED. Meanwhile, the low thickness of 0.5 nm with high Al composition difference in LED B presents contradictory characteristics compared to LED C. In this simulation, LED A, with uniform thickness for each Al composition grading in the QWs, acts as the reference for the performance of LED B and LED C. Thus far, it has exhibited intermediate characteristics compared to those two.

Fig. 3 shows the electron and hole concentrations across the active region of all five QWs. As illustrated in Fig. 3(a), LED C has the highest average electron concentration compared to LED A and B. Additionally, Fig. 3(b) reveals that LED C has the highest peak hole concentration among all five QWs. Conversely, both electron and hole concentrations decrease in LED A, with LED B having the lowest average carrier concentration. As expected, the greater depth of the QWs in LED C, as shown in Fig. 2(c), has enhanced its overall electron confinement. With increased electron confinement, more electrons are trapped inside the QW, resulting in a higher carrier density within the QW [33].

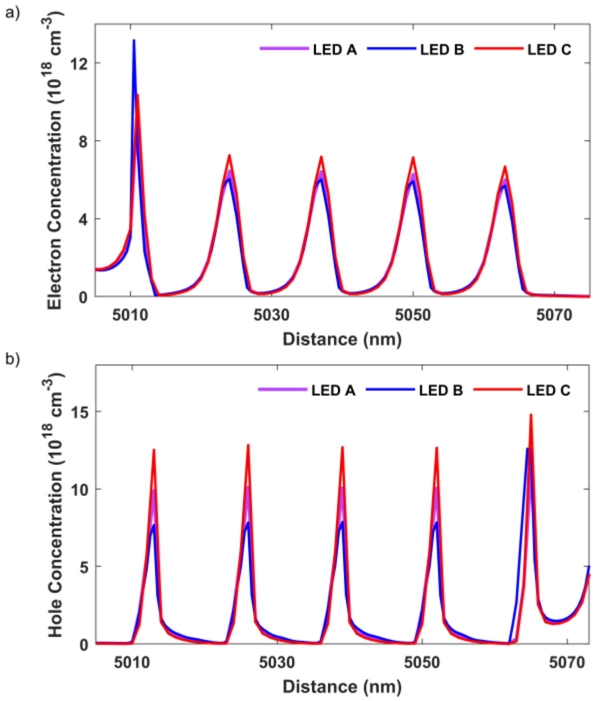

Fig. 3. The (a) electron concentration and (b) hole concentration for LED A, B, and C.

Fig. 4(a) depicts the radiative recombination rate of the MQW in all LEDs. Overall, LED C shows the highest radiative recombination rate compared to LED A and B. The radiative recombination rate in LED C is approximately uniform in each MQWs. The bimolecular rate equation in Eq. (1) states that the recombination rate is proportional to the product of electron and hole concentration [34]. B is the bimolecular recombination coefficient, and n and p are the concentration of electrons and holes, respectively.

$$R = -\frac{\mathrm{d}n}{\mathrm{d}t} = -\frac{\mathrm{d}p}{\mathrm{d}t} = Bnp \qquad \text{Equation 1}$$

Thus, carrier distribution, as well as carrier concentration for LED C structure, can also be inferred to be in the best performance compared to LED A and LED B. Uniform carrier distribution across the active

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region and high carrier concentration density in LED C leads to higher radiative recombination and reduces the polarization effect leading to less bend bending and simultaneously enhance the carrier transport across the active region.

Based on the luminescence spectrum in Fig. 4(b), the emission peak of the LEDs only varies between 281.02 nm for LED B and 283.33 nm for LED C. This indicates that the thickness variation for step Al-graded QWs does not significantly impact the emission peak. Nonetheless, LED C presents a higher luminescence intensity of 6.92×10^{19} a.u., which is ~8.68% higher than LED A and ~16.85% higher than LED B. The high-intensity emission is due to the densely uniform holes and electron confinement, thus improving the radiative recombination rate in the active region in LED C.

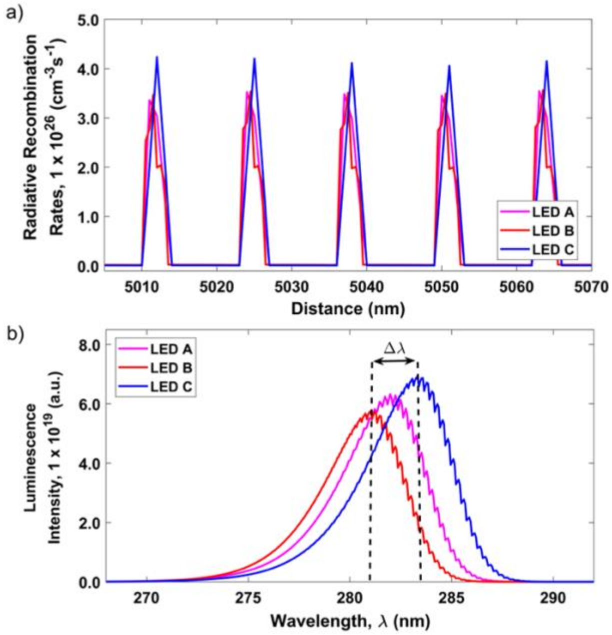

Fig. 4. The (a) radiative recombination rate and (b) luminescence spectrum for LED A, B, and C, respectively.

The IQE and current density-voltage (J-V) characteristics are plotted in Fig. 5. From the results, LED C has a higher IQE of 53.06% at ~130 Acm^{-2}, which is 8.05% higher than LED A and 15.72% higher than LED B. An essential consideration is that each QWs in the proposed LEDs have an overall uniform thickness of 3 nm, but with the thickness variation at different Al composition grading. The total thickness of QW plays a role in achieving high optical performance by increasing the radiative recombination since it has been found in the previous works by other researchers that the QW with a thickness lower than 5 nm can decrease the effect of spatial separation between the electron and hole wavelength [27], [34]. This implies that the optical performance of LED C benefits from its thin QW structure, which is further enhanced by having the highest thickness at the lowest Al composition grading of 0.43 within the QW. Hence, the step Al graded QWs design that leads to the high IQE is linked to an increased radiative recombination rate, resulting from improved carrier concentration due to the reduction of polarization effect in the DUV-LED. The enhanced carrier confinement within each QW also promotes more electrons and holes to recombine radiatively, leading to higher luminescence intensity.

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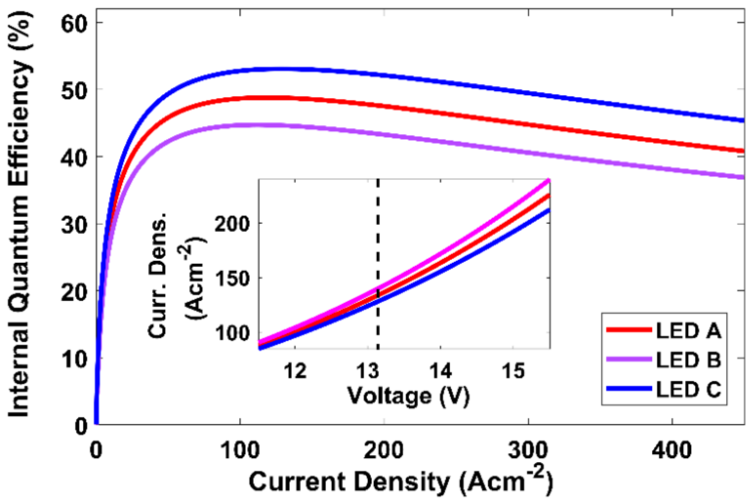

Fig. 5. The internal quantum efficiency (IQE) and inset of current density-voltage (J-V) characteristics for LED A, LED B, and LED C, respectively.

CONCLUSION

In conclusion, the thickness impact for step Al graded QWs for AlGaN-based DUV LEDs is investigated. Our simulation results show that LED with step-graded QWs of 1.5 nm thickness at $X_{Al} = 0.43$ exhibits a higher IQE at 53.06%, surpassing LED with QWs thicknesses of 0.5 nm and 1 nm at $X_{Al} = 0.43$ by 15.72% and 8.05%, respectively. The LED with step-graded QWs of 1.5 nm thickness at $X_{Al} = 0.43$ exhibits a wavelength of 283.33 nm. This design effectively reduces polarization effects in the DUV-LED and minimizes band bending in the active region. Consequently, it enhances carrier injection efficiency into the active region and improves carrier transport and confinement within each QW. The overall carrier concentration in the LED increases significantly, resulting in a higher radiative recombination rate and a luminescence intensity of 6.92×10^{19} a.u., which exceeds LED with 0.5 nm and 1 nm at $X_{Al} = 0.43$ grading by 16.85% and 8.68%, respectively. Therefore, research on the optimal thickness for each graded aluminium composition in QW can pave the way for the high efficiency of AlGaN-based DUV-LED.

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CONFLICT OF INTEREST STATEMENT

The authors declare the absence of conflicting interests.

AUTHORS' CONTRIBUTIONS

Wan Nur Amierha Wan Ibrahim researched, wrote, and revised the article. Muhammad Amirul Hairol Aman provided the visualization. Faris Azim Ahmad Fajri and Muhammad Amirul Hairol Aman conceptualized the central research idea and reviewed the article. Wan Nur Amierha Ibrahim provided the theoretical framework. Faris Azim Ahmad Fajri supervised the progress of the research. Ahmad Fakhrurrazi Ahmad Noorden anchored the review and approved the article submission.

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