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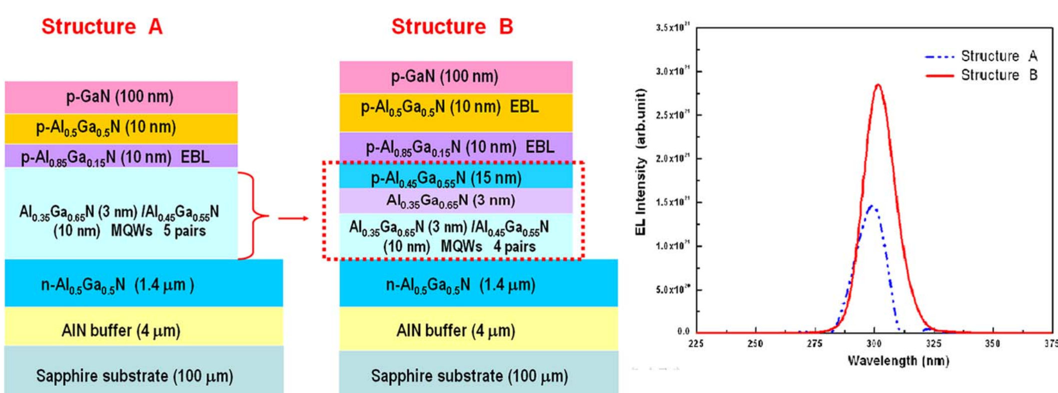

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Performance Improvements for AlGaN-Based Deep Ultraviolet Light-Emitting Diodes With the p-Type and Thickened Last Quantum Barrier

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Abstract: In order to improve the performance of AlGaN-based deep ultraviolet light-emitting diodes (UV LEDs), the optical and physical properties of AlGaN-based deep UV LEDs with a p-type and thickened last quantum barrier (LQB) are studied numerically. The output power–current performance curves, internal quantum efficiency, electroluminescence intensity, energy band diagrams, distributions of carrier concentrations, and the radiative recombination rates in the active region are investigated by Advance Physical Model of Semiconductor Devices (APSYS) software. The results reveal that, compared with the conventional one, the AlGaN-based deep UV LED with a p-type and thickened LQB achieves a remarkable improvement in performance, which is mainly attributed to the enhancement of hole injection and electron confinement.

Index Terms: Deep UV LED, last quantum barrier, p-type, thickening, improvement.

1. Introduction

It is well known that III-nitride light-emitting diodes (LEDs) have a wide range of applications in areas such as solid-state lighting, full color display, medical treatment, and back lighting, due to their energy-saving capacity, small size, high efficiency, and long lifetime [1]–[5]. Particularly, with the development of technology in recent years, deep ultraviolet light-emitting diodes (UV LEDs) based on high Al content AlGaN materials have attracted considerable attention, because ultraviolet (UV) LEDs are considered to be the pumping source for procuring white-light emission with high color rendering index, which is thought to play a role in the general illumination one day [6], [7]. In addition, deep UV LEDs also show many other potential applications such as UV sensing, air and water purification [8], curing [9], medical treatment, biochemical detection, and optical data storage [10]. However, although it really seems that there are tremendous opportunities for AlGaN-based deep UV LEDs, some challenging issues in technology still remain for AlGaN-based deep UV LEDs, especially the relatively low internal quantum efficiency (IQE) and emission power [11], [12]. Many causes have been proposed as being responsible for the relatively low IQE and emission power, such as the high dislocation density in AlGaN materials [13], [14], the spontaneous and piezoelectric polarizations [15], carrier delocalization [16], and Auger recombination [17], [18]. Among the various causes, it is widely regarded that the strong electron leakage and poor hole injection efficiency may play an important role, owing to the large imbalance in electron and hole injection in AlGaN-based deep UV LEDs [19]–[23].

To date, some methods have been suggested to resolve the issues, mainly aimed at improving the internal quantum efficiency (IQE) and emission power for AlGaN-based deep UV LEDs. For example, Hirayama *et al.* [24] reported that the efficiency of AlGaN-based deep-ultraviolet LEDs could be improved significantly by using a multi-quantum-barrier electron blocking layer (EBL). Li *et al.* [25] enhanced hole injection and suppressed electron overflow out of the active region by employing a graded-composition electron blocking layer (EBL) for 310 nm AlGaN LEDs. Yan *et al.* [26] proposed $Al_xGa_{1-x}N$-$Al_yGa_{1-y}N$-$Al_xGa_{1-x}N$ $(y < x)$ complex barriers in the active region of AlGaN-based UV-LEDs to enhance hole injection. Zhang *et al.* [27] proposed inserting an AlN layer between the active region and p-type hole-injection layer, which would suppress the escape of electrons out of the active region and improve the output power of the device. In general, on the basis of previous research, we can find in order to improve the performance of AlGaN-based deep UV LEDs, much attention has been paid to the EBL and the multiple quantum wells (MQWs, the active region). Besides, the multiple methods used can be summarized as the energy band engineering, which improves electrical and optical properties of AlGaN-based UV LEDs through optimizing the band structure of the active region.

In fact, when it comes to InGaN-based LEDs, the energy band engineering has been studied and experimentally demonstrated fully. Zhao *et al.* [28] investigated the approaches based on quantum well structures with large overlap design to enhance the internal quantum efficiency (IQE) for InGaN-based QWs LEDs. Thin AlInN barriers was proposed to be employed in InGaN QWs to suppress the efficiency-droop phenomenon significantly [29]. G. Lin *et al.* pointed that thin quantum barriers (QBs) could provide an efficient and practical way for enhancing efficiency performance of InGaN/GaN LEDs [30]. Meanwhile, it was found that p-doping in the barriers of InGaN/GaN MQWs could enhance photoluminescence intensity, thermal stability and internal quantum efficiency of InGaN-based LEDs [31]. Lei *et al.* [32] found an increased p-doping concentration in the last barrier (LB) in multiple quantum wells (MQWs) could enhance the output power and could improve the efficiency droop behavior of GaN-based blue LEDs, and after blue InGaN/GaN MQW LEDs with varying thickness and p-doping concentration for the LB was numerically investigated, the conclusion that thin LB was more beneficial to improving the performance at low p-doping concentration while at high p-doping concentration, thick LB was much better was made by Xia *et al.* [33]. Actually, as we all know, carriers tend to accumulate in the last quantum wells (QW) next to the p-type layer, since it is more difficult to inject holes from p-type layer into quantum wells (QWs), which results in the dominant role of the last quantum well in the radiative recombination [34], [35]. In the meantime, it also means the last barrier (LB) in MQWs plays a significant role in the hole transport of this kind of devices, including AlGaN-based deep UV LEDs. Hence, it is supposed that the p-doping concentration and the thickness of the last quantum barrier (LQB) have an effect on the energy band structure of the active region for GaN-based LEDs. Furthermore, even though the method of energy band engineering has been used in AlGaN-based MQW deep UV LEDs, little attention has been paid to the thickness and p-doping concentration of the last quantum barrier (LQB).

Therefore, in this study, we focus on the last quantum barrier (LQB) of AlGaN-based deep UV LEDs. After research and analysis, we propose a new structure with p-type and thickened last quantum barrier (LQB) for AlGaN-based deep UV LEDs to improve the performance. The optical and electrical properties of the conventional structure and the proposed structure for AlGaN-based deep UV LEDs are investigated numerically in detail with the Advance Physical Model of Semiconductor Devices (APSYS) simulation program developed by Crosslight Software, Inc. It should be noted that it is still challenging to obtain a highly conductive p-type $Al_xGa_{1-x}N$ layer with high Al content experimentally until now, due to the larger acceptor ionization energy and lower formation energy of compensation defects in the AlGaN materials with higher Al content

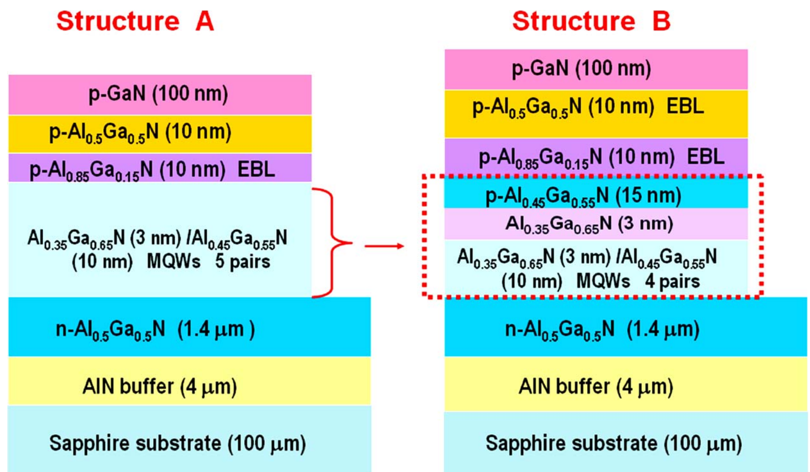

Fig. 1. Schematic diagrams of structure A and structure B in the study.

[36]–[39]. However, much effort has been devoted to increasing the concentration of hole carriers in p-type AlGaN materials in theory and experiment [40]–[42], and p-type AlGaN materials with relatively high Al content has been employed in many photoelectron devices [44]–[47], especially deep UV LEDs [48]–[52]. Thus, for making the proposed structure possible in reality, we have chosen the AlGaN-based deep MQW UV LED emitting at around 300 nm to simulate, since the wavelength is just in deep UV region and compared with other AlGaN-based deep UV LEDs, the Al content in AlGaN materials and the concentration of hole carriers required are relatively low when emitting wavelength is just around 300 nm.

2. Model and Parameters

As shown in Fig. 1, the conventional AlGaN-based deep UV LED used as reference in the simulation is labeled as structure A, which is designed to be grown on a c-plane sapphire substrate, followed by a 4-μm-thick undoped AlN buffer layer and a 1.4-μm-thick n-doped $Al_{0.5}Ga_{0.5}N$ layer (n-doping $= 5 \times 10^{18}$ cm^{-3}). The active region consists of five 3-nm thick $Al_{0.35}Ga_{0.65}N$ QWs separated by six 10-nm-thick $Al_{0.45}Ga_{0.55}N$ barriers. A 10-nm-thick p-type $Al_{0.85}Ga_{0.15}N$ EBL (p-doping $= 5 \times 10^{17}$ cm^{-3}) is grown on the top of the active region, followed by a 10-nm-thick p-type $Al_{0.5}Ga_{0.5}N$ (p-doping $= 5 \times 10^{17}$ cm^{-3}) and a 100-nm-thick p-type GaN layer (p-doping $=$ 2×10^{18} cm^{-3}) for making contact. The proposed structure for AlGaN-based deep UV LEDs is labeled as structure B, which is very similar to structure A from the overall, except the last quantum barrier (LQB) of the active region. To be specific, in structure B, the last quantum barrier (LQB) of the active region is p-type doped (p-doping $= 5 \times 10^{17}$ cm^{-3}) and the thickness of the last quantum barrier (LQB) is increased from 10 nm to 15 nm.

In the simulation, the device geometry is designed as a rectangular shape of 300×300 um^2. The Shockley-Read-Hall (SRH) recombination time is set to be 1.5 ns, and the internal loss is 2000 m^{-1} [53]. The surface fixed interface charge densities are calculated from the method proposed by Fiorentini *et al.* [54]. Taking the screening by defects into account, the surface charges densities are set to be 40% of the calculated values [55]. As the experiment described, the Auger recombination coefficient is set to be 1×10^{30} cm^6/s [56]. The band-offset ratio is assumed to be 0.7/0.3 for AlGaN materials [57] and the device operating temperature is assumed to be 300 K [58]. Most of the parameters in this paper are the same as those in [59]. The other material parameters of the devices used in the simulations can be found in [60].

3. Results and Discussions

To compare the performance of the two deep UV LED structures, we describe the optical power, the internal quantum efficiency (IQE), and the electroluminescence intensity (EL) of the

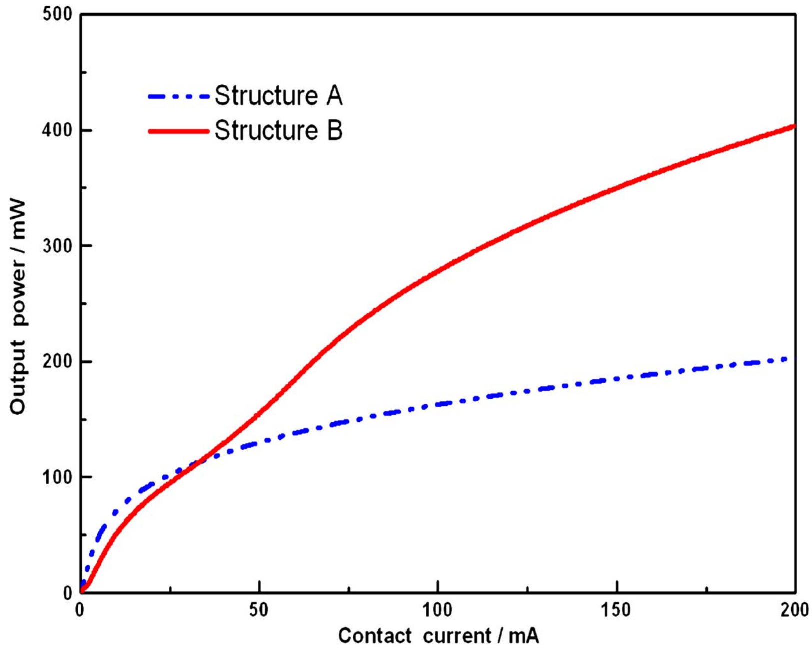

Fig. 2. Light output power as a function of current for structure A and structure B in the study.

structures A and B, hoping to probe into the advantages of AlGaN-based deep UV LEDs with p-type and thickened last quantum barrier (LQB) in depth.

Fig. 2 presents the curves of the light output power versus the increasing injection current for structures A and B. It can be clearly seen that the light output power of the two structures both increase with the increasing current. However, in comparison with structure A, the light output power of structure B is significantly higher. Moreover, the increase is more obvious when the injection current get higher. When the injection current rises to 200 mA, the light output power of structure A is just about 202 mW, while that of structure B rises to 404 mW, which means the light output power of structure B is twice as high as that of structure A at the current of 200 mA, from which it seems to be very useful to improve the light output power at a high injection current by p-type doping and thickening the last quantum barrier (LQB) of the active region for AlGaN-based deep UV LEDs.

The plots of IQE as a function of the injection current for the structure A and B are shown in Fig. 3. Obviously, as the forward current increases, structure A exhibits an efficiency droop behavior in the IQE. Only when the injection current is just about 2.5 mA has the IQE of structure A reached 80% that is the maximum value. Then, it drops rapidly as the current increases. Finally, when the current rises to 100 mA, the IQE drops down to nearly 11%, which is too low to work for UV LEDs. As to structure B, though it shows a similar behavior in terms of the IQE, the situation seems totally distinct from structure A. When the injection current is up to about 8 mA, the IQE of structure B reaches the maximum value 81% that is a little greater than that of structure A. Most importantly, after the current exceeds 8 mA, the IQE of structure B decreases more slowly than that of structure A all the time and even keeps the value of IQE approximately above 30% at the current of 100 mA. Correspondingly, in the whole range of current from 0 mA to 200 mA, the efficiency droop of structure A is drastically more grave than that of structure B. It is clear that compared with structure A, structure B not only has a little higher maximum IQE, but also presents much lower efficiency droop. Thus, for AlGaN based deep UV LEDs, it is wise to adopt a p-type and thickened LQB to alleviate the efficiency droop behavior and to increase the value of IQE.

Fig. 4 shows the electroluminescence (EL) spectra of the two structures at injection current of 200 mA. From it, we can find the peak wavelengths of the two AlGaN-based LEDs are both

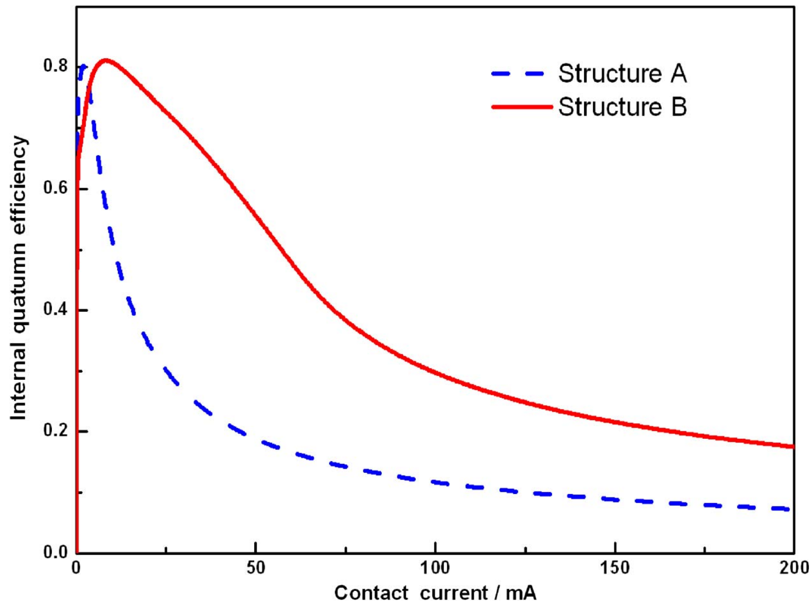

Fig. 3. IQE as a function of current for structure A and structure B in the study.

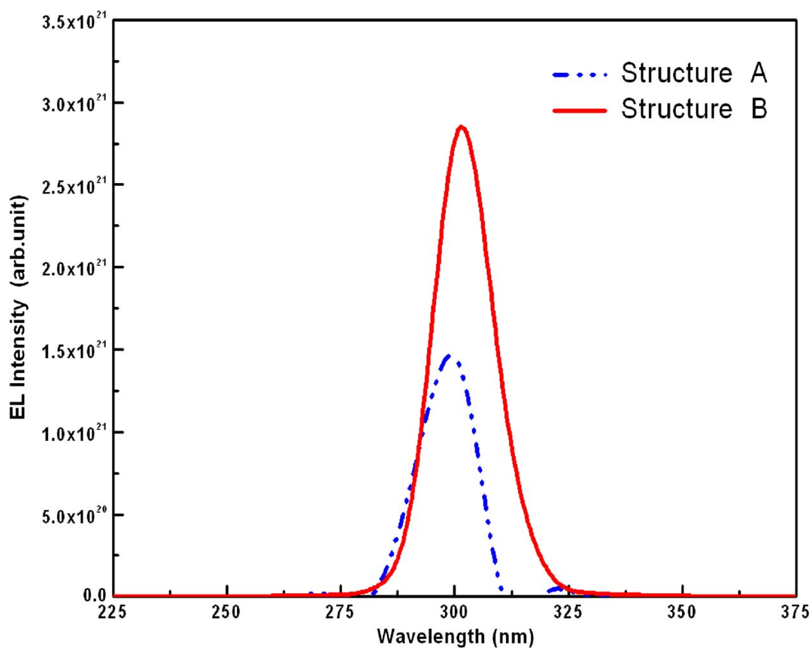

Fig. 4. Electroluminescence (EL) spectra of structure A and structure B at injection current 200 mA in the study.

around 300 nm, indicating the light produced by the two structures lies in deep UV region indeed. Nevertheless, in contrast with structure A, the peak wavelength of structure B is slightly shifted by 1–2 nm, which can be mainly attributed to a slight change of energy band gap in the active region of LED caused by the influence of p-type and thickened LQB. Besides, as shown in Fig. 4, the EL intensity of structure B is almost as twice as that of structure A, which means that for an AlGaN-based UV LED, if the LQB is p-type doped and thickened, the luminescent intensity will be enhanced to some degree.

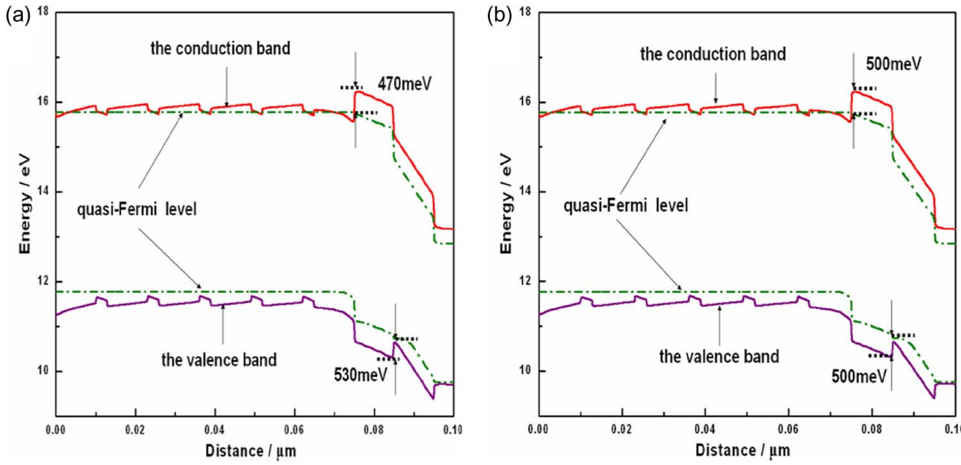

Fig. 5. Calculated energy band diagrams of a structure A (a) and structure B (b) at 200 mA forward current.

Based on the descriptions of the optical power, the internal quantum efficiency (IQE) and the electroluminescence intensity (EL) of structures A and B above, as for AlGaN-based deep UV LEDs, the performance of structure B (the structure with p-type and thickened LQB) is more excellent than structure A (the conventional structure). However, the mechanism in it seems a little puzzling. Then in order to shed light on the mechanism as much as possible, we investigate the energy band diagrams, the electrostatic fields, carrier concentrations, and radiative recombination rates in the active region of the structures A and B further.

Fig. 5 shows the energy band diagrams and quasi-Fermi levels for structures A and B at injection current of 200 mA. As we all know, for conventional UV LEDs, because of the lattice mismatch, the piezoelectric and spontaneous polarization fields will pull down the energy band at the interface of the last quantum barrier (LQB) and the electron blocking layer (EBL) [61]. In addition, due to the bending of quantum wells in the conduction band and valence band, the electron wave function and the hole wave function are separated seriously. As a result, it is more difficult to confine electrons in the active region and to inject holes into the active region so as to achieve recombination luminescence. As depicted in Fig. 5(a) and (b), the band profiles of structure A (the conventional structure) and structure B (the structure with p-type and thickened LQB) for AlGaN-based UV LEDs are presented as mentioned above. However, from Fig. 5(a) and (b), we can find that the effective potential heights for electrons in the conduction band of structures A and B are 470 meV and 500 meV, respectively. It reflects p-type doping and thickening the LQB can increase the effective electron potential height and then enhance the electron confinement and suppress electron overflow more effectively. At the same time, as demonstrated in Fig. 5(a) and (b), the effective potential height for holes in valence band reduces from 530 meV to 500 meV by adopting the p-type and thickened LQB. Accordingly, except the enhancement of the electron confinement, compared with structure A (the conventional structure), structure B (the structure with p-type and thickened LQB) is helpful for hole transportation into the active region with lower effective potential height for holes.

The electrostatic fields in the active region of the two structures for AlGaN-based UV LEDs are shown in Fig. 6. As depicted in Fig. 6, the electrostatic fields of the LQB and the EBL in structure B are remarkably smaller than that of structure A. It is worthy to note that a stronger electrostatic field in the active region will lead to the bending band and poor overlap of electron and hole wave functions. Especially, the band tends to bend downward at the interface of the LQB and the EBL, due to the big electrostatic field caused by the big spontaneous polarization and piezoelectric polarization. As a result, radiative recombination rates will be reduced and the performance of the structure will be influenced remarkably as well. Therefore, from Fig. 6, we can confirm that structure B (the structure with p-type and thickened LQB) for AlGaN-based UV

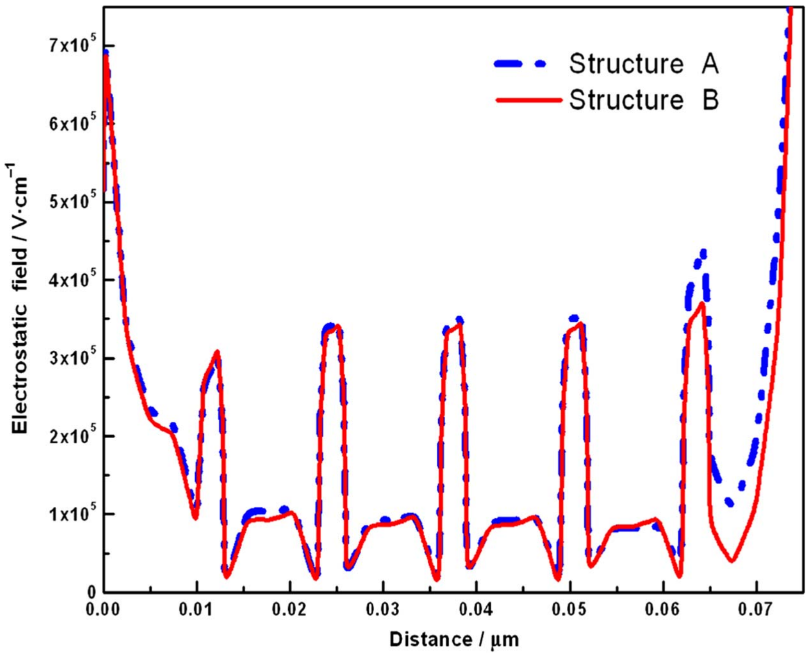

Fig. 6. Simulated electrostatic fields of structure A and structure B at injection current 200 mA in the study.

LEDs will have an advantage over structure A (the conventional structure) in performance, since the electrostatic fields of the LQB and the EBL in structure B are significantly smaller.

Fig. 7 shows the profiles of carrier concentrations in the active region at injection current of 200 mA for the two structures. As shown in Fig. 7(a), the distributions of holes in the quantum wells for the two structures seem to be uniform on the whole. But the hole concentrations of the quantum wells in structure B are noticeably higher than that in structure A, which can be ascribed to the mitigated band bending at the interface of the LQB and the EBL. And then, the p-type LQB can also act as a hole injection layer, which can increase the hole-injection efficiency. As demonstrated in Fig. 7(b), the electron concentrations of structure B are higher in most parts of multiple quantum wells. Whereas the electron concentrations of structure B in the last quantum barrier are abruptly lower than that of structure A. It indicates that the electron leakage in the active region of AlGaN-based deep UV LEDs has been decreased markedly by p-type and thickened LQB on account of the more efficient confinement of electrons.

According to a series of analysis about the energy band diagrams, the electrostatic fields and carrier concentrations of structures A and B above, it is believed that due to the change of effective potential barriers and the reduced electrostatic field, more electrons and holes survive and accumulate in the active region of structure B, which will contribute to the radiative recombination directly. The radiative recombination rates of the two structures are plotted in Fig. 8. It can be seen that compared with structure A, the radiative recombination rates in the active region of structure B keep distinctly higher all the time, which is in accordance with the conclusions of other analysis, and it is further proof that structure B (the structure with p-type and thickened LQB) is superior to structure A (the conventional structure) on the whole, indicating that it is effective to p-type dope and thicken the last quantum barrier (LQB) in the active region for improving performance of conventional AlGaN-based deep UV LEDs.

4. Conclusion

In summary, we have numerically investigated the performance of AlGaN-based deep UV LEDs with the p-type and thickened last quantum barrier (LQB). The results show that the structure with the p-type and thickened last quantum barrier has a great advantage in improving the device

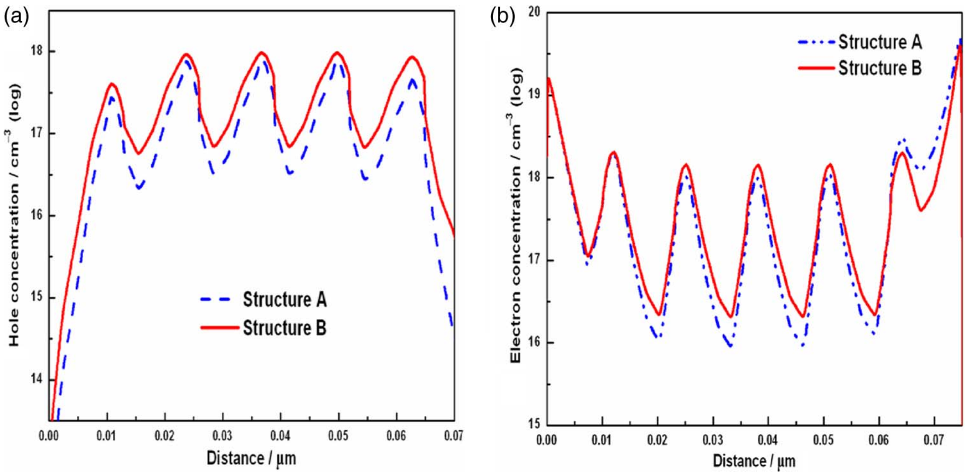

Fig. 7. Distributions of (a) hole concentrations and (b) electron concentrations of structure A and structure B at injection current of 200 mA.

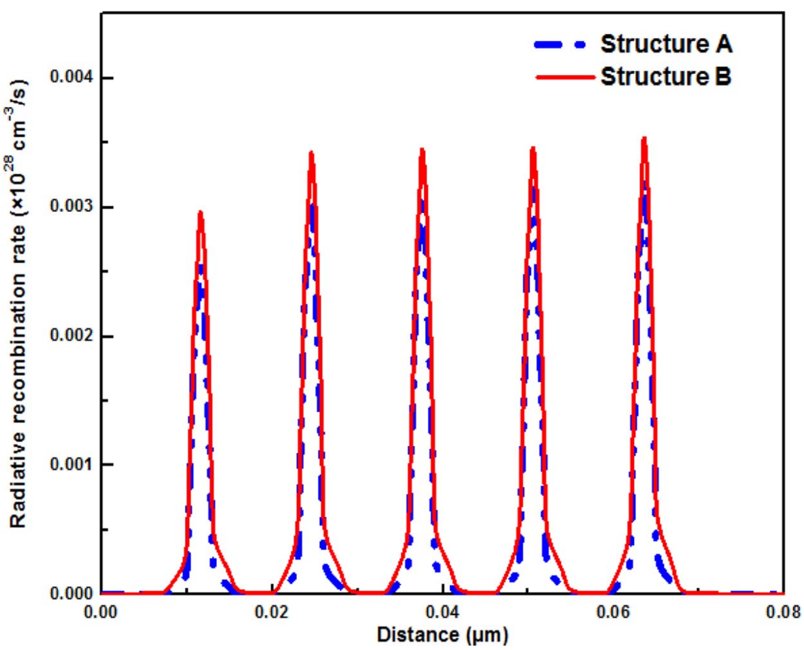

Fig. 8. Radiative recombination rates in the active region of structures A and B at injection current of 200 mA.

performance, including internal quantum efficiency (IQE), output power-current performance curves, and electroluminescence intensity (EL). Considering the analysis of the energy band diagrams, the electrostatic fields in the active region, the profiles of carrier concentrations and the radiative recombination rates in the active region, the significant improvements of the proposed structure can be attributed to the increase of effective potential height for electrons and the reduction of effective potential height for holes. Moreover, p-type doping and thickening the last quantum barrier (LQB) for AlGaN-based deep UV LEDs will lead to the obvious reduction of electrostatic field around the regions of the LQB and the EBL, resulting in more efficient electron blocking, lower electron leakage and improved hole injection. Therefore, in a conclusion, the adoption of p-type and thickened LQB in the structure of AlGaN-based deep UV LEDs is reasonable and promising. Although it is still challenging to obtain p-type AlGaN materials with high Al content in experiment currently, the proposed structure in the paper provides a new method of achieving high efficient AlGaN-based deep UV LEDs indeed, and we hope the results will motivate further research in the area of deep UV LEDs.

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