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Suppression of electron and hole overflow in GaN-based near-ultraviolet laser diodes*

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In order to suppress the electron leakage to p-type region of near-ultraviolet GaN/$In_xGa_{1-x}N$/GaN multiple-quantum-well (MQW) laser diode (LD), the Al composition of inserted p-type $Al_xGa_{1-x}N$ electron blocking layer (EBL) is optimized in an effective way, but which could only partially enhance the performance of LD. Here, due to the relatively shallow GaN/$In_{0.04}Ga_{0.96}N$/GaN quantum well, the hole leakage to n-type region is considered in the ultraviolet LD. To reduce the hole leakage, a 10-nm n-type $Al_xGa_{1-x}N$ hole blocking layer (HBL) is inserted between n-type waveguide and the first quantum barrier, and the effect of Al composition of $Al_xGa_{1-x}N$ HBL on LD performance is studied. Numerical simulations by the LASTIP reveal that when an appropriate Al composition of $Al_xGa_{1-x}N$ HBL is chosen, both electron leakage and hole leakage can be reduced dramatically, leading to a lower threshold current and higher output power of LD.

Keywords: GaN-based ultraviolet LD, electron and hole leakage

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1. Introduction

Recently, the GaN-based ultraviolet laser diodes have attracted much attention due to their massive potential applications in high-density optical storage technology, chemical analysis, photolithography, bio-agent detection and sterilization, which can create great interest.[1–5] Compared with GaN-based green or blue LDs, near-ultraviolet LDs have shallower quantum wells, resulting in more electrons leaking to p-type region[6,7] even some holes leaking to n-type region. It is known that the problem of electron leakage current has a considerable influence on the optical performance of III-nitride laser diode. Therefore, a large number of proposals have been given to reduce the electron leakage by inserting an electron blocking layer (EBL), including optimizing the thickness and composition of $Al_xGa_{1-x}N$ EBL,[8] adding tapered EBL[9] and step graded Al composition EBL,[10,11] p-$Al_xIn_yGa_{1-x-y}N$/GaN superlattice structure EBL,[12] $Al_xGa_{1-x}N$/GaN multi-quantum barriers (MQBs) EBL,[13] $Al_xIn_yGa_{1-x-y}N$ EBL,[14] etc.

However, there are limited studies of hole transport in near-ultraviolet LD.[15] For blue LD, it is reported that it suffers low hole injection efficiency because of inefficient Mg doping in wide band-gap nitrides.[9] Meanwhile, after inserting $Al_xGa_{1-x}N$ EBL, the valence band offset at the interface will form a barrier to block the transport of holes. However, according to the study of Cheng *et al.*,[16] holes can overflow from the green double quantum well (DQW) at high current density, which reduces carrier injection efficiency of *c*-plane $In_xGa_{1-x}N$-based green LD. For the near-ultraviolet LDs, the QWs are too shallow, and holes are easier to overflow from the DQWs. To improve the performance of near-ultraviolet LD, it is necessary to investigate the properties of hole transport.

In this study, the Al composition of $Al_xGa_{1-x}N$ EBL is optimized to better suppress the large electron leakage. Specifically, an additional $Al_xGa_{1-x}N$ hole blocking layer (HBL) is inserted between n-type waveguide and the first quantum barrier to reduce the hole leakage current effectively. The optical and electrical characteristics of LDs are theoretically simulated by the software LASTIP. Based on these numerical data, it is found that by using a 20-nm $Al_{0.27}Ga_{0.73}N$ EBL and inserting a 10-nm $Al_{0.23}Ga_{0.77}N$ HBL, the electron and hole leakage current can be reduced tremendously. As a result, the

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threshold current density and output power of newly-designed LD are improved.

2. Device structure and numerical simulation

The original LD structure used in our simulations is shown in Fig. 1, which, in accordance with the order of growth, is composed of a 1-μm Si-doped n-type GaN substrate with a doping concentration of 3×10^{18} cm^{-3}, a 1-μm Si-doped n-type $Al_{0.08}Ga_{0.92}N$ cladding layer with a doping concentration of 3×10^{18} cm^{-3}, a 0.12-μm Si-doped n-type GaN lower waveguide with a doping concentration of 5×10^{17} cm^{-3}, a two-period unintentionally-doped 2.5-nm $In_{0.04}Ga_{0.96}N$/14-nm GaN MQW active region, a 0.1-μm unintentionally-doped GaN layer, a 20-nm Mg-doped p-type $Al_{0.2}Ga_{0.8}N$ EBL with a doping concentration of 5×10^{19} cm^{-3}, a 0.6-μm Mg-doped p-type $Al_{0.08}Ga_{0.92}N$ cladding layer with a doping concentration of 2×10^{19} cm^{-3}, a 0.04-μm Mg-doped p-type GaN contacting layer with a doping concentration of 2×10^{20} cm^{-3}. There are two series of new LD structures that are studied in our calculations. The series one is similar to the original structure of $Al_xGa_{1-x}N$ EBL with different Al compositions, changing from 0.2 to 0.3. Based on the optimal results of series I, in series II, a 10-nm Si-doped n-type $Al_xGa_{1-x}N$ HBL is inserted between n-type waveguide and the first quantum barrier, and the Al composition is varied from 0.15 to 0.25.

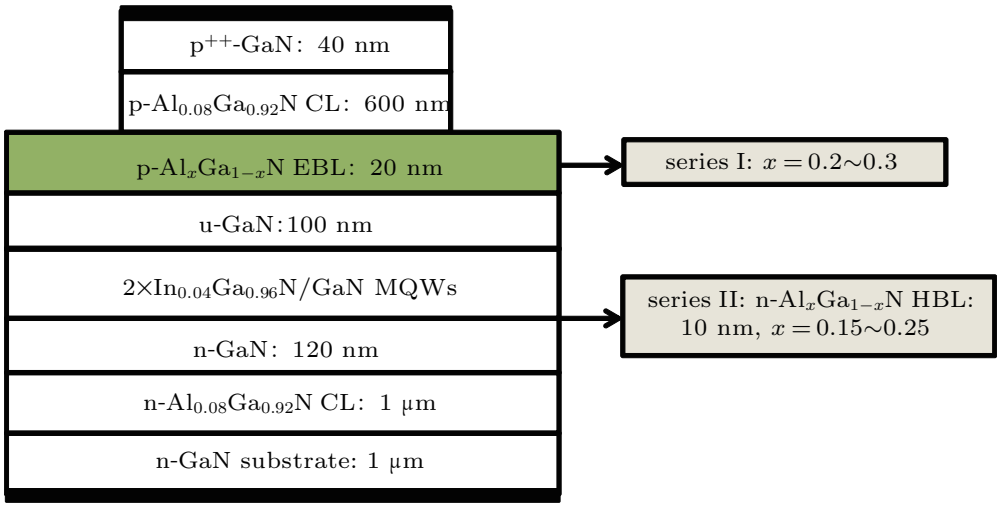


Fig. 1. (color online) Schematic diagrams of LD structures in series I and II. CL: cladding layer.

Here, the two-dimensional (2D) simulator LASTIP (crosslight Software Inc.) is employed to calculate the optical and electrical characteristics, in which the Poisson's equation and the current continuity equations are self consistently solved to obtain the states of QW levels and the carrier distributions at a specific bias voltage.[17] Meanwhile, the built-in polarization, including spontaneous and piezoelectric polarization, is considered in this software as well. In our simulations, the n-type and p-type electrodes are all set to be ideal ohmic contacts. The cavity length and the ridge width of these LDs are 600 μm and 3 μm, respectively. Considering partial compensation for the built-in polarization by charged defects, the screening factor is set to be 0.25, and the band offset ratio ($\Delta E_c/\Delta E_g$) of GaN/$In_xGa_{1-x}N$ heterojunction is 0.67. In addition, the activation energy of Mg acceptor in $Al_xGa_{1-x}N$ is regarded as 170 meV, which is supposed to increase 3 meV along with the addition of 1% Al composition of $Al_xGa_{1-x}N$ material. The absorption coefficients of n-type layers are taken to be approximately 5 cm^{-1}, and the absorption coefficients of all p-type layers are assumed to be 50 cm^{-1} except the one of the most heavily Mg-doped GaN contacting layer which is set to be 100 cm^{-1}. The refractive indexes of $In_xGa_{1-x}N$ and $Al_xGa_{1-x}N$ for $\lambda = 370$ nm are cited from Ref. [18].

3. Results and discussion

3.1. $Al_xGa_{1-x}N$ EBL

Figure 2(a) shows calculated *P–I–V* curves for different Al compositions of $Al_xGa_{1-x}N$ EBL. As the barrier height of EBL increases with Al composition increasing, it is easy to understand why the values of turn-on voltage and resistance of these samples become larger along with increasing Al composition of $Al_xGa_{1-x}N$ EBL. The *P–I* curves in Fig. 2(b) demonstrate that when the Al composition of $Al_xGa_{1-x}N$ EBL is less than 0.2, the threshold current is as large as 78.4 mA, and then it decreases sharply when the Al composition of $Al_xGa_{1-x}N$ EBL increases from 0.2 to 0.25. Finally, it increases again when the Al composition of $Al_xGa_{1-x}N$ EBL is higher than 0.25. At the same time, the output power under a fixed 120-mA injected current condition changes in a similar trend. The highest output power, 65.3 mW, and the lowest threshold current, 72.9 mA, are obtained simultaneously when the Al composition of $Al_xGa_{1-x}N$ EBL is 0.25. The reason for this phe-

nomenon will be explained in the following paragraph.

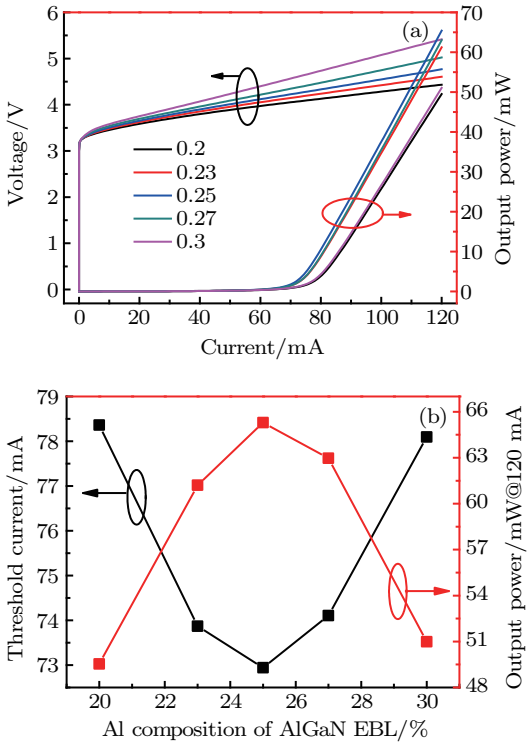


Fig. 2. (color online) (a) Curves of voltage and output power versus current injection of ultraviolet LDs with different Al compositions of $Al_xGa_{1-x}N$ EBL; (b) curves of threshold current (black line) and output power (red line) versus Al composition of $Al_xGa_{1-x}N$ EBL at a fixed current of 120 mA when the Al composition of $Al_xGa_{1-x}N$ EBL varies from 0.2 to 0.3.

Figure 3(a) shows the profiles of vertical electron current density near the active region at 120 mA. It can be seen that the electron current density decreases apparently with Al composition of EBL changing from 0.2 to 0.27. Figure 3(b) shows the plots of the percentage of electron leakage current on the basis of Fig. 3(a), which is defined as the ratio of the current overflowed outside the active region to the total current injected into the active region of the laser device. It can be seen that the percentage of electron leakage current decreases considerably from 25% to 2.4% along with the increase of Al composition from 0.2 to 0.27, and then it remains almost unchanged when the Al composition is higher than 0.27, which surely indicates that an increasing Al composition has a positive effect on the leakage current suppression. However, as shown in Fig. 2(b), when the Al composition increases from 0.25 to 0.3, the threshold current rises from 72.9 mA to 78.1 mA and output power decreases from 65.3 mW to 51.0 mW. It is known that a higher Al composition provides a higher density of positive polarization charges at the interface between u-GaN layer and $Al_xGa_{1-x}N$ EBL, which can attract more electrons accumulating at the interface, and thus bend the energy band more. As for injected holes, they will be attracted by the accumulated electrons and stay at the interface between $Al_xGa_{1-x}N$ EBL and $Al_{0.08}Ga_{0.92}N$ CL, leading to a hole accumulation and hindering holes from being injected into the active region.[19] Therefore, when choosing the aluminum composition of the barrier layer, a compromise between reducing the electron overflow and avoiding the carrier accumulation is required.

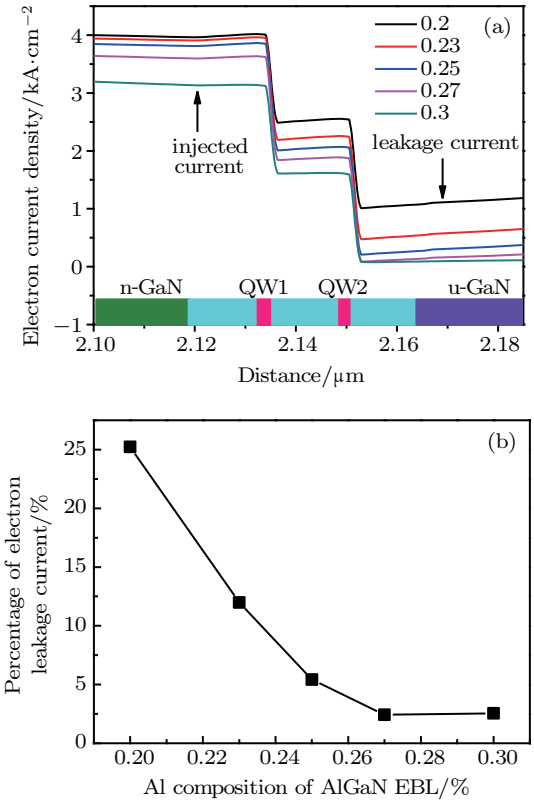


Fig. 3. (color online) (a) curves of vertical electron current density versus position for LDs with different Al compositions of $Al_xGa_{1-x}N$ EBL in LDs at 120 mA; (b) curve of percentage of electron leakage current as a function of Al composition of $Al_xGa_{1-x}N$ EBL at 120 mA.

Actually, other factors, such as the optical confinement of quantum wells and the optical loss, do not change too much with Al composition of $Al_xGa_{1-x}N$ EBL in our simulation results. When Al composition increases from 0.2 to 0.3, the optical confinement factor increases from 2.285% to 2.295%, and the optical loss decreases from 8.34477 cm^{-1} to 8.07967 cm^{-1}. Owing to the difference in effective refractive index between active and p-type layers, the majority of optical field is confined between upper and lower GaN. After enhancing the Al composition of $Al_xGa_{1-x}N$ EBL, the effective refractive index of p-type layer decreases. Consequently, it is reasonable to attribute the small improvement of optical characteristics to the smaller refractive index of higher Al composition.

3.2. $Al_xGa_{1-x}N$ HBL

Through the optimization of Al composition of $Al_xGa_{1-x}N$ EBL, we can obtain better LD performance, which reveals that the threshold current can be 7.0% lower than that of the original LD structure without EBL. However, compared with blue LDs, we think the ultraviolet LDs in our simulations still have a lot of room for improvement, which means that it is not enough to improve LD performances only by optimizing

Al composition of $Al_xGa_{1-x}N$ EBL. Note that near-ultraviolet GaN/$In_xGa_{1-x}N$ QW LDs have shallow quantum wells in both conduction and valence bands, and not only electrons but also holes might overflow outside the quantum wells, causing a hole leakage, and thus deteriorating the performances of LDs. Based on this analysis and the optimal result of Al composition of $Al_xGa_{1-x}N$ EBL, that is, 0.25, (the LD is taken as an reference LD in the following simulation analysis), an additional 10-nm $Al_{0.23}Ga_{0.77}N$ hole blocking layer is inserted between n-type waveguide and the first quantum barrier (this LD is regarded as a new LD later in the following simulation analysis).

The *P–I–V* results are exhibited in Fig. 4, showing that both turn-on voltage and resistance of new LD slightly increase in comparison with reference LD. As for the *P–I* curves, the threshold current of reference (Ref) LD is 72.9 mA, while for new LD, it reduces to 60.9 mA, 16.5% lower than that of reference LD. Meanwhile, the output power under 120-mA injected current condition of new LD is 79 mW, 20.1% higher than that of reference LD. It is obvious that the performance of new LD is significantly better.

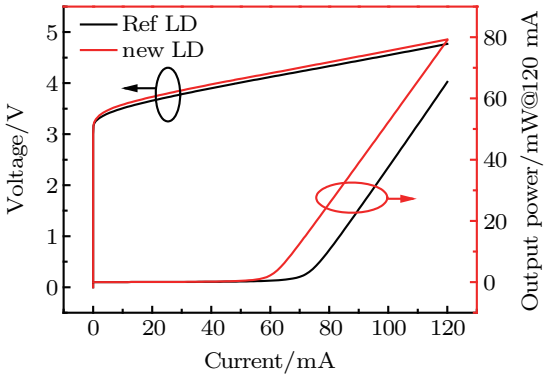


Fig. 4. (color online) The *P–I–V* results of reference LD and new LD.

To find out the reason, we plot the vertical hole and electron current density profiles of two structures in Fig. 5. It can be seen from Fig. 5(b) that under the 120-mA injected current condition, holes are injected into p-type layers, and recombine with electrons in the quantum wells and end up with a dramatic reduction of hole current density outside the active region near the p-type layer. The holes leaking into p-type layers will recombine with electrons nonradiatively, leading to a hole loss,[20] which will increase the threshold current of LD. Obviously, for new LD, the reductions of both hole and electron current densities in two quantum wells are all bigger than that of the reference LD. Specifically, 14.4% injected holes leak into n-side for reference LD, reduces to 6.0% for new LD, and 7.8% injected electrons leak into p side for reference LD, reduces to 5.1% for new LD. It indicates that it may be due to the fact that more holes recombine with electrons in the quantum wells radiatively, and thus the efficiency of new LD is enhanced impressively.

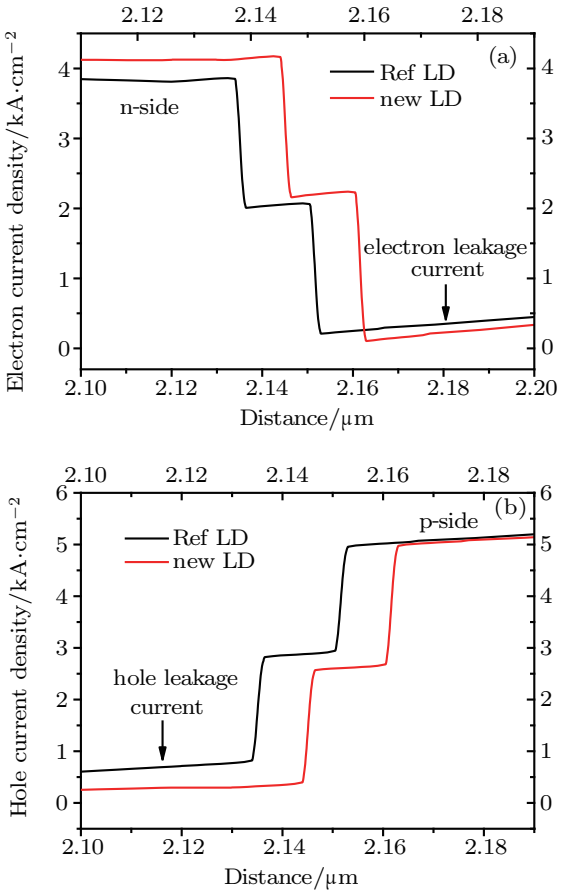


Fig. 5. (color online) Plots of vertical hole (a) and electron (b) current density versus distance of reference LD and new LD.

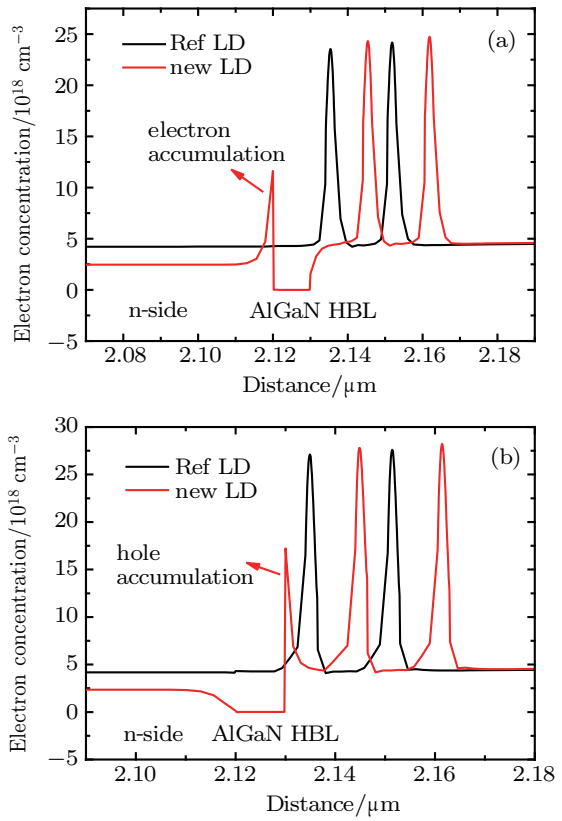


Fig. 6. (color online) (a) Electron and (b) hole concentration distributions near the active region of reference LD and new LD at 120 mA.

Figure 6 shows the electron and hole concentration dis-

tributions near the active region of two LDs at 120 mA. For reference LD, as shown in Fig. 6, there is neither electron nor hole accumulation in the n-type region. While for new LD, it can be seen that after inserting an $Al_xGa_{1-x}N$ HBL, there is a barrier at HBL for injected electrons which can block the injecting of electrons into the active regions to some extent. Due to the polarization effect between the n-GaN waveguide and n-$Al_xGa_{1-x}N$ HBL layer, there is a lower potential region in the conduction band, thereby electrons are easy to capture and result in an electron accumulation. For holes, as shown in Fig. 6(b), they will be blocked by the barrier of HBL which is beneficial to the enhancement of the optical performance of new LD. On the other hand, the holes tend to accumulate at the interface between the HBL and the first quantum barrier due to the polarization mismatch. Furthermore, with increasing Al composition of HBL, firstly, the carrier accumulation of both electrons and holes becomes much more severe and may induce more nonradiative recombination. Secondly, the whole electrical resistance of LD rises, the voltage applied to LD increases under the same injected current. These are harmful to the lasing operation of LDs.

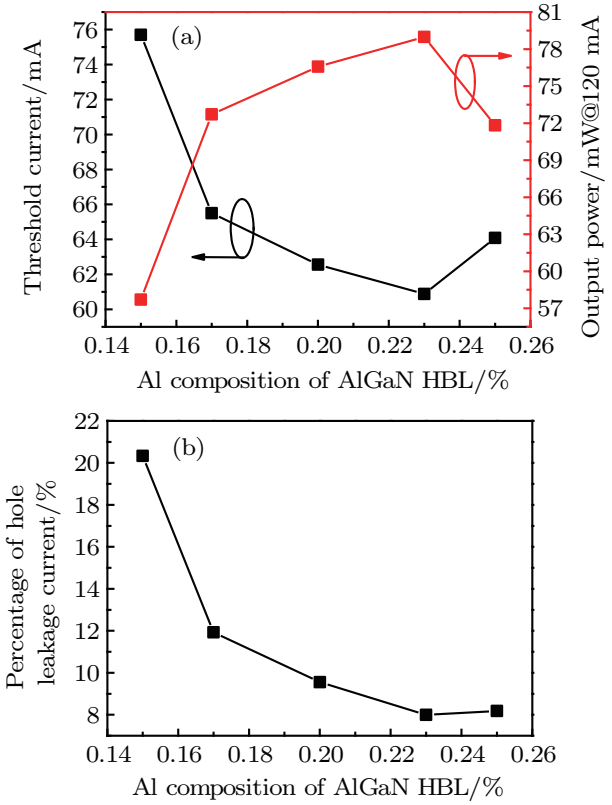


Fig. 7. (color online) (a) Threshold current (black line) and output power (red line) at 120 mA when Al composition of HBL changes from 0.15 to 0.25; (b) percentage of hole leakage current as a function of Al composition of HBL.

Therefore, as a compromise, it is essential to find an appropriate Al composition for Al_xGa_{1-x}NHBL. Figure 7(a) shows the variations of threshold current and output power at a fixed current of 120 mA along with increasing Al composition from 0.15 to 0.25. It is found that when Al composition is less than 0.23, the threshold current decreases and the output power increases, and a too high Al composition over 0.23 will bring about a negative effect, leading to the deterioration of LD performance. Referring to Fig. 7(b), through the optimization of Al composition, the percentage of hole leakage current can decrease from 20.3% to 8.0% when Al composition changes from 0.15 to 0.23.

Additionally, in the aspect of optical characteristics, the optical confinement factor of new LD decreases from 2.29% to 2.06%. The total optical loss induced by free carrier absorption increases from 7.67 cm^{-1} to 8.17 cm^{-1}. It can be seen that the optical characteristics deteriorate. For analysis, after inserting an HBL near the active region, the optical field can be influenced and the center of it moves from the first QW to the second QB due to the changed effective refractive index, which means that the whole optical field moves to the p-type region, leading to a reduced optical confinement of QWs and an increased optical loss. Nevertheless, the new LD still shows a better performance than the reference LD, which indicates that the decreasing of hole leakage is exceedingly important for improving the near-ultraviolet LDs.

4. Conclusions and perspectives

In this work, the effects of different Al compositions of inserted $Al_xGa_{1-x}N$ EBL and HBL on LD performance are investigated. Through optimizing the $Al_xGa_{1-x}N$ EBL alone, and additionally inserting an $Al_xGa_{1-x}N$ HBL with suitable Al composition between the n-GaN waveguide and the first quantum barrier, the threshold current could decrease by 7.0% and 16.5%, respectively, and the output power at 120 mA increases by 31.8% and 20.1%, leading to a better performance of near-ultraviolet LD.

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