Proposed performance enhancement of GaN-based blue light-emitting diodes with a step-graded electron-blocking layer

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The properties of GaN-based blue light-emitting diodes (LEDs) with a step-graded AlGaN electron-blocking layer (EBL) are investigated numerically. The proposed design exhibits a improved efficiency droop and superior optical characteristics compared with the conventional LEDs. The simulation results indicate that a reduction of electron spillover and a higher efficiency of hole injection can be achieved by using the proposed design. Furthermore, it is found that the significant decrease of electrostatic fields near the last quantum barrier and the EBL might be one of the key reasons for these improvements.

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1. Introduction

Recently, high-brightness GaN-based light-emitting diodes (LEDs) are investigated extensively due to their applications in automotive lightings, back-lighting, full color displays and domestic illumination [1-3], etc. However, the issue of efficiency droop has become a key stumbling block for the development of high power devices which are required in commercial fields. However, the issue of efficiency droop prevents the development of high power devices. It is widely regarded that the electron leakage may play an a crucial role for the issue. Therefore, an AlGaN layer as an electron-blocking layer (EBL) is inserted between the last quantum barrier (QB) and the p-GaN layer to suppress the electron spillover. However, due to the severe lattice mismatch between the last QB and EBL, this conventional EBL can not effectively suppress electrons overflow from the p-GaN layer and even act as a large potential barrier for holes injection. As a result, the issue of efficiency droop can not be mitigated effectively. Many published works suggest some specific designs of LEDs can improve the issue, such as the p-doped in last QB and EBL [4], the staggered QWs or delta-QWs [5-8], the polarization-doped p-type AlGaN EBL [9,10], the InGaN [11], AlGaN [12] or InAlGaN QB [13,14], graded thickness QB [15], etc.

In this paper, with the purpose of improving the efficiency droop and the optical performance of LEDs, a specific EBL with step-graded AlGaN layers is

investigated numerically in detail. The possible mechanisms are also discussed based on the simulation results of electrostatic fields, emission spectra, carrier concentrations, electron current density, radiative recombination rate and internal quantum efficiency (IQE).

2. Structure and parameters

The conventional LEDs (denoted as structure A) used in this paper as a reference is grown on a c-plane sapphire substrate with metal-organic chemical vapor deposition (MOCVD), followed by a 0.02-µm-thick undoped GaN nucleation layer, and then a 4.5-µm-thick n-type GaN layer (n-doping = 5×10^{18} cm⁻³). The active region consists of 4-pairs In_{0.1}Ga_{0.9}N/GaN multiple quantum wells (MQWs) with four 2.2-nm-thick wells sandwiched by five 15-nm-thick barriers. On the top of the active region are a 0.02- μ m-thick p-type Al_{0.18}Ga_{0.82}N EBL and a 0.2- μ m-thick p-type GaN cap layer(p-doping=7 \times 10^{17} cm⁻³). The area of the device geometry is designed into a rectangular shape of 300µm×300µm. To improve the performance of the LEDs, another LED epitaxial structure(denoted as structure B) is designed, which has the similar structure except for the rectangular AlGaN EBL using in the conventional LEDs is replaced by a p-type step-graded AlGaN EBL(p-doping= 7×10^{17} cm⁻³). This EBL structure consists of three step-graded Al_xGa_{1-x}N layers, the Al mole fraction x is set to 0.04(5 nm), 0.09(5

nm) and 0.18(10 nm), respectively. The total thickness of step-graded EBL is the same as conventional one. The two

structures are shown in Fig. 1.

structure A: conventional structure				structure B		
	p-GaN	0.2µm		p-Al _{0.18} Ga _{0.82} N	10nm	
	p-Al _{0.18} Ga _{0.82} N	0.02µm	>	p-Al _{0.09} Ga _{0.91} N	5nm	
	MQW	4-pairs		p-Al _{0.04} Ga _{0.96} N	5nm	
	n-GaN	4.5 μm				
	i-GaN	0.02µm				
	Sapphire substrate					

Fig. 1. Schematic diagrams of the LED structures.

The physical properties of the LEDs are investigated numerically with the APSYS (Advanced Physical Models of Semiconductor Devices) [16] simulation software. In the simulation, the light extraction efficiency is assumed to be 0.78 in order to match the experimental data [17]. The band offset ratio is assumed to be 0.7/0.3 [18]. Note that the surface charges could be screened due to the defects inside the device [19,20]. The 40% of the calculated surface charge density is assumed in our simulation to approach experimental results [21]. The epitaxial material parameters are chosen to be the same as in Ref [22]. The other simulation parameters are set to be the same as Ref [23].

The strong electrostatic fields generated by the polarization near the last quantum barrier(QB) and the EBL in LEDs are shown in Fig. 2(a). This piezoelectric polarization effect appears due to the severe lattice mismatch at the interface between the last QB and AlGaN EBL. The traditional ways of increase of Al mole fraction in AlGaN EBL can only increase the mismatch at the interface and result in worse downward band-bending. As a result, the performance of LEDs will be deteriorated with this conventional EBL structure. However, when the conventional EBL is replaced by a step-graded EBL (structure B), the specific three step-graded layers structure might disperse the strong polarization field at the interface between last QB and EBL. Accordingly, the electrostatic field near the last QB and the EBL is apparently alleviated compared with the conventional LEDs as shown in Fig. 2(b).



Fig. 2. The electrostatic fields of two LEDs with (a) the conventional EBL and (b) the step-graded EBL at 150 mA.

The energy band diagrams of two structures at 150 mA are shown in Fig. 3. As shown in Fig. 3(a), the effective barrier height for electrons of the EBL reduce significantly (408 meV) due to the severe band-bending of the conduction band. It makes the EBL fail its purpose for blocking the electrons. Moreover, conventional EBL also acts as a high potential barrier (537 meV) for holes, as a result, the hole injection from the p-layer become difficult. On the contrary, the severe band-bending near the last QB and EBL is mitigated by using the step-graded AlGaN

layers as an EBL. The effective potential height for electrons (526 meV) in conduction band is higher than that of conventional LEDs as shown in Fig. 3(b). The effective potential height for holes (448 meV) is also been reduced. Fig. 3(c) and (d) show the enlarged band diagrams near the EBL. Because of the smaller polarization field near the last QB and EBL, the band-bending in structure B is slighter than that of the conventional LEDs.

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Fig. 3. Energy band diagrams of two LEDs with (a) the conventional EBL (b) the step-graded EBL (c) the enlarged conduction band near EBL and (d) the enlarged valence band near EBL at 150 mA.

Fig. 4 shows the electron and hole concentrations of two structures at 150 mA. It can be seen that electron leakage concentration in conventional LEDs is two orders of magnitude greater than that of the structure B. It demonstrates that the electron spillover can be suppressed due to the higher effective potential barrier from modification of EBL. Moreover, we found that the average hole concentration in structure B is more than one orders of magnitude larger than that of the conventional LEDs. It indicates that the specific EBL in structure B might promotes the efficiency of hole injection because of a lower effective potential height for holes compared with conventional LEDs.



Fig. 4. The carrier concentration distribution of two LEDs with (a) the conventional EBL and (b) the step-graded EBL at 150 mA.

Fig. 5(a) shows the radiative recombination rate around the active region of two structures at 150 mA. Note that the horizontal positions in the plot have been shifted slightly for better observation. In Fig. 5(a), due to the reduction of electron spillover as well as the improved hole injection in structure B, more electrons and holes can participate in recombination in QWs. As a result, the radiative recombination rate of structure B by employing the step-graded AlGaN EBL is enhanced significantly compared with the conventional LEDs. Fig. 5(b) shows the vertical electron current density near the active region of two structures at 150mA. The electrons are injected from the n-GaN layer and take part in recombination with holes in QWs, which results in the reduction of electron current. The electron current that escapes from the active region and then overflows from the p-GaN layer is viewed as the electron leakage current. As shown in Fig. 5(b), fewer electrons contributed to the recombination in QWs, which result in severe leakage current in conventional LEDs. However, after employing the step-graded EBL in structure B, the electron spillover can be remarkably suppressed.



Fig. 5. (a) The radiative recombination rate and (b) vertical electron current density of two LEDs at 150 mA.

The spectra, IQE and light-current(*L-I*) performances of the two structures are plotted in Fig. 6. It can be found that the spectrum intensity of structure B is almost twice as much as that of the structure A as shown in Fig. 6(a). It indicates that a better radiative recombination rate can prominently enhance the luminescence of LEDs. From the IQE curves in Fig. 6(b), we can see that the efficiency droop of structure B is slighter than the conventional LEDs (i.e.,19.3% versus 65.2%). Moreover, as shown in Fig. 6(c), the light output power of structure B keeps almost the linear increase versus the current, the stronger intensity can be achieved even at the large current. Under the injection current of 250 mA, the light output power can be enhanced more than 81.7% by using step-graded AlGaN EBL compared with the conventional LEDs.



Fig. 6. (a) Spectra at 150 mA (b) IQE and (c) Light output versus current(L-I) for two structures.

4. Conclusions

The characteristics of LEDs with conventional EBL and step-graded EBL are investigated numerically. The specific EBL of structure B can significantly alleviate the electrostatic fields near the last QB and EBL. As a result, the efficiency of hole injection is enhanced and electron spillover can be suppressed. The LEDs with a step-graded EBL have better optical and electrical performance such as stronger spectrum intensity, higher IQE and larger light output power compared with the conventional LEDs. Furthermore, the troublesome issue of efficiency droop at the large injection current can be effectively improved.

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