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Enhanced performance of AlGaN-based ultraviolet light-emitting diodes with linearly graded AlGaN inserting layer in electron blocking layer*

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The conventional stationary Al content AlGaN electron blocking layer (EBL) in ultraviolet light-emitting diode (UV LED) is optimized by employing a linearly graded AlGaN inserting layer which is 2.0 nm $Al_{0.3}Ga_{0.7}N$/5.0 nm $Al_xGa_{1-x}N$/8.0 nm $Al_{0.3}Ga_{0.7}N$ with decreasing value of x. The results indicate that the internal quantum efficiency is significantly improved and the efficiency droop is mitigated by using the proposed structure. These improvements are attributed to the increase of the effective barrier height for electrons and the reduction of the effective barrier height for holes, which result in an increased hole injection efficiency and a decreased electron leakage into the p-type region. In addition, the linearly graded AlGaN inserting layer can generate more holes in EBL due to the polarization-induced hole doping and a tunneling effect probably occurs to enhance the hole transportation to the active regions, which will be beneficial to the radiative recombination.

Keywords: ultraviolet light-emitting diode, electron blocking layer, internal quantum efficiency

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1. Introduction

The AlGaN-based ultraviolet light-emitting diodes (UV LEDs) have attracted great attention due to their wide applications, such as anti-counterfeiting recognition, air and water purification, chemical sensors, UV curing, and data storage.[1–3] In theory, the deep UV LEDs can be realized by increasing the aluminum composition in the quantum well. Nevertheless, the large activation energy of Mg in high Al content AlGaN layer and strong polarization induced electric field result in low hole concentration in the p-type AlGaN layer and serious electron leakage.[4] Consequently, the internal quantum efficiency (IQE) of the UV LEDs is far less than that of visible LEDs. In addition, the UV LEDs also face the problem of efficiency droop, the IQE of the UV LEDs obviously decreases at high current, which further restricts the commercial application of the UV LEDs. Some methods have been proposed to solve the above problems, such as adopting polarization-induced hole doping to enhance the hole concentration in p-type AlGaN,[5] designing a special electron blocking layer (EBL) to reduce electron leakage,[6–8] proposing special quantum well structures to depress the polarization effect in the active region.[9] In UV LEDs, a high Al content p-type AlGaN EBL is normally used to enhance the restriction of electrons and reduce electron leakage to the p-type layer.[10] However, it also creates a hole potential barrier in the valence band, which causes a low hole injection efficiency. On the other hand, the p-type AlGaN layer with high Al content is hardly realized due to the large activation energy of Mg, which also results in a low hole injection efficiency and a poor performance. Accordingly, researchers have put forward some new EBL structures to further improve the carrier injection, such as the polarization-reversed[11] or polarization-reduced[12] AlInGaN EBL, a gradually decreasing Al-content AlGaN EBL,[13] an inverted-V-shaped graded Al composition EBL,[14] and a p-AlInN/AlGaN superlattice EBL.[15] In this work, we numerically investigate and theoretically study the influence of a linearly graded AlGaN inserting layer in EBL on the performance of AlGaN-based UV LEDs. We find that the LED with the linearly graded AlGaN inserting layer in EBL shows markedly improved light output power and mitigated efficiency droop compared to that with the conventional stationary Al content AlGaN EBL. Further research shows that these improvements are attributed to the enhanced hole injection efficiency and the suppressed electron overflow simulta-

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neously due to the optimized energy band structure. In addition, the linearly graded AlGaN inserting layer can generate more holes in EBL due to the polarization-induced hole doping and a tunneling effect probably occurs to enhance the holes transportation to the active regions.

2. Structure and parameters

The original structure (sample A) consists of a 3 μm thick Si-doped $Al_{0.15}Ga_{0.85}N$ layer (2×10^{18} cm^{-3}), 5 periods of $In_{0.02}Ga_{0.98}N$ (3 nm)/$Al_{0.15}Ga_{.85}N$ (8 nm) multiple quantum wells (MQWs), a 15 nm p-type $Al_{0.3}Ga_{0.7}N$ EBL layer, a 100 nm p-type $Al_{0.15}Ga_{0.85}N$ layer (hole concentration of 1.0×10^{17} cm^{-3}), and then a 10 nm highly Mg-doped p-GaN contact layer. The proposed structures (samples B and C) consist of an identical structure to the original one except that a linearly graded $Al_xGa_{1-x}N$ layer is inserted in the p-type $Al_{0.3}Ga_{0.7}N$ EBL. Specifically, the EBLs of samples B and C are composed of a 2 nm $Al_{0.3}Ga_{0.7}N$/5 nm $Al_xGa_{1-x}N$/8 nm$Al_{0.3}Ga_{0.7}N$ structure. The Al composition in the $Al_xGa_{1-x}N$ layer of sample B is linearly decreased from 30% to 15%. The Al composition in the $Al_xGa_{1-x}N$ layer of sample C is linearly decreased from 30% to 5%. The structures of the three samples are shown in Fig. 1 in detail.

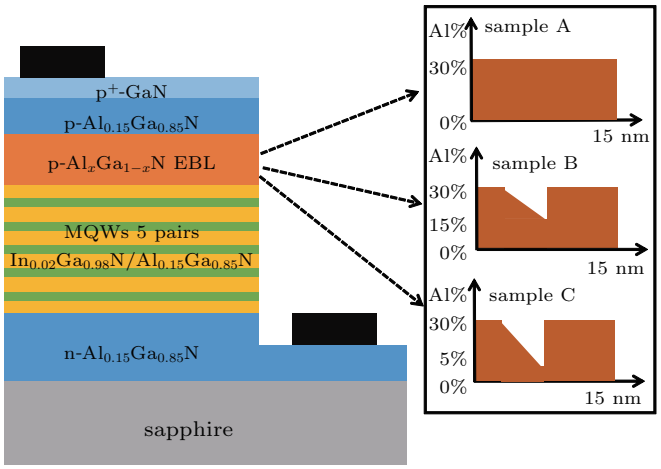


Fig. 1. Schematic diagram of UV LED structures with linearly graded AlGaN inserting layer in EBL.

In this paper, optical and electrical properties, band diagrams, radiative recombination efficiencies, electrostatic fields, and carrier concentrations of all UV LED structures are simulated by calculating the Schrödinger equation, Poisson's equation, the carrier transport equations, and the current continuity equation self-consistently with appropriate boundary conditions by using the advanced physical models of semiconductor devices (APSYS) numerical simulation program. The device geometry is designed into a rectangular shape of 300 μm×300 μm. In the carrier recombination model, the Shockley–Read–Hall (SRH) recombination lifetime in the active region is evaluated to be 5.0 ns and the internal loss is 1000 m^{-1}. The built-in interface polarization charges owing to the spontaneous and piezoelectric polarizations are calculated based on the methods proposed by Fiorentini *et al.*, and scaled down by a fit factor of 0.4 accounting for the partial compensation of them by fixed defects and other interface charges.[16] The Auger recombination coefficient is set to be 1×10^{-30} cm$^{-6}\cdot$s^{-1} and the operating temperature is set to be 300 K for simplification.[17] The band-offset ratio is supposed to be 0.7/0.3 for AlGaN materials.[18] More detailed descriptions of the model and material parameters applied in the simulation could be found in Ref. [19].

3. Results and discussion

The output power and IQE of the proposed structures are numerically investigated. As shown in Fig. 2(a), within the injection current range, the light output power of the three structures increases almost linearly with increasing injection current. However, the proposed UV LED structures with linearly graded AlGaN inserting layer in EBL exhibit clearly enhanced output compared to the original structure. Figure 2(b) shows the simulated results of IQE vs. injection current for the three samples. When the conventional stationary Al content AlGaN EBL is replaced by the proposed structures, the IQE of the UV LED increases significantly. At around 40 mA, the maximum IQEs of samples B and C increase to 37.4%, 52.4%, respectively. The IQEs of samples B and C increase by

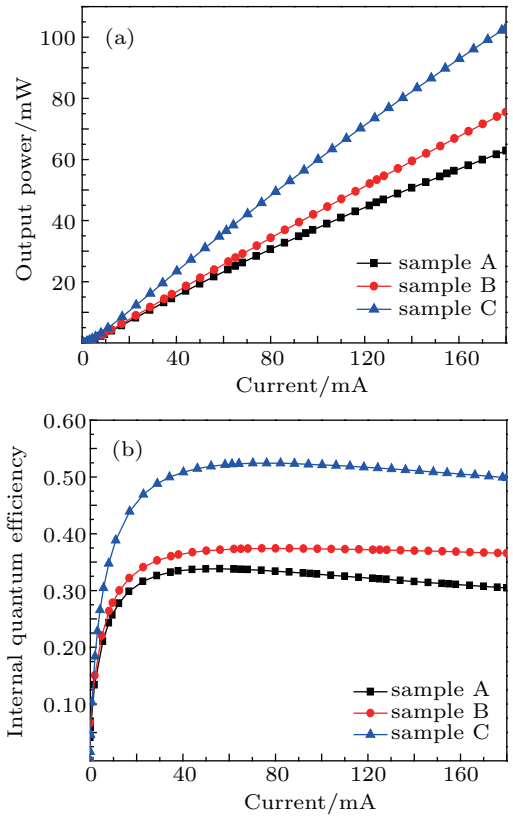


Fig. 2. (a) Light output power and (b) internal quantum efficiency as a function of injection current for the three samples.

10.6% and 55.0% compared with the maximum value of sample A (33.8%). Apart from that, we calculate the efficiency droop of sample C at the injecting current of 180 mA, and we find that the efficiency droop decreases from 9.8% (sample A) to 4.8% (sample C). All these data demonstrate the effectiveness of improving LED performances by adopting the linearly graded AlGaN inserting layer in EBL.

To clarify the mechanism of the above UV LEDs improvements, we have further studied the energy band diagrams and quasi-Fermi levels of the three samples, which are plotted in Fig. 3. From Fig. 3(a), it can be found that the band diagram of sample A severely bends both in the EBL and the last quantum barrier (LQB), which leads to the decreased ability of UV LEDs for electron restriction. However, the effective electron barrier heights of samples B and C are 270.8 meV and 306.9 meV, respectively, which are enhanced compared to that of sample A (264.8 meV). Since samples B and C have higher electron barrier heights, they can effectively restrict electrons and reduce the leakage of electrons to the p-type layer, and electrons are more fully compounded with holes in the MQWs region. On the other hand, it is noted that the effective hole barrier heights of sample B (260.7 meV) and sample C (258.4 meV) are lower than that of sample A (268.3 meV), indicating that holes in the p-type layer are more easily injected into the active region. In addition, the Al content in the inserting layer is linearly graded, which will realize a polarization-induced hole doping effect. This doping technology was first put forward by Simon *et al.*[20] to promote the generation of holes in AlGaN by polarization-induced effect. We believe that the linearly graded AlGaN inserting layer can generate more holes in EBL, which contributes to the radiative recombination. Therefore, samples B and C can not only enhance the ability of electronic restriction, but also generate more holes. At the same time, we also analyze the electron current density distributions versus distance at the MQWs of the three samples under 180 mA, which are plotted in Fig. 3(d). The electron leakage currents in the p-type layer of samples A, B, and C at 180 mA are 375 A/cm^2, 275 A/cm^2, and 40 A/cm^2, respectively. The electron leakages of samples B and C are lower than that of sample A due to the sufficient radiation recombination of the electrons and holes in the MQWs.

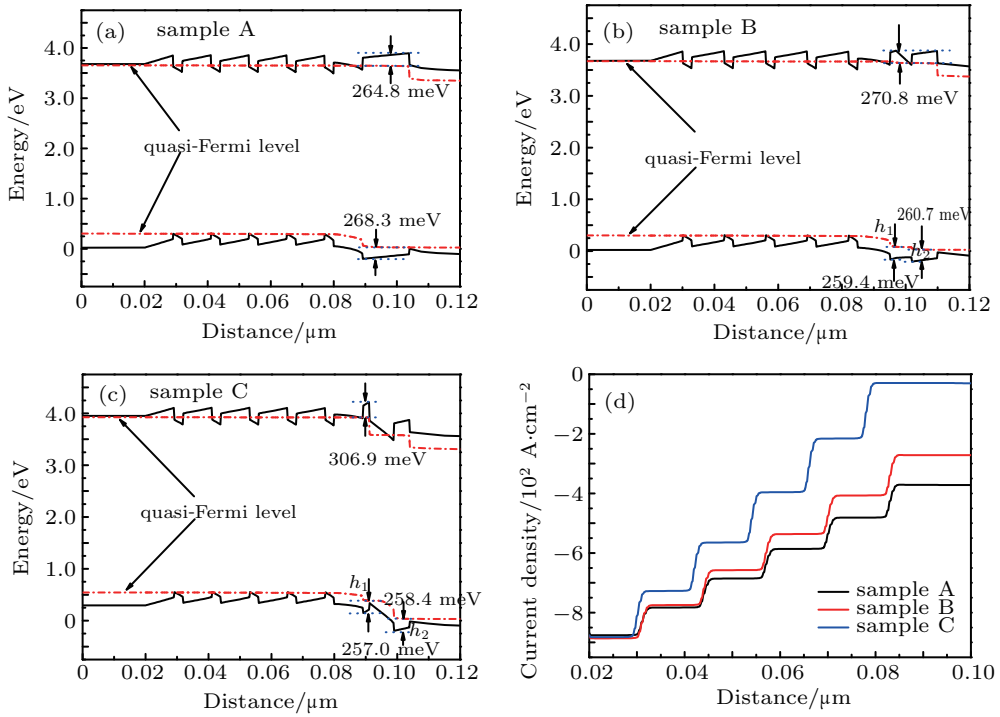


Fig. 3. (a)–(c) Energy band diagrams, quasi-Fermi levels, and (d) electron current density distributions at the injection current of 180 mA for the three samples.

The above energy band diagram analysis can be verified by the distributions of electrons and holes in the active region, which are plotted in Fig. 4. Note that the horizontal positions of samples B and C in Figs. 4(a) and 4(b) are shifted slightly for better analysis. According to Fig. 4(a), it can be found that the concentrations of electrons in the active regions of samples B and C are higher than that of sample A. And sample C has the highest electron concentration. At the same time, we can easily find that the changes of holes in the active regions of samples B and C are consistent with the changes of electrons. In addition, in our proposed structure, the thickness of the $Al_{0.3}Ga_{0.7}N$ layer between the last barrier of MQWs and the linearly graded AlGaN inserting layer is only 2.0 nm. Zhang *et al.*[21] managed to enhance

the hole injection efficiency via employing a p-$Al_{0.60}Ga_{0.40}N$ (2.0 nm)/$Al_{0.50}Ga_{0.50}N$ (3.0 nm)/p-$Al_{0.60}Ga_{0.40}N$ (5.0 nm) EBL structure, in which the very thin $Al_{0.50}Ga_{0.50}N$ layer was able to achieve a high local hole concentration, which was very effective in reducing the effective barrier height of the p-EBL for holes. More importantly, such a thin $Al_{0.60}Ga_{0.40}N$ (2.0 nm) layer between the last quantum barrier and the $Al_{0.50}Ga_{0.50}N$ layer in EBL can realize a strong intraband tunneling process for holes. As a result, it can obtain a more efficient hole injection into the quantum wells, leading to a remarkably improved optical power for the DUV LED. In our work, the tunneling effect probably occurs since the thickness of the $Al_{0.3}Ga_{0.7}N$ layer is only 2.0 nm between the last quantum barrier and the $Al_xGa_{1-x}N$ layer, which can enhance the hole transportation to the active region and be beneficial to the recombination of carriers in MQWs. Just as the analysis above, the improvements of electron and hole concentrations in MQWs are due to the adoption of the linearly graded AlGaN inserting layer in EBL, which enhances the capability of electron confinement and hole transportation to the active region of the UV LEDs simultaneously.

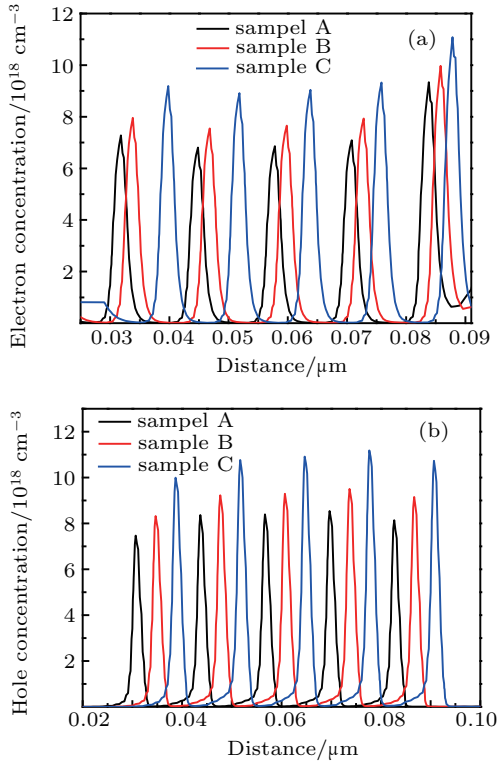


Fig. 4. Simulated distributions of (a) electron and (b) hole concentrations nearby MQWs of the three samples at 180 mA.

The radiative recombination rates and spontaneous emission rates of the three samples are studied, which are shown in Fig. 5. According to the above analyses, with the reduction of electron leakage and the enhancement of hole injection, more carriers in the active region contribute to the radiative recombination. As a result, the radiative recombination rates of samples B and C are higher than that of sample A. Sample C has the highest radiative recombination rate, which is an average enhancement of 68% compared with that of sample A. From Fig. 5(b), it is obvious that the spontaneous emission rates of samples B and C are higher than that of sample A, with estimated enhancement factors of 7% and 27%, respectively.

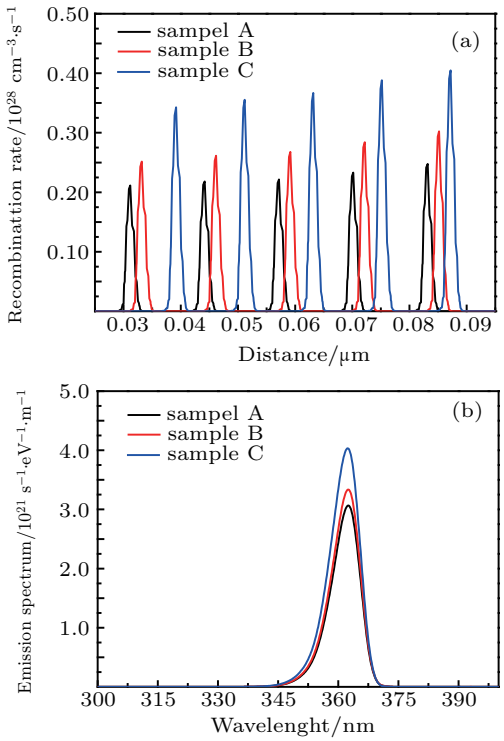


Fig. 5. (a) Radiative recombination rates distribution and (b) spontaneous emission spectrum for the three samples at 180 mA.

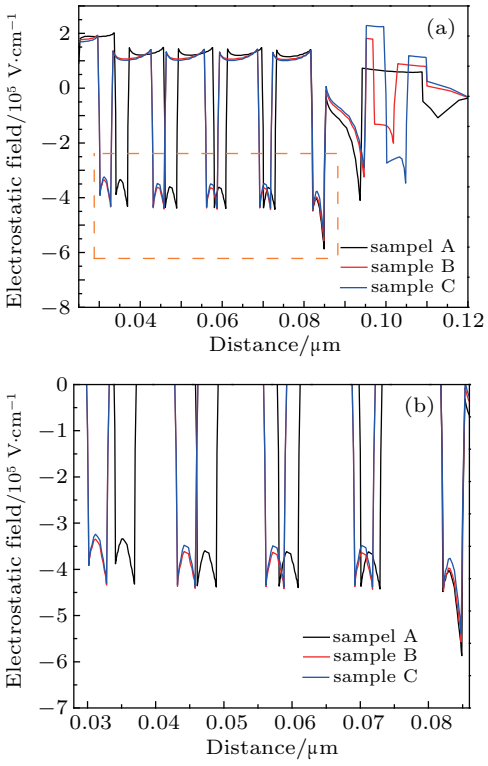


Fig. 6. (a) The electrostatic field distributions in LED structures of the three samples, (b) the electrostatic fields in the MQWs of the three samples at 180 mA.

In addition, the electrostatic fields of the three samples at 180 mA are shown in Fig. 6. It is found that the electrostatic fields in EBL (shown in Fig. 6(a)) are increased by using a linearly graded AlGaN inserting layer which can produce an extra polarization field. The large electrostatic fields contribute to form 2DHG, which can enhance the mobility of holes and improve the concentration of carriers (shown in Fig. 4). On the other hand, we also find that the electrostatic fields in the MQWs (shown in Fig. 6(b)) of samples B and C are obviously much smaller than that of sample A, which are beneficial to the overlap of electrons and holes wavefunctions and can also enhance the radiative recombination of electrons and holes in the MQWs (shown in Fig. 5). In a word, the results in these figures are consistent with the previous explanations.

According to a series of analyses about the light output power and internal quantum efficiency, the energy band diagrams, the distribution of carriers, and the radiative recombination rate of the three samples, it is believed that due to the application of the linearly graded AlGaN inserting layer in EBL, the effective potential barrier of electron is increased, the effective potential barrier of the hole is reduced, and more electrons and holes accumulate into the active region. In addition, the linearly graded AlGaN inserting layer can generate more holes in EBL due to the polarization-induced hole doping and a tunneling effect probably occurs to enhance the hole transportation to the active region because of the thin $Al_{0.3}Ga_{0.7}N$ barrier between last barrier of MQWs and the linearly graded AlGaN inserting layer.

4. Conclusion

To solve the problems of low quantum efficiency and efficiency droop in UV LEDs, we have proposed and numerically investigated the effects of the linearly graded AlGaN inserting layer in EBL. Through the careful analysis of the numerical results, it is found that the IQE, carrier concentrations, and radiative recombination rates in the MQWs are improved for the proposed structures compared to those of the original UV LEDs with conventional stationary Al content AlGaN EBL. These improvements are attributed to that the proposed structure can increase the effective barrier height for electrons and reduce the effective barrier height for holes, which obviously lead to the enhanced electron and hole concentrations in MQWs. At the same time, more holes can be generated by the polarization-doping in EBL and a tunneling effect probably occurs to enhance the hole transportation to the active regions, which will also contribute to the radiative recombination.

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