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PAPER

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IOP Publishing

Semiconductor Science and Technology

Semicond. Sci. Technol. **38** (2023) 125003 (9pp)

https://doi.org/10.1088/1361-6641/ad03fd

Simulation of performance enhancement of GaN-based VCSELs by composition gradient InGaN last-quantum barrier

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Received 6 August 2023, revised 1 October 2023

Accepted for publication 17 October 2023

Published 27 October 2023

Abstract

Electron leakage in the active region decreases the internal quantum efficiency and impedes the performance of gallium nitride (GaN)-based vertical-cavity surface-emitting lasers (VCSELs). In this study, we propose a novel InGaN last-quantum barrier (LQB) structure with gradient indium (In) composition, and the device performance was simulated by the commercial software PICS3D. Compared with the device with conventional GaN LQB, the electron leakage is greatly reduced and the hole injection efficiency is also improved by the graded LQB structure. Consequently, the threshold current is reduced by 44%, and output power is increased by 392% in GaN-based VCSEL based on composition gradient InGaN LQB. The composition gradient InGaN can also allow us to increase the thickness of the LQB in epitaxy without degrading the carrier injection efficiency due to the reduced polarization in the LQB. The results of this study suggest that the composition gradient InGaN LQB is promising for the realization of high-performance GaN-based VCSELs.

Keywords: simulations, GaN, VCSELs

(Some figures may appear in colour only in the online journal)

1. Introduction

Gallium nitride (GaN)-based vertical-cavity surface-emitting lasers (VCSELs) are attracting increasing attention due to their circular beam profile, low threshold current, high coupling efficiency with optical fiber, and ease of realization of two-dimensional arrays [1–3]. They have great potential for solid-state lighting [4], displays [5], data communications [6], and high-density optical storage [7]. However, electron leakage in the active region is an important problem limiting GaN-based VCSELs from achieving higher output power. The AlGaN electron blocking layer (EBL) on top of the last-quantum barrier (LQB) can reduce the electron leakage from active region due to the conduction band difference between the EBL and the LQB [8]. Although the leakage current can be reduced by increasing the bandgap of the EBL by a larger aluminum (Al) content, it also increases the hole injection barrier and reduces the hole injection efficiency. In order to solve this problem, researchers have proposed many optimization designs, including superlattice EBL [9], Al composition gradient EBL [10, 11], stepped EBL [12], and multi-quantum barrier EBL [13], etc. However, these studies mainly focus on the modification of EBL. It should be noted that the LQB between quantum well (QW) and EBL also has a significant impact on the performance of the device. The energy band structure of LQB directly affects the electron leakage in the active region. The

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thickness of the LQB must also be carefully designed. In the point of protecting active region, it is often preferred to grow a thicker LQB during epitaxy, which on the one hand can avoid the degradation of the crystal quality of InGaN QW during the high-temperature growth of AlGaN EBL. On the other hand, it can also reduce the diffusion of Mg atoms form the p-type EBL into the active region. However, a thicker LQB will decrease the carrier injection efficiency [14]. Therefore, a suitable LQB structure is particularly important to enhance the performance of GaN-based VCSEL, but there is a lack of research in this area.

In this study, we propose an LQB structure based on the composition gradient InGaN (Graded). The composition gradient can increase the band offset between LQB and EBL, consequently enhance the electron blocking ability of EBL. At the same time, the conduction band offset between LQB and last QW (LQW) is unchanged, so it will not lead to additional electron leakage. More importantly, it will not introduce additional hole potential barrier, which can lead to a decrease in hole injection efficiency. The influence of LQB thickness on the device performance is also investigated. It is found that, due to the reduced polarization, there is no significant degradation of device performance by increasing the thickness of the Graded-LQB.

The performance of GaN-based VCSELs with both Graded and conventional (Flat) LQB structures was simulated by using commercial software Crosslight PICS3D. The results show that the Graded-LQB structure can significantly reduce electron leakage and improve the hole injection efficiency into the multi-QWs (MQWs) compared with the Flat-LQB. Therefore, the performance of GaN-based VCSELs based on the Graded-LQB is significantly improved, as the output power increases by 392% at 20 mA while the threshold current decreases by 44%.

2. Device structures and simulation parameters

The structures of GaN-based VCSEL with two different LQB are shown in figure 1. Flat-LQB consists of GaN, and Graded-LQB consists of InGaN with the indium (In) composition increasing from 0 to 0.15 along the growth direction. The thickness of the two different LQB are both 4 nm. The device composed a 5.5 λ-thick cavity and features a dual dielectric distributed Bragg reflectors (DBRs) structure with 12.5 periods of SiO_2/TiO_2 at bottom and 6 periods of SiO_2/TiO_2 on top. A 20 nm-thick indium tin oxide (ITO) is employed as the current spreading layer, and a 10 nm-thick SiO_2 is used as the current confinement layer. The device has an optical emission aperture (current confinement aperture) with a diameter of 5 μm, and the emission wavelength (λ) is 502 nm. The detailed parameters of the epi-layers and others are given in table 1. The bandgap of $In_xGa_{1-x}N$ alloy can be expressed as follows [15]:

$$E_g\left(In_xGa_{1-x}\right) = xE_g\left(InN\right) + (1-x)\,E_g\left(GaN\right) - bx\,(1-x)$$

where E_g (InN) and E_g (GaN) is 0.71 and 3.42 eV at 300 K. Bowing parameter $b = 1.43$ eV [16]. The material parameter used in this work are list in table 2 [17].

Crosslight PICS3D was used to simulate the optical and electrical properties of VCSELs, which contain current continuity equations, drift–diffusion equations, Schrödinger and Poisson's equations, etc [18]. The Auger recombination coefficient was set to be 1.4×10^{-31} $cm^6\,s^{-1}$ to account for Auger recombination in the material, while the Shockley–Read–Hall (SRH) lifetime is 1×10^{-8} s, which consist with the previous results [19–23]. The polarization level was set as 40% to approximate the polarized charge at the interface. The conduction/valence band offset ratio was set to be 70:30 for MQWs and 50:50 for AlGaN/GaN interface [18, 24]. The average optical background loss of the n-GaN, MQWs, EBL, and p-GaN layers in the cavity was set to 1000 m^{-1} [22, 25].

3. Results and discussion

Figure 2 shows the optical output power (P) as a function of injection current (I) for the two VCSELs. The output power of the Graded-LQB VCSEL is 2.36 mW at 20 mA, which is 392% higher than the 0.48 mW of the Flat-LQB VCSEL. In addition, the threshold current of the Graded-LQB VCSEL is 4.5 mA, which is reduced by 44% compared to the 8.0 mA for the Flat-LQB VCSEL. The performance of the Graded-LQB VCSEL is significantly improved. For green VCSELs in this study, compared to blue VCSELs, they require more In composition in the InGaN/GaN QWs layer, resulting in a larger polarization electric field and lattice-mismatch-induced defects. These will strongly reduce the emission efficiency and therefore lower output power. The output power for GaN-based green VCSELs using double dielectric DBRs, similar to the present paper, were much lower, in the order of ~nW, and the structure in this paper is expected to drastically increase the output power. Based on other structures, the output power of green VCSELs can achieve several mW, such as Nichia [26] and Sony [27]. With the QW structure of this manuscript, it is believed that there will be a further improvement in output power.

The energy band was analyzed to reveal the detailed reason for the improved performance of the Graded-LQB VCSEL. Figures 3(a) and (b) show the energy band diagrams of the Graded-LQB VCSEL and the Flat-LQB VCSEL at 4 mA (below threshold), respectively. The potential barrier for electron leakage (ΔE_c) is 150 meV for Flat-LQB and 278 meV for Graded-LQB, which is improved by 85%. The increased ΔE_c means that the Graded-LQB can prevent electron leakage more effectively. The electron concentration in p-GaN is reduced by about 100 times in the Graded LQB structure compared to the Flat LQB, as shown in figure 3(c). The reduced electron leakage indicates that more electrons are confined in the MQWs, as shown in figure 3(d). Although the potential barrier of EBL for hole injection (ΔE_v) is almost the same in

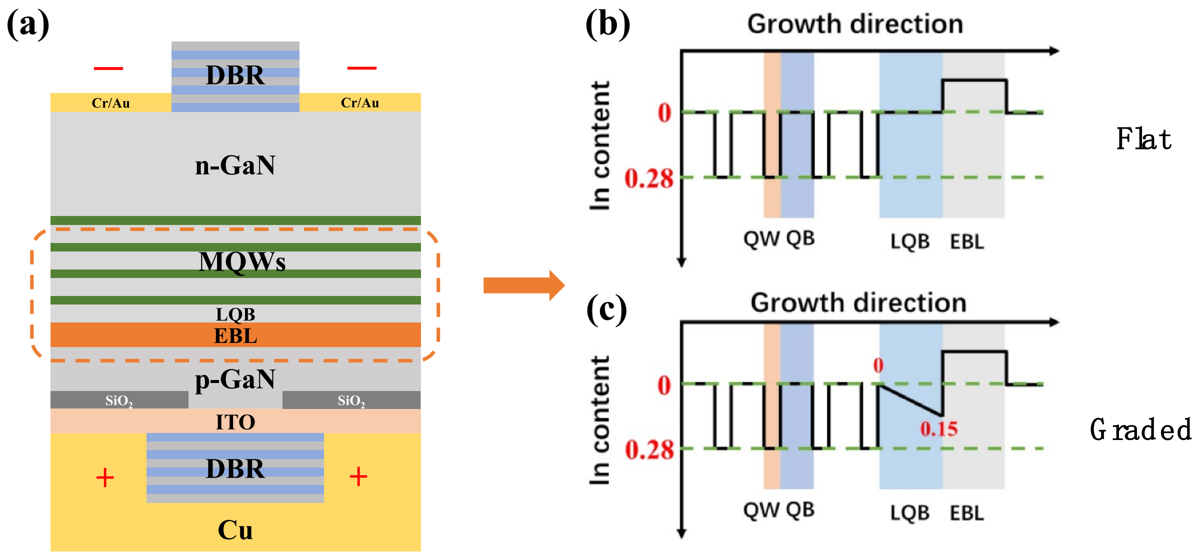

Figure 1. (a) Schematic diagram of GaN-based VCSEL with two different LQB structure; (b) Flat-LQB; (c) Graded-LQB.

Table 1. Detailed parameters of the epi-layers.

Type	Material	Thickness (nm)	Doping concentration (cm^{-3})
Top-DBRs	SiO_2/TiO_2	(87/52)*6 pairs	
	n-GaN	944	n:5e18
MQW	$In_{0.28}Ga_{0.72}N/GaN$	(2/4)*4 pairs	—
EBL	$Al_{0.2}Ga_{0.8}N$	15	p:3e18
	p-GaN	106	p:5e18
Passivated region	SiO_2	10	
Current spreading layer	ITO	20	
Bottom-DBRs	SiO_2/TiO_2	(87/52)*12.5 pairs	

Table 2. Material parameters for wurtzite nitride binaries at 300 K.

Parameter	GaN	InN	AlN
a_0 (Å)	3.189	3.545	3.112
c_0 (Å)	5.185	5.703	4.982
α (meV K^{-1})	0.909	0.245	0.019
β (K)	830	624	1462
$m_e^{\parallel}$	0.2	0.12	0.28
$m_e^{\perp}$	0.2	0.12	0.32
A_1	−7.21	−8.21	−3.86
A_2	−0.44	−0.68	−0.25
A_3	6.68	7.57	3.58
A_4	−3.46	−5.23	−1.32
A_5	−3.40	−5.11	−1.47
A_6	−4.90	−5.96	−1.64

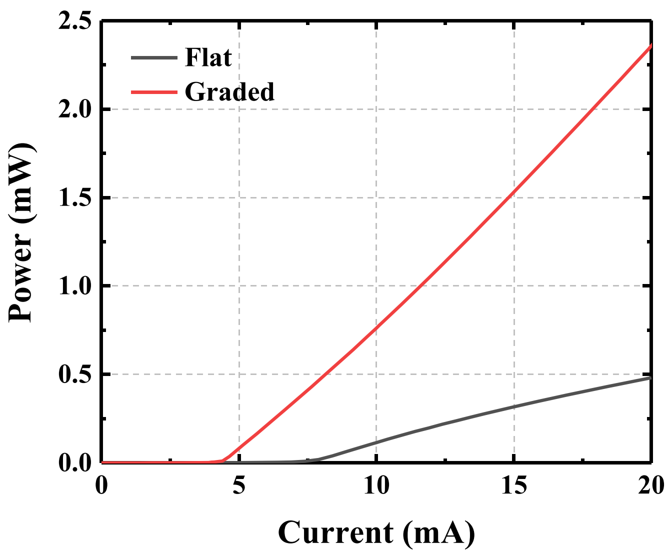

Figure 2. *P–I* curves for Graded-LQB VCSEL and Flat-LQB VCSEL.

both VCSELs, the composition gradient InGaN leads to a larger valence band difference between the LQB and EBL, so that the hole can obtain greater kinetic energy at the interface of EBL and the Graded-LQB, which makes it easier to inject into the MQW [28]. Figures 3(e) and (f) show the hole concentration in logarithmic and linear coordinate, respectively. The hole concentration in the active region is larger in the Graded-LQB VCSELs. And due to the bulk polarization, the hole will accumulate in the graded layer, as shown in the blue dashed frame in figure 3(e).

Figure 4 shows the normalized electron current density in Flat and Graded LQB VCSELs at 4 mA. The electron leakage

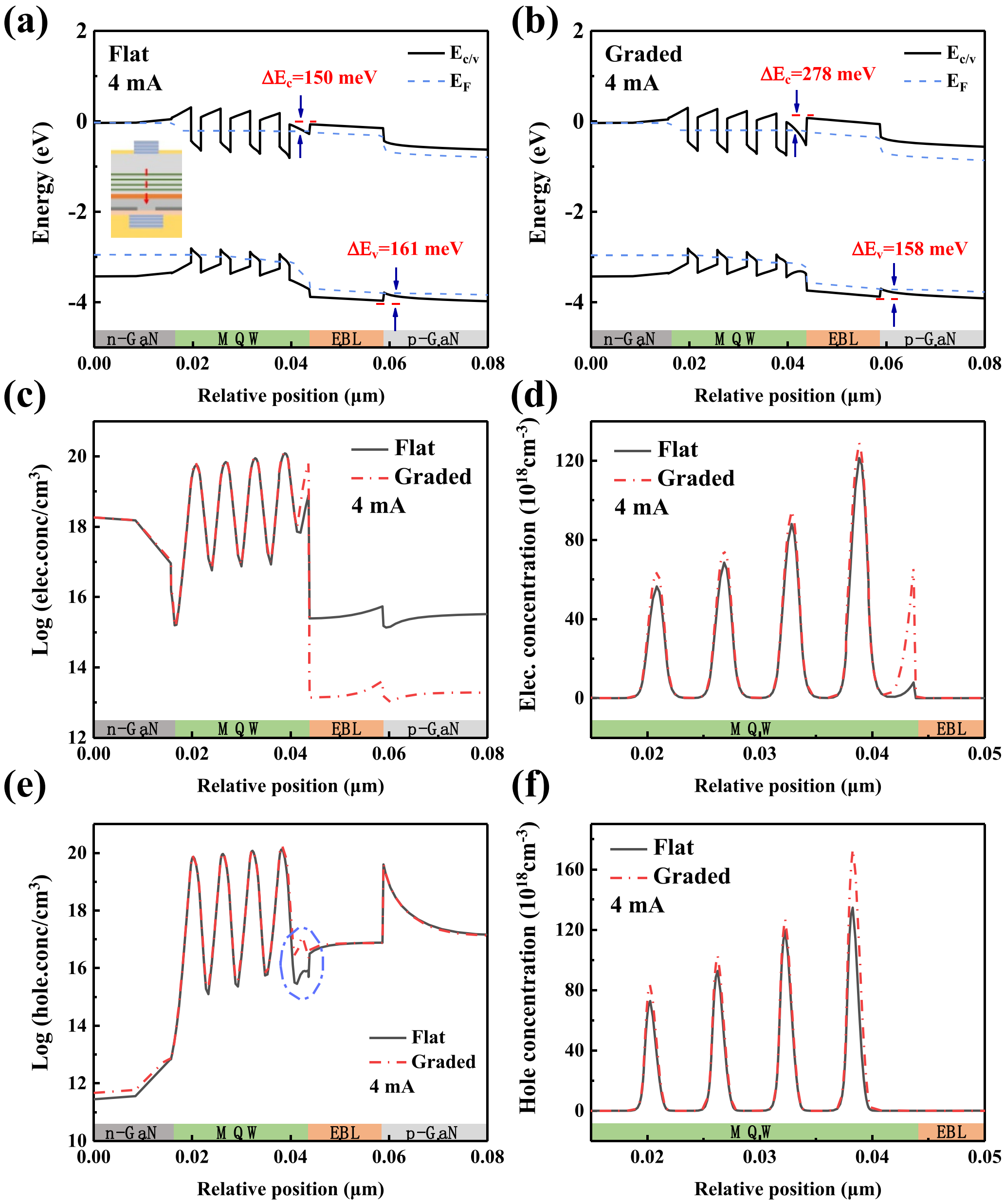

Figure 3. (a) Energy band diagram at 4 mA in Flat-LQB VCSEL, the dashed line is the quasi-Fermi level; (b) energy band diagram at 4 mA in Graded-LQB VCSEL; electron concentration distribution in (c) logarithmic coordinates and (d) linear coordinates; hole concentration distribution in (e) logarithmic coordinates and (f) linear coordinates.

current in the VCSEL with Graded-LQB is reduced significantly compared to that in the Flat-LQB VCSEL. These results suggest that Graded-LQB can effectively confine the electron in the MQWs region and improve the hole injection efficiency.

Figures 5(a) and (b) show the electron-hole wave function distribution within the LQW in the Flat-LQB VCSEL and Graded-LQB VCSEL at 4 mA, respectively. The overlap of wave functions is defined as the area of the yellow section divided by the total area of the curve integral, and it is improved by 18.1% in the Graded-LQB VCSEL compared to Flat-LQB VCSEL. This improvement can be attributed to the more carrier injection in the LQW with graded LQB, and the carrier screening effect reduces the QCSE and consequently diminishes the energy band tilt in the LQW. Due to the more efficient carrier injection in the MQWs and the larger wave function overlap, the spontaneous (as shown in figure 5(c)) and stimulated radiative recombination rate of Graded-LQB VCSEL can be increased at the same time. At the same time, the threshold current of Graded-LQB VCSEL is reduced. Figure 5(d) shows the stimulated radiative recombination rate at 20 mA (above threshold). Compared with the Flat-LQB VCSEL, the stimulated radiative recombination rate of the MQWs in the Graded-LQB VCSEL is much higher, significantly improving the optical output power.

The thickness of the LQB is also an important parameter for epitaxial structure design. The effect of LQB thickness

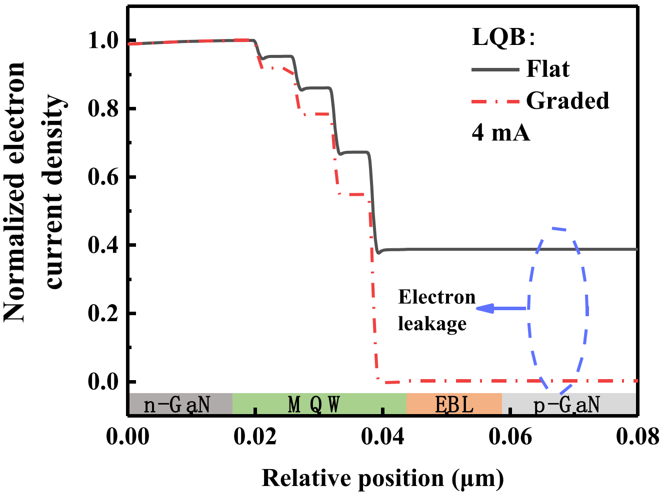

Figure 4. Normalized electron current density at 4 mA in Flat and Graded-LQB VCSEL.

on the performance of the devices was investigated. The *P–I* curves of the Flat-LQB and Graded-LQB VCSELs are shown in figures 6(a) and (b). As the LQB thickness is increased from 4 nm to 12 nm, the performance of the Flat-LQB VCSEL including both threshold current and output power are deteriorated remarkably. In contrast, the performance of the Graded-LQB VCSEL is more stable and less affected by the thickness of LQB. This means that it is possible to weaken the deterioration of crystal quality of the QWs during high-temperature growth of EBL, as well as to prevent the diffusion of Mg atoms from the p-EBL into the active region by increasing the thickness of the LQB without degrading the performance. This is helpful for improving the quality of the wafer epitaxy.

To explain the different behavior between the two VCSELs with increasing the LQB thickness, the energy band diagram of the two VCSELs with different LQB thicknesses was analyzed. Figures 7(a), (c) and (e) shows the energy band of Flat-LQB, and (b), (d), (f) shows the energy band of Graded-LQB VCSELs with different LQB thickness below the threshold current. As the LQB thickness increases, ΔE_c in the Flat-LQB VCSEL gradually decreases from 212 meV (4 nm-LQB) to 167 meV (12 nm-LQB). The reduction of ΔE_c means that the electrons can be more easily leaked out of the MQWs. On the other hand, ΔE_v in the Flat-LQB VCSEL gradually increase with increasing the LQB thickness, which means that the hole injection becomes more and more difficult. The increase of electron leakage and the decrease of hole injection efficiency lead to a significant deterioration of the performance of Flat-LQB VCSEL with the increase of LQB thickness. In the Graded-LQB VCSEL, the values of ΔE_c and ΔE_v do not show large difference and thus the performance is stable with the increase of LQB thickness.

The main reason for such discrepancy between ΔE_c and ΔE_v in the two types of VCSEL is caused by the difference of polarization in the LQB. In simulation, all layers are fully strained and assumed to be coherently grown on GaN template. For the Graded-LQB, the compressive strain is larger than the Flat-LQB, and is gradually increased along the [0001] direction because of the gradient In composition. As the piezoelectric polarization (P_{pz}) caused by the compressive strain is along the [0001] direction, opposite to the direction of spontaneous polarization (P_{sp}). The total polarization in the Graded-LQB is smaller than that of Flat LQB and is continuously diminished along [0001] direction. The P_{sp} and P_{pz} of GaN and $In_xGa_{1-x}N$ alloy can be calculated as [29–32]:

$$P_{sp}\left(\mathrm{In}_x\mathrm{Ga}_{1-x}\mathrm{N}\right) = -0.042x - 0.034\left(1-x\right) + 0.038x\left(1-x\right)$$

$$P_{pz}\left(\mathrm{In}_x\mathrm{Ga}_{1-x}\mathrm{N}\right) = xP_{pz}\left(\mathrm{InN}\right) + \left(1-x\right)P_{pz}\left(\mathrm{GaN}\right)$$

where

$$P_{pz}\left(\mathrm{InN}\right) = -1.373\varepsilon + 7.559\varepsilon^2$$

$$P_{pz}\left(\mathrm{GaN}\right) = -0.918\varepsilon + 9.541\varepsilon^2$$

and the basal strain for the $In_xGa_{1-x}N$ alloy is defined as:

$$\varepsilon = \frac{\left[a_{sub} - a\left(x\right)\right]}{a\left(x\right)}$$

a_{sub} and $a_{(x)}$ is the lattice constants of the substrate and alloy at composition x. According to the Vegard's law, the lattice constants of $In_xGa_{1-x}N$ alloy can be calculated and expressed as [33]:

$$a_{\mathrm{In}_x\mathrm{Ga}_{1-x}\mathrm{N}(x)} = 0.3189\left(1-x\right) + 0.3545x.$$

The P_{sp} and P_{pz} in the two LQB can be calculated based on the above formula. Figure 8 shows the total polarization (P_{sp} + P_{pz}) inside the two VCSELs, where the polarization along the [0001] direction is defined as positive. The total polarization in the Graded-LQB shows an obvious reduction compared to that of the Flat-LQB (area of yellow section). The small polarization presents a small electric field and a weak band tilting in the LQB. ΔE_{c1} is defined as the value of the difference between the conduction band energy levels at the n-side and p-side of the LQB, and can reflect the degree of energy band tilt of the LQB. The value of ΔE_c, ΔE_v and ΔE_{c1} are listed in table 3. For Flat-LQB VCSEL, ΔE_{c1} increases with a thicker LQB, indicating that the energy band tilt becomes more serious. The electrons can transport from the active region to the p-side of the LQB more easily and accumulate at the LQB/EBL interface. And the quasi-Fermi level for electron rises as the electron concentration increases, reducing the difference between quasi-Fermi level and the top of the EBL conduction band (ΔE_c). The electron leakage is therefore more serious, and this will also increase the difficulty of hole injection at the same time, inducing a larger ΔE_v. As for the Graded-LQB VCSEL, the energy band tilt is weaker because of the lower polarization electric field in the LQB. Therefore, as the LQB thickness increases,

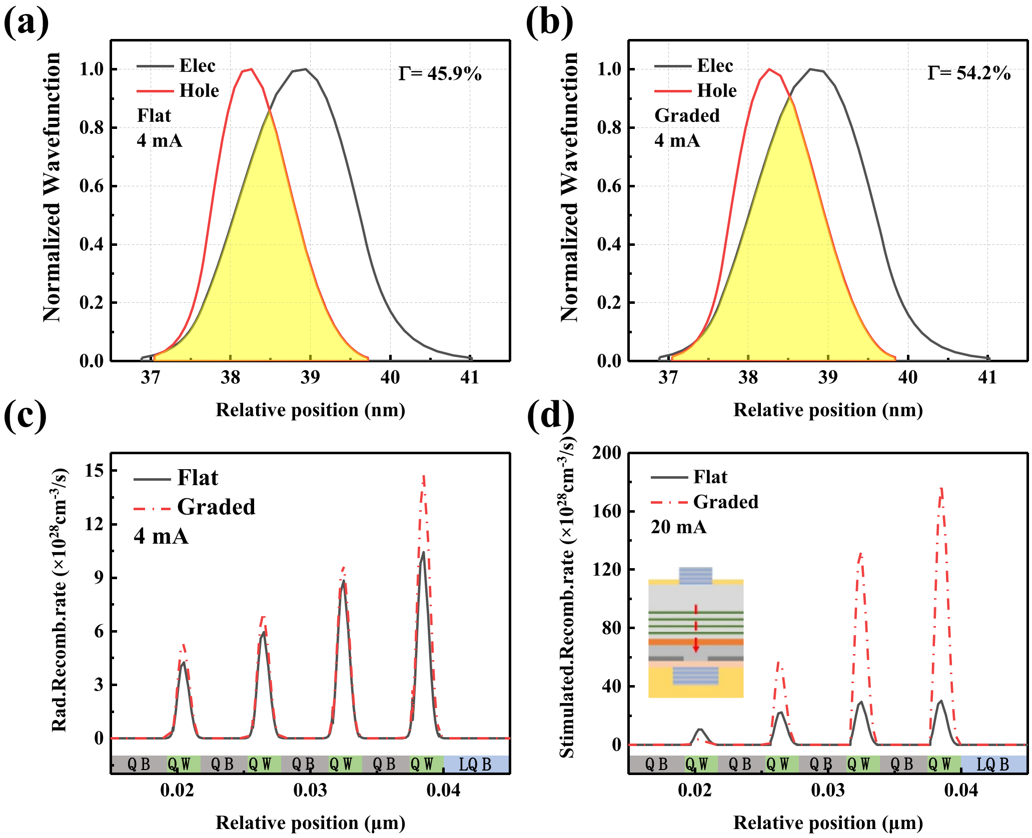

Figure 5. Electron and hole wave functions at 4 mA (a) in LQW of Flat-LQB VCSEL; (b) in LQW of Graded-LQB VCSEL; (c) spontaneous radiative recombination rate; (d) stimulated radiative recombination rate at 20 mA.

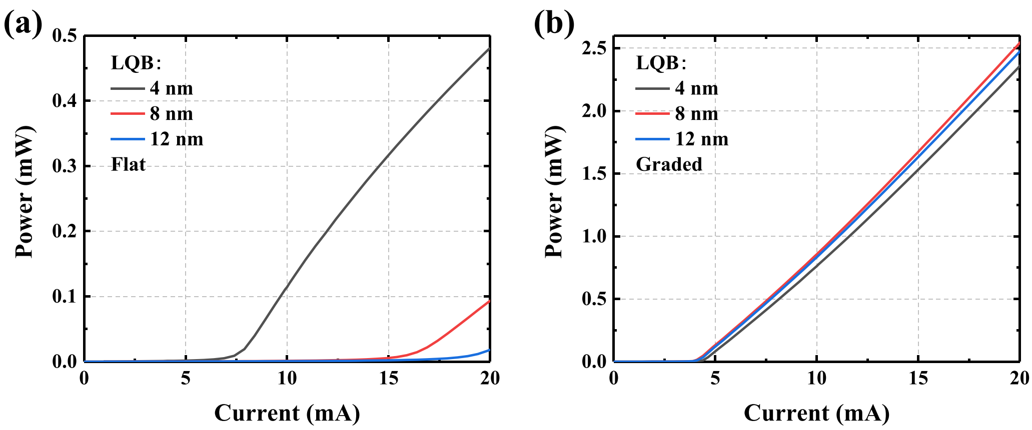

Figure 6. (a) *P–I* curves of Flat-LQB VCSEL with different LQB thickness; (b) *P–I* curves of Graded-LQB VCSEL with different LQB thickness.

the value of ΔE_{c1}, ΔE_c and ΔE_v remains almost the same, and the device performance is less influenced. By weakening the polarization electric field, a thicker LQB is allowed during device design. This is preferred for the wafer epitaxy to protect the QWs during high-temperature growth of EBL, and reduce the diffusion of Mg atoms form the p-type. And we have grown epi-wafers based on the concepts proposed in this paper and device preparation is currently underway to verify the validity of Graded-LQB GaN-based gain structure.

To evaluate the effect of composition gradient LQB, the *P–I* curves of VCSELs based on conventional structure (Flat), composition gradient LQB, and composition gradient EBL (Al composition gradient from 0.2 to 0 along the growth direction), and composition gradient LQB plus EBL are shown in figure 9. It can be seen that both Graded-LQB and

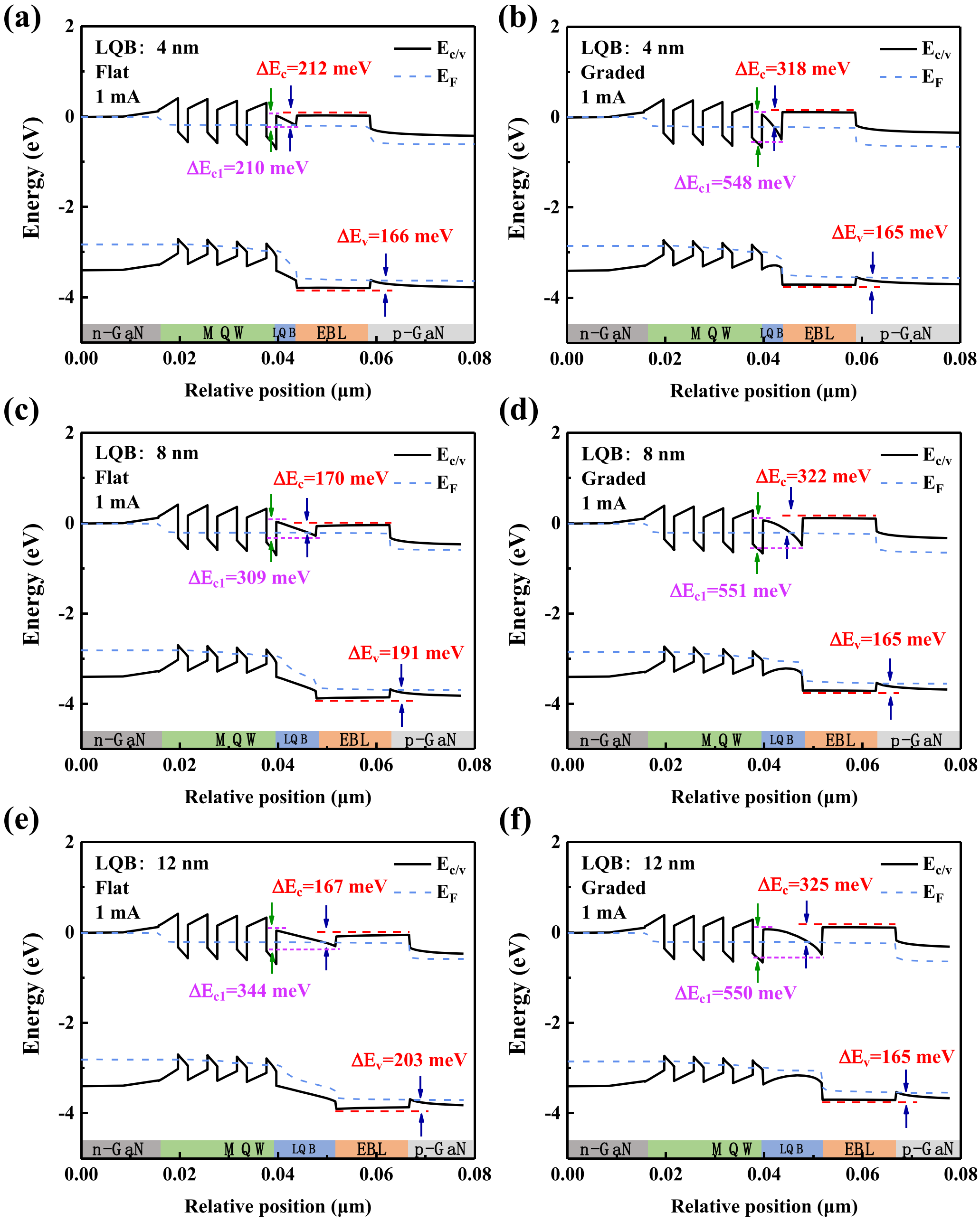

Figure 7. (a), (c), (e) Energy band of Flat-LQB VCSEL with different LQB thickness; (b), (d), (f) energy band of Graded-LQB VCSEL with different LQB thickness.

Graded-EBL can improve the output power of the device. And the device based on Graded-LQB has more power enhancement than based on Graded-EBL, which may be attributed to its higher electron-blocking barrier and more efficient hole injection from the p-region into the active region. More importantly, the combination of the two can further enhance the device output power, which means that it is compatible with the current EBL-based improvement methods, providing us with another way of improving the performance of GaN-based VCSELs.

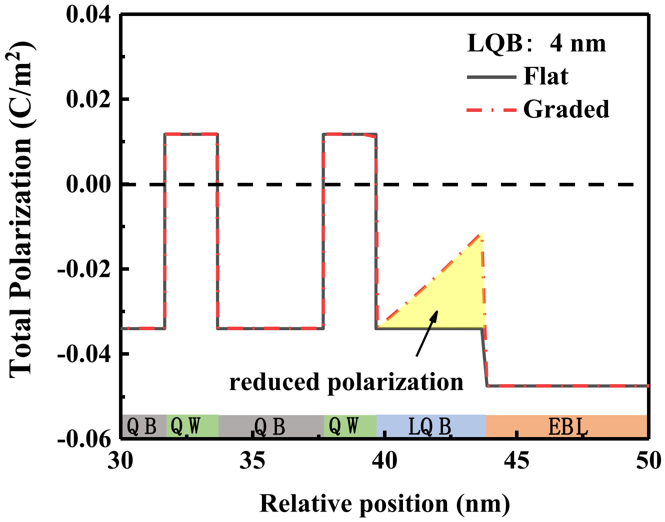

Figure 8. Total polarization inside the VCSELs.

Table 3. The value of ΔE_c, ΔE_v and ΔE_{c1} for Flat-LQB and Graded-LQB VCSEL with different LQB thickness.

Thickness (nm)	Device (for each thickness)	ΔE_c (meV)	ΔE_v (meV)	ΔE_{c1} (meV)
4	Flat	212	166	210
	Graded	318	165	548
8	Flat	170	191	309
	Graded	322	165	551
12	Flat	167	203	344
	Graded	325	165	550

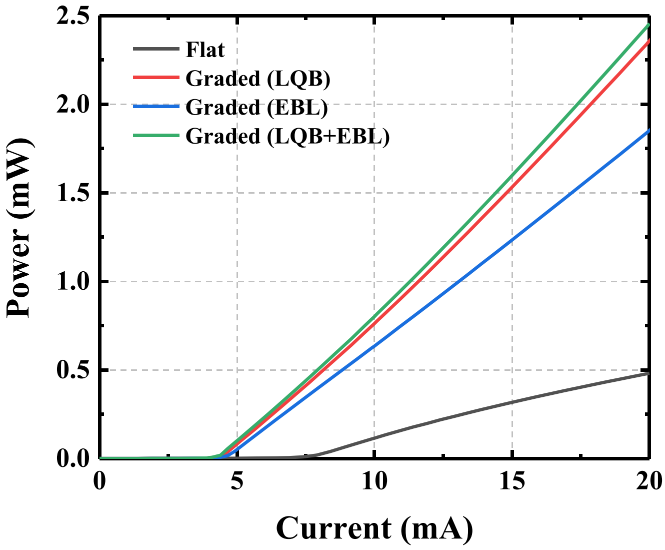

Figure 9. $P-I$ curves of VCSELs based on conventional structure (Flat), composition gradient LQB, composition gradient EBL, and composition gradient LQB plus EBL.

4. Conclusions

In summary, a GaN-based VCSEL based on composition gradient InGaN LQB structure was designed, and the device performance was theoretically calculated by PICS3D. Compared with the conventional LQB, the Graded-LQB can effectively reduce the electron leakage and increase the hole injection efficiency. Consequently, the threshold current reduced by 44%, and output power increased by 392% in GaN-based VCSEL based on composition gradient InGaN LQB. Moreover, the composition gradient InGaN can significantly reduce the polarization of LQB, which is helpful to increase the thickness of LQB to meet the requirement of epitaxial growth without degrading the performance. This study provides an in-depth analysis of the effect of LQB structure on the performance of GaN-based VCSELs, which is helpful for the development of GaN-based optoelectronic devices.

Data availability statement

All data that support the findings of this study are included within the article (and any supplementary files).

Acknowledgment

This work was supported by the National Natural Science Foundation of China (Nos. U21A20493, 62234011 and 62104204), the National Key Research and Development Program of China (No. 2017YFE0131500) and the President's Foundation of Xiamen University (No. 20720220108).

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