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Efficiency enhancement of ultraviolet light-emitting diodes with segmentally graded p-type AlGaN layer*

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AlGaN-based ultraviolet light-emitting diodes (UV-LEDs) have attracted considerable interest due to their wide range of application fields. However, they are still suffering from low light out power and unsatisfactory quantum efficiency. The utilization of polarization-doped technique by grading the Al content in p-type layer has demonstrated its effectiveness in improving LED performances by providing sufficiently high hole concentration. However, too large degree of grading through monotonously increasing the Al content causes strains in active regions, which constrains application of this technique, especially for short wavelength UV-LEDs. To further improve 340-nm UV-LED performances, segmentally graded Al content p-$Al_xGa_{1-x}N$ has been proposed and investigated in this work. Numerical results show that the internal quantum efficiency and output power of proposed structures are improved due to the enhanced carrier concentrations and radiative recombination rate in multiple quantum wells, compared to those of the conventional UV-LED with a stationary Al content AlGaN electron blocking layer. Moreover, by adopting the segmentally graded p-$Al_xGa_{1-x}N$, band bending within the last quantum barrier/p-type layer interface is effectively eliminated.

Keywords: AlGaN, ultraviolet light-emitting diodes, polarization-doped p-type layer

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1. Introduction

AlGaN-based ultraviolet light-emitting diodes (UV-LEDs) have attracted great research interest due to their wide ranges of application fields, such as purification for air or water, disinfection, anti-counterfeiting recognition, chemical sensors, and medical equipment.[1–3] However, they are suffering from much lower light output power (LOP) and internal quantum efficiency (IQE) compared to InGaN-based visible LEDs, while they share the common problem of efficiency droop, which further restricts the commercialization process of AlGaN-based solid-state UV light sources.[4,5] The root causes with respect to the unsatisfactory LOP and IQE, and the troublesome efficiency droop issues have been investigated by many groups. Several reasons have been proposed, including Auger recombination,[6] severe electron leakage, high density of threading dislocations,[7] carrier delocalization,[8] Shockley–Read–Hall recombination,[9] asymmetry of carriers transport,[10] etc. The lack of balanced injection of electrons and holes caused by the light effective mass of electrons and the low concentration of holed has been considered as one of the most important roles. Hence, an electron blocking layer (EBL) with relatively high Al content AlGaN layer is often employed to strengthen electron restriction. However, the introduction of EBL with stationary Al composition is often accompanied with downward band-bending, thus leading to electron accumulation in the last quantum barrier (LQB)/EBL interface, induced by the large polarization field formed by the sharp change of Al content between the LQB and EBL. At the same time, the EBL acts as a high potential barrier for hole injection. In previous work, we have demonstrated the effectiveness of lowering polarization field in EBL and active regions as well as alleviating band bending within the EBL/p-type layer interface by engineering the band structures with gradually decreased Al content EBL.[11] Further, by gradually decreasing the Al content in p-AlGaN layer, we have experimentally confirmed that the forward voltage could be reduced and the LOP could be improved even without an EBL layer.[12] This technique was also known as polarization-doping, which

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was first put forward by Simon *et al.*[13] Using the polarization field formed through grading the element composition instead of thermal energy to ionize Mg acceptors, a high-density three-dimension hole concentration as high as 2×10^{18} cm^{-3} is achieved. By applying this technique to LEDs, promisingly, we can have the hole concentration in active regions improved and the interfacial band structures smoothed. It was pointed out that the hole concentration produced via polarization-doping was in close relation with the degree of AlGaN gradation, i.e., the change of Al content in unit thickness, according to the formula of $\sim 10^{13}(\Delta x/d)$ cm^{-2} (here Δx is the variation of Al composition and d (nm) is the thickness of AlGaN layer). However, a too large degree of gradation through increasing the initial Al content impeded further improvements of the overall LED performance, such as electroluminescence (EL) and external quantum efficiency (EQE).[14–18] This may be attributed to the increased alloy scattering and strain within multiple quantum wells (MQWs) active regions induced by high Al compositionally grading, thus weakening the radiative recombination.[14,15] Therefore, structure designs aiming at retarding this contradiction for further performance improvements of LEDs, especially for UV-LEDs in need of relatively high Al content in active regions, are extremely deserved to be investigated.

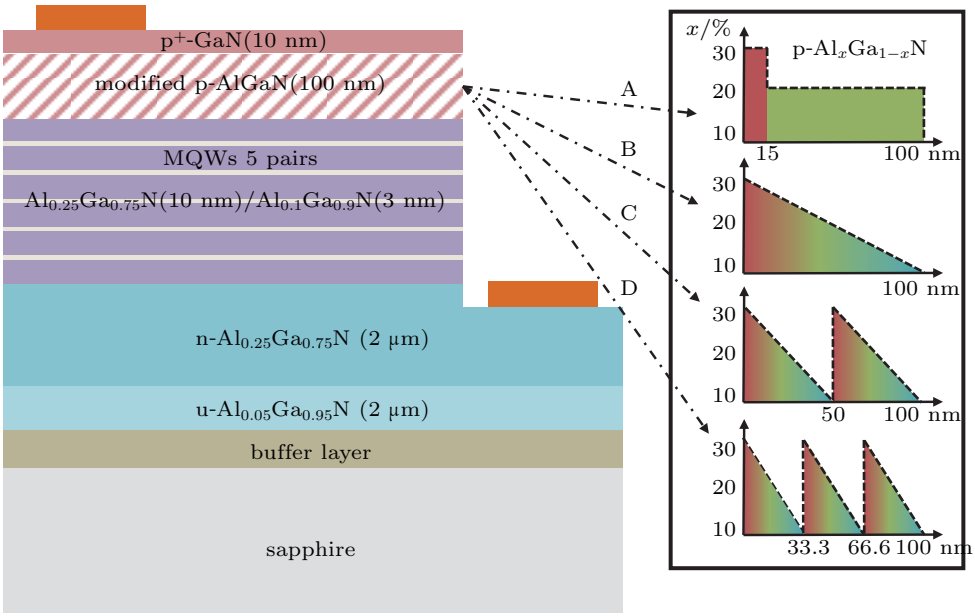


Fig. 1. Schematic diagram of UV-LED structures with different p-$Al_xGa_{1-x}N$: the original structure (a) with 15 nm $Al_{0.3}Ga_{0.7}N$ EBL and 85 nm $Al_{0.2}Ga_{0.8}N$, and the three modified p-type layer with respectively one section (b), two sections (c), and three sections (d) of linearly graded Al content from 30% to 10%.

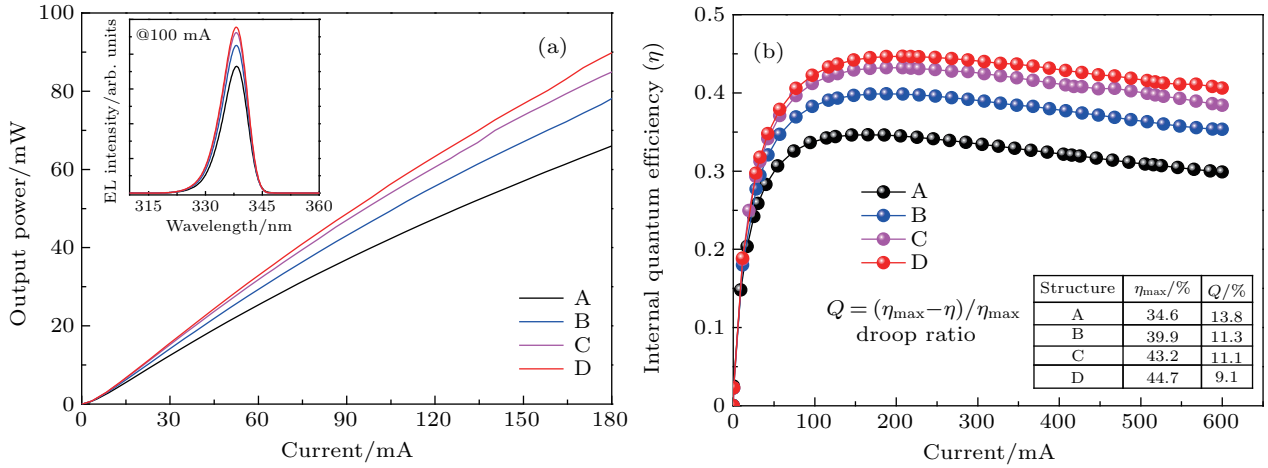


Fig. 2. (a) Light output power and (b) normalized internal quantum efficiency as a function of injection current for the four LEDs. The inset in panel (a) is the EL spectrum collected at injection current of 100 mA.

In this contribution, we proposed UV-LED designs with segmentally graded Al content p-type AlGaN layer, where the linearly decreased Al content in p-$Al_xGa_{1-x}N$ layer was divided into multiple segments of the same thickness. This system has been numerically investigated using the advanced physical models of semiconductor devices (APSYS) simulation program. Results indicate that the IQE and LOP are improved with the increase in the number of grading seg-

ments. The overall performance of LED can be improved by polarization-doping the enhanced hole concentration and modifying band structures to eliminate the band bending within the last QB/p-type layer interfaces and reduce electrostatic field in active regions, thus strengthening hole injection, electron blocking, and radiative recombination.

2. Structure and parameters

As a reference in this study, the original structure (denoted as A in Fig. 1) consists of a 25.0-nm-thick low-temperature nucleation layer, a 2.0-μm unintentionally doped $Al_{0.05}Ga_{0.95}N$ layer, a 2.0-μm n-type $Al_{0.25}Ga_{0.75}N$ layer (n-doping: 2.0×10^{18} cm^{-3}), 5 periods of $Al_{0.1}Ga_{0.9}N/Al_{0.25}Ga_{0.75}N$ (MQWs) with 3.0-nm-thick well and 10.0-nm-thick barrier, a 15.0-nm Mg-doped $Al_{0.3}Ga_{0.7}N$ EBL layer, a 85.0-nm p-doped $Al_{0.2}Ga_{0.8}N$ (p-doping: 1.0×10^{17} cm^{-3}), and a 10.0-nm highly Mg-doped p-GaN contact layer. The proposed structures B, C, and D are composed of the structure similar to the original structure, except that the 100 nm p-type layer was replaced by segmentally polarization-doped $Al_xGa_{1-x}N$ layer, with Al composition linearly decreasing from 30% to 10%, as shown in Fig. 1. The average Al component and doping concentration in p-type layers of all structures keep the same.

Optical and electrical properties, band diagram, and carrier concentration of all LED structures in this work are simulated by solving Poisson's equation, Schrödinger equation, the carrier transport equations, and the current continuity equation self-consistently with proper boundary conditions via APSYS numerical simulation program. The device geometry is designed into a rectangular shape of 300×300 μm. In the carrier recombination model, the Shockley–Read–Hall (SRH) recombination lifetime in the active region is estimated to be 5.0 ns and the internal loss is 1000 m^{-1}. The Auger recombination coefficient is set to be 1×10^{-30} cm^{-6}/s and the operating temperature is set to be 300 K for simplification. The built-in interface polarization charges induced by spontaneous and piezoelectric polarization are calculated by Fiorentini *et al.* Their partial compensation caused by fixed defects and other interface charges is scaled down by introducing a fitting factor of 0.4. The band-offset ratio is assumed to be 0.7/0.3 for AlGaN materials. More detailed descriptions of the model and material parameters used in the simulation can be found in Ref. [15].

3. Simulation results and discussion

To evaluate the effect of proposed structures on the LED performance improvements, the output power and IQE of modified structures compared with the original structure have been investigated. As shown in Fig. 2(a), the total output power increases nearly linearly for all structures within the injection current range.

With segmentally polarization-doped p-$Al_xGa_{1-x}N$, structures B, C, and D exhibit clearly enhanced output ability than that of conventional structure A. As the injection current increases to 180 mA, the enhancement factors are 18.4%, 28.7%, and 36.1%, respectively, for structure B, C, and D. The inset in Fig. 2(a) shows the EL spectrum at injection of 100 mA, which indicates the modification of structures has little influence on the luminous wavelength centered at around 340 nm. The improved LOP may originate from more carriers confined in active regions, thus enhancing the radiative recombination.

Figure 2(b) shows the normalized IQE as a function of injection current. With three segments of Al content grading repetitively with the 100 nm p-$Al_xGa_{1-x}N$, structure D exhibits the highest IQE. The value of η_{max} is enhanced by about 44.7% compared with that of the original device. At the same time, the improvement trend slows down as the graded segments increase. The efficiency droop ratio Q has also been improved for the modified samples. As listed in the table in the inset of Fig. 2(b), the Q values at injection current of 180 mA are reduced from 13.8% (structure A) to 9.1% (structure D), while the injection level which drops at the beginning delays from 49.6 mA to 62.4 mA (i.e., increased by 25.8%). All these data demonstrate the effectiveness to further improve LED performances by adopting segmentally decreased Al composition in the p-type layer, while the initial grading point of Al content remains at a relatively high value.

To shed light on the underlying mechanisms responsible for the overall device improvements, energy band profiles and quasi-Fermi levels, as well as electrostatic field distribution at 180 mA have been calculated, as plotted in Fig. 3. For the reference structure, the typical downward energy band-bending between the last QB and the EBL can be clearly seen in Fig. 3(a), as also verified in the correspondingly reversed electrostatic field within this region in Fig. 3(e). This bending arising from the sharp change of Al composition induces an energy valley in the last QB, which causes electron leakage and hence lowers the efficiency of electron utilization. However, by linearly decreasing the Al content of p-$Al_xGa_{1-x}N$ along the growth direction to eliminate sharp interfaces, the variation of electrostatic field slows down (see Figs. 3(f)–3(h)), and the energy band at the last QB recovers its upward bending states, as indicated in Figs. 3(b)–3(d). The modification of interfaces has a great influence on the effective barrier for electron blocking and hole injection. The effective potential barrier for electrons is raised from 241 meV (sample A) to 268 meV, 287 meV, and 293 meV for structure B, C, and D, respectively, while that for holes decreases from 257 meV to 161 meV, 144 meV, and 136 meV. Compared to the increase of electron barrier, the decease of hole injection barrier undergoes a two times greater change, which should be a very important characteristic that determines LED device performances since the hole injection plays a more important role to some degree. Moreover, the segmentally graded designs

benefits the radiative recombination process via the reduction of built-in field in active regions, as demonstrated in the inset of Fig. 3(h), which should be one of droop remedies accounting for the reduced efficiency droop presented in Fig. 2(b). The reduced built-in electrostatic field is related to the relaxed strain in MQWs, which confirms that the segmentally grading Al content in p-type region effectively helps to release accumulated strains.

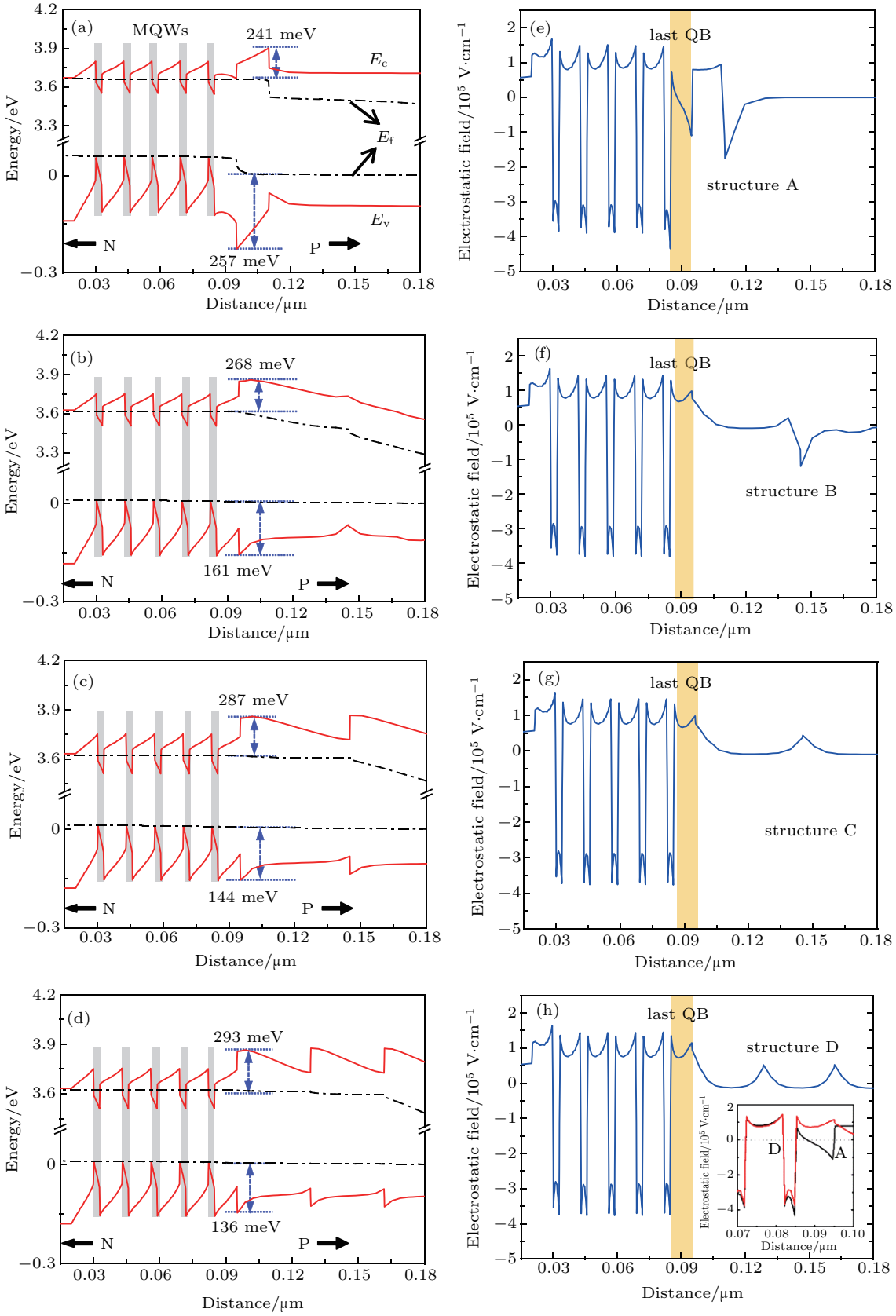


Fig. 3. (a)–(d) Energy band diagrams of UV-LEDs with different structures; (e)–(h) corresponding electrostatic field profiles. The inset in panel (h) is the enlarged electrostatic field distribution diagram within the last QW and QB of structure A and D.

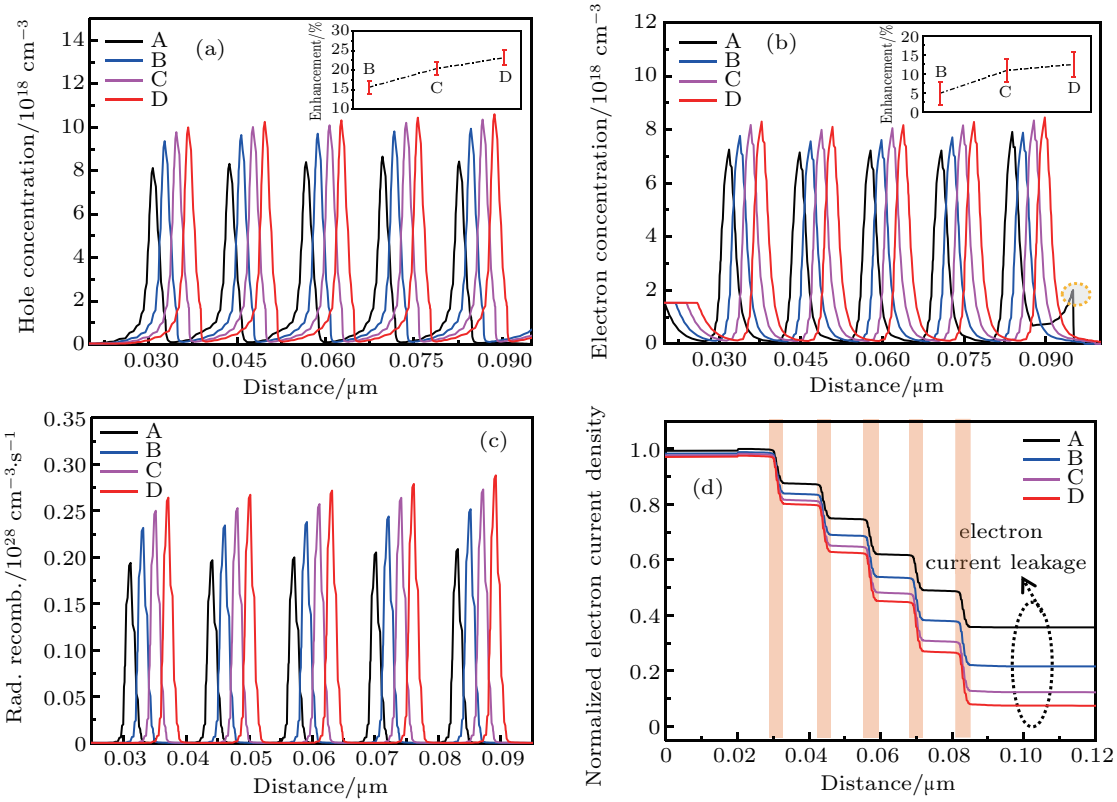


Fig. 4. Simulated distribution of electron (a), hole (b), and radiation recombination rate (c) for the four different UV-LEDs. (d) Normalized electron current density throughout the four structures at injection current of 180 mA.

The smoothed band structures and modified effective carrier barriers for proposed LED structures are verified by the carrier concentration variations in active regions. The hole and electron concentration distributions are presented in Figs. 4(a) and 4(b). Note that the horizontal position has been shifted slightly for better observation. By applying segmentally graded Al composition p-$Al_xGa_{1-x}N$, both hole and electron in the five MQWs are improved apparently. The enhancement of hole confinement is more remarkable, with average enhancement factors of 15.7%, 20.4%, and 23.2% for structure B, C, and D, compared to the hole concentration in the original structure. The average enhancement of electron concentration is 4.9%, 10.9%, and 12.5% for structure B, C, and D, respectively, as plotted in the insets of Figs. 4(a) and 4(b). These results are consistent with the above analysis of band structures. It is worth noting that for the original device, another electron concentration peak is observed in the last QB, as labeled in the dashed box in Fig. 4(b), which is in agreement with the electrostatic field profile and band bending effects at the last QB/EBL interface. However, no such peaks are observed out of active regions, both for electrons and holes in the other three structures, which should be ascribed to the tuned interfacial energy bands. Thanks to the enhanced hole concentration and electron confinement, the radiative recombination rate for proposed LED devices is improved significantly (Fig. 4(c)). Meanwhile, the recombination is only observed in the active regions, which demonstrates that the improvement of light output power results from the enhanced radiative recombination. The electron current overflowing to the p-type layers is defined as the electron leakage current. As shown in Fig. 4(d), the normalized electron current density in p-type region is reduced significantly for modified LED structures.

4. Conclusion

To relieve the contradiction between the degradation of UV-LED performances with large degree of Al content gradation polarized-doped p-type layer and the need of high Al composition EBL, segmentally graded Al content p-$Al_xGa_{1-x}N$ is applied and investigated in this work. By carefully analyzing the numerical results, we found that the IQE, LOP, electron current leakage, carrier concentrations, and radiative recombination rate in the MQWs are improved for modified structures compared to those of the conventional UV-LED with a stationary EBL layer. These improvements are attributed to the enhanced hole concentration and the engineered interface band structures, which obviously leads to increased effective electron blocking barrier and lowered hole injection barrier, as well as eliminated band bending within the LQB/p-type layer interface.

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