Blue InGaN light-emitting diodes with dip-shaped quantum wells*

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InGaN based light-emitting diodes (LEDs) with dip-shaped quantum wells and conventional rectangular quantum wells are numerically investigated by using the APSYS simulation software. It is found that the structure with dip-shaped quantum wells shows improved light output power, lower current leakage and less efficiency droop. Based on numerical simulation and analysis, these improvements on the electrical and the optical characteristics are attributed mainly to the alleviation of the electrostatic field in dip-shaped InGaN/GaN multiple quantum wells (MQWs).

Keywords: GaN-based light-emitting diodes, dip-shaped quantum wells

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1. Introduction

InGaN/GaN-based high-brightness light-emitting diodes (LEDs) have attracted much attention because of their applications in signage, back lighting and general illumination. However, a well-known fundamental problem, referred to as "efficiency droop", needs to be solved, which is that the quantum efficiency decreases monotonically as the injection current increases. The "efficiency droop" is a major obstacle for the further application of high power GaN-based light emitting diodes. Many investigations have suggested that the polarization field is one of the main mechanisms of efficiency droop.[1−6] The conventional growth direction for a GaN-based LED is along the polar (0001) axis. Large piezoelectric and spontaneous polarization exists in GaN-based LEDs. The spontaneous polarization field in GaN-based material is caused by a lack of inversion symmetry along the [0001] orientation. The piezoelectric polarization in an InGaN-based quantum well (QW) arises due to different indium components inducing lattice mismatch between the quantum well (QW) and the quantum barrier (QB). The piezoelectric effect eventually leads to a strong electrostatic field and band bending situation within the active region. The large electrostatic field within the active region pulls the electrons and holes to the opposite sides, resulting in 'charge separation', which leads to spatial separations of the electrons and holes in the QW, and thus a severe reduction of electron–hole wave function overlap ($\Gamma_{\mathrm{e_hh}}$), consequently, a reduction in the radiative recombination rate and the internal quantum efficiency of the optoelectronic devices. Several methods have been proposed to alleviate the effect of the internal field due to piezoelectric polarization in blue InGaN LEDs, such as nonpolar (a-planes and m-planes) QWs grown on r-plane sapphire,[7,8] semi-polar QWs grown on m-plane sapphire,[9,10] and polarization-matched AlGaInN layers.[1−3] In addition, specific designs of non-rectangular QWs have been proposed, including triangular QWs,[11] staggered QWs,[12−14] trapezoidal QWs,[15] and dip-shaped QWs.[16] Recently, Zhao *et al.*[14,17] independently proposed a staggered QW structure which employs three InGaN layers, which is basically identical to the dip-shaped QW structure. Their results indicated that a dip-shaped QW structure showed improvements on the spontaneous recom-

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bination rate and output power. Park *et al.*'s[16] research showed that a dip-shaped QW structure had a smaller effective heavy hole mass, a larger spontaneous emission coefficient and optical matrix elements produced by Kane's parameter. However, many of the fundamental properties of dip-shaped QW structures are not yet well understood, because studies based on these structures are at an early developmental stage. Thus, the study of dip-shaped QW structures is quite necessary to obtain high internal quantum efficiency and output power. For the exploration of efficiency droop in blue InGaN LEDs, the reduction of the polarization field in the active region and electron leakage in p-type layer may be a key issue.

2. Structure and parameters

In this paper, the optical and electrical properties of conventional rectangular InGaN/GaN multiple quantum well (MQW) LEDs and the newly designed LEDs with dip-shaped quantum wells were investigated numerically with the APSYS simulation program, developed by the Crosslight Software Inc.[18] The blue InGaN-based LED was grown on a *c*-plane sapphire substrate. The structure consisted of a 4.0-μm-thick n-GaN layer (n-doping = 5×10^{18} cm^{-3}). The active region consisted of six 3-nm-thick $In_{0.16}Ga_{0.84}N$ QWs or 0.5-nm $In_{0.09}Ga_{0.91}N$/2 nm-$In_{0.18}Ga_{0.82}N$/0.5 nm-$In_{0.09}Ga_{0.91}N$ dip-shaped QWs, separated by six 10-nm-thick GaN barriers. On the top of the last QB was a 20-nm thick p-$Al_{0.1}Ga_{0.9}N$ (p-doping = 5×10^{17} cm^{-3}) electron blocking layer (EBL), and a 170-nm thick p-GaN (p-doping = 1×10^{18} cm^{-3}) was deposited finally. The device geometry was designed to be a rectangular shape of 300 μm×300 μm. The device structure is shown in Fig. 1.

The bandgap energies of InGaN and AlGaN ternary alloys can be expressed, respectively, as[19]

$$E_g(In_xGa_{1-x}N) = x\cdot E_g(InN) + (1-x)\cdot E_g(GaN) - 1.4x\cdot(1-x), \quad (1)$$

$$E_g(Al_xGa_{1-x}N) = x\cdot E_g(AlN) + (1-x)\cdot E_g(GaN) - 0.7x\cdot(1-x), \quad (2)$$

where E_g(InN), E_g(AlN), and E_g(GaN) are the bandgap energies of InN, AlN, and GaN, with values of 0.78, 6.25, and 3.51 eV, respectively.[19] The internal absorption within the LED device is assumed to be 500 m^{-1} and the operating temperature is assumed to be 300 K. To simplify the simulation, the light extraction efficiency is assumed to be 0.78. Other material parameters of the semiconductors used in the simulation can be found in Ref. [20]

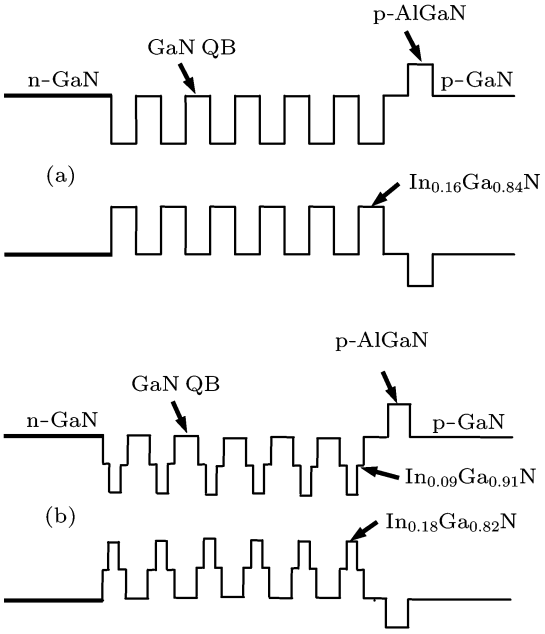


Fig. 1. Schematic diagram of GaN-based LED structures (a) with rectangular QWs, and (b) with dip-shaped QWs.

3. Results and discussion

The simulated light–current (L–I) performance curves of the two samples are plotted in Fig. 2. It can be seen that the difference between the two structures is very small at a low injection current. With the injection current further increasing, the difference between the two LEDs is enlarged. The output power of the dip-shaped QW LED increases linearly as the forward current increases, but for the rectangular QW LED, the output power slowly increases. The light output power of the dip-shaped QW LED is about twice as large as that of the rectangular QW LED at 200 mA.

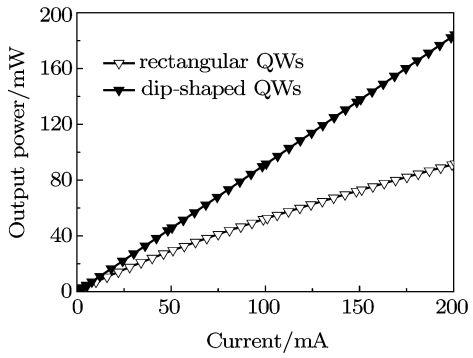


Fig. 2. Simulated L–I characteristics of two samples.

The simulated carrier concentrations of the two samples in MQWs cut from n-side to p-side at 200 mA

are plotted in Fig. 3. It can be seen that the difference between the two structures is obvious. The electron concentration in the rectangular QW is relatively uniformly distributed, but for the dip-shaped MQW, the electron concentration decreases sharply from the n-side to the p-side. In contrast to the distribution of electron concentration, the hole concentration in the dip-shaped QW is relatively uniformly distributed, but for the rectangular QW, the hole concentration decreases drastically from the p-side to the n-side.

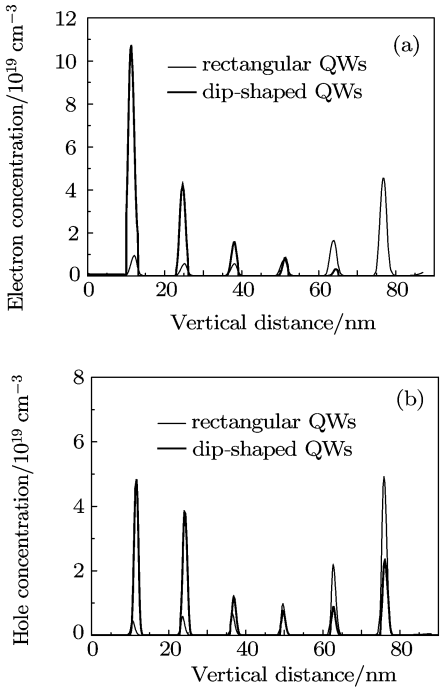


Fig. 3. (a) Electron and (b) hole concentration distributions in MQW at 200-mA forward current.

The spontaneous emission spectra of the two structures are plotted in Fig. 4. The spontaneous emission rates of the two structures both increase as the forward current increases from 50 mA to 200 mA, the peak wavelengths of the rectangular QWs and the dip-shaped QWs are 460 nm and 455 nm at 200 mA, respectively. The spontaneous emission rate of the dip-shaped QWs is larger than that of the rectangular QWs at each forward current. The ratio of the peak spontaneous emission rate intensity between the dip-shaped QWs and the rectangular QWs augments from 2 to 2.5 as the forward current increases from 50 mA to 200 mA.

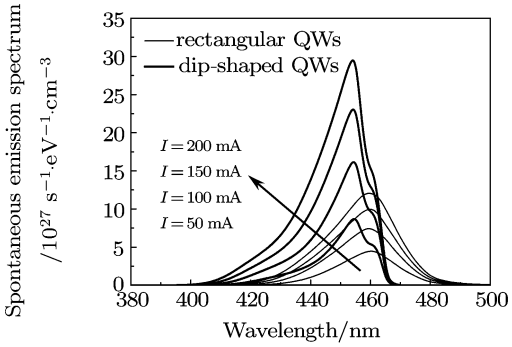


Fig. 4. Calculated spontaneous emission spectra of the two structures.

Simulated electrostatic fields throughout the two LED structures are shown in Fig. 5. The electrostatic field is uniformly distributed in rectangular QWs under 200 mA. The values of electrostatic field in the rectangular QWs is about 1 MV/cm, which is larger than that in QBs. In contrast to the rectangular QWs, the dip-shaped QWs have a smaller field strength compared with that of QBs. The electrostatic field is suppressed apparently in dip-shaped QWs, which is because the dip-shaped QWs include three layers, that is, two 0.5-nm thick $In_{0.09}Ga_{0.91}N$ layers sandwiched with a 2-nm-$In_{0.18}Ga_{0.82}N$ layer and thus the polarization field can be greatly reduced. We also notice that because a large electrostatic field exists at the interface between the last QB and the p-AlGaN EBL in rectangular QWs, the conduction band may be highly downward, which might cause the severe electron leakage current at a high level of current injection.

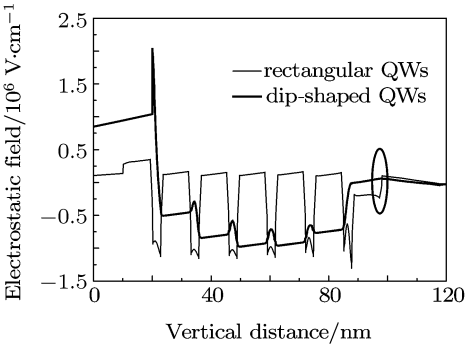


Fig. 5. Simulated electrostatic fields throughout the two LED structures under 200 mA forward current.

The calculated electron–hole wave function is plotted in Fig. 6. By the use of dip-shaped QWs, the electrostatic field in the active region can be effectively suppressed, hence, the overlap between electron and hole wave functions and the probability of radiative recombination can be markedly enhanced. The overlaps between electron and hole wave functions are 33.1%

for the rectangular QWs and 47.4% for the dip-shaped QWs. The increase of the overlap between electron and hole wave functions results in more electrons contributing to radiative recombination. Therefore, the issue of electron leakage, accordingly, is diminished.

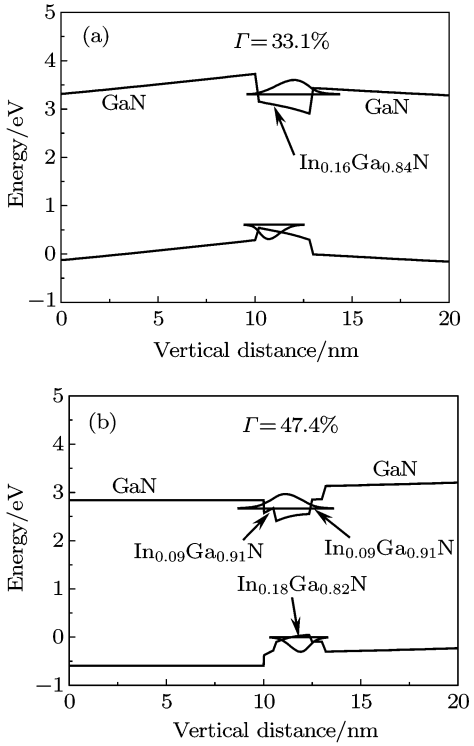


Fig. 6. Calculated band diagrams with ground-state electron and hole wave functions of (a) rectangular QWs and (b) dip-shaped QWs.

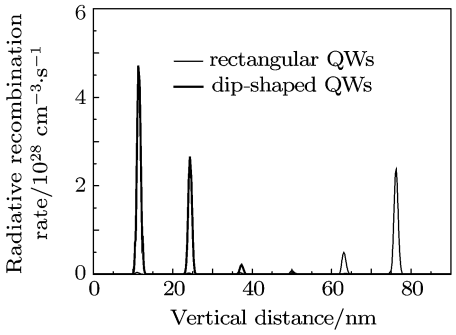


Fig. 7. Calculated radiative recombination rates in MQWs of two structures at 200-mA forward current.

The radiative recombination rates of the two structures are plotted in Fig. 7. It can be seen that the two structures show different characteristics in recombination rate distribution in the active region. For conventional rectangular QWs, the radiative recombination occurs mainly in QWs adjacent to p-side, but for dip-shaped QWs, the radiative recombination happens dominantly in QWs close to n-side. This phenomenon can be explained by the larger overlap between electron and hole concentrations, which results in a larger radiative recombination rate in these QWs. The total radiative recombination rate in dip-shaped QW is about three times larger than that in a rectangular QW.

The electron current density distributions of the two structures under 200 mA are shown in Fig. 8. For dip-shaped QWs, due to a lack of electrons in the QWs adjacent to the p-side, the electrons can be confined in QWs efficiently and the electron leakage can be neglected. It is noted that the first QW along the growth direction is located at 20 nm and a dramatic reduction in the electron density of dip-shaped QWs can be attributed to much more electron recombination with holes in these QWs compared with that in its counterpart. The larger electron density of dip-shaped QWs in the n-GaN region indicates that the holes can be recombined with electrons in MQWs more efficiently and less holes are injected into n-GaN area, thus inducing a higher electron current. Due to the large polarization field induced band bending in the active region, the QB and EBL can hardly block the electron overflow from QWs to p-type layer, and thus a severe electron current leakage in conventional structure with rectangular QWs is observed. However, for dip-shaped QWs, the inserted $In_{0.09}Ga_{0.91}N$ layer can reduce the lattice mismatch between the QW and QB, and thus alleviate the polarization field induced band bending and the electrons can be efficiently confined in MQWs, and finally the electron leakage current can be dramatically reduced. The electrons escaping from MQW active region can be recombined with holes in p-type region and thereby lower the LED efficiency. This reveals that the electron leakage current due to polarization fields is one of the main mechanisms that result in efficiency droop.

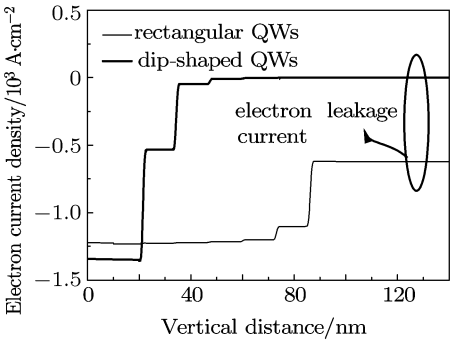


Fig. 8. Simulated electron current density throughout the two LED structures under 200-mA forward current.

The dependences of output power and internal quantum efficiency (IQE) on forward current are shown in Fig. 9. As the forward current increases, the two LED structures show different characteristics.

Due to the poor electron–hole overlap induced poor radiative recombination in the active region and the electron overflow, an obvious efficiency droop in the IQE of rectangular QW LEDs is observed, but for dip-shaped QWs, the IQE barely decreases. This can be explained by the dip-shaped QWs that can alleviate polarization field induced band bonding and the poor electron–hole wave function overlap, which leads to the effective blockage of electrons and the enhancement of the radiative recombination in the active region.

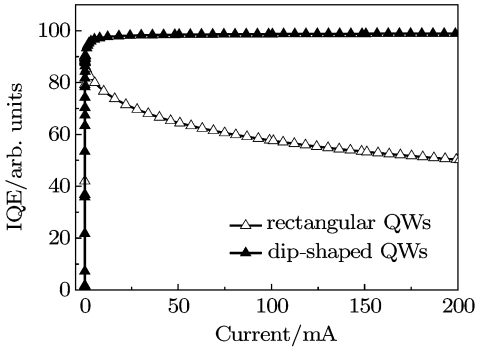


Fig. 9. IQE versus current for the two LED structures under study.

Our theoretical calculation indicated that dip-shaped QWs have many advantages over traditional rectangular QWs and Zhao's experimental results also demonstrated that dip-shaped QWs can be employed in green-emitting LEDs to improve the LED performance.[14] Compared to green-emitting LEDs, the low In-content and high quality InGaN QWs can be obtained relatively easily, and the reduction in technical challenge for growing dip-shaped QWs would be anticipated. So, it may become possible to employ dip-shaped QWs to improve the optical and electrical performance of InGaN-based blue LEDs.

4. Conclusions

In this paper, InGaN-based LEDs with traditional rectangular QWs and dip-shaped QWs are numerically investigated by using APSYS simulation software. It is found that the conventional structure with rectangular QWs has severe electron leakage, shows inferior light output power and has a dramatic efficiency droop. In contrast to rectangular QWs, an LED with dip-shaped QWs shows improved light output power, lower current leakage and less efficiency droop. Based on numerical simulation and analysis, these improvements on electrical and optical characteristics are attributed mainly to the alleviation of the electrostatic field in InGaN/GaN MQWs by using dip-shaped QWs.

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