Efficiency droop alleviation in blue light emitting diodes using the InGaN/GaN triangular-shaped quantum well*

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The InGaN/GaN blue light emitting diode (LED) is numerically investigated using a triangular-shaped quantum well model, which involves analysis on its energy band, carrier concentration, overlap of electron and hole wave functions, radiative recombination rate, and internal quantum efficiency. The simulation results reveal that the InGaN/GaN blue light emitting diode with triangular quantum wells exhibits a higher radiative recombination rate than the conventional light emitting diode with rectangular quantum wells due to the enhanced overlap of electron and hole wave functions (above 90%) under the polarization field. Consequently, the efficiency droop is only 18% in the light emitting diode with triangular-shaped quantum wells, which is three times lower than that in a conventional LED.

Keywords: efficiency droop alleviation, InGaN/GaN triangular quantum well, blue light emitting diode

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1. Introduction

In recent years, GaN-based light emitting diodes (LEDs) have attracted considerable attention due to their high potential efficiencies. This solid lighting source is expected to be a substitute for conventional incandescent and fluorescent lamps.[1,2] However, the further wide application of GaN-based blue LEDs is hindered by some critical unsolved problems, one of which is the efficiency droop, a phenomenon which shows that the internal quantum efficiency sharply decreases with increasing injection current under a high current density. Although various explanations are proposed, including carrier overflow from quantum wells (QWs),[3] Auger scattering,[4] junction heating,[5] and a piezoelectric polarization field,[6] controversies still exist in understanding the physical mechanisms. It seems that the efficiency droop can be alleviated by improving the quantum confinement in QWs.

The quantum confined Stark effect (QCSE) induced by the strong piezoelectric polarization field in the QWs decreases the overlap of electron and hole wave functions,[7] leading to the reduction of the radiative recombination rate, which is a direct factor influencing the efficiency of the LED. Several methods were proposed to reduce the QCSE, such as growing QWs along a nonpolar orientation, using the p-AlInN electron blocking layer,[8,9] and using the ultrathin InGaN QW and the quaternary AlInGaN barrier.[10,11] Recently, many researchers have focused on modifying the band profile shapes of the QWs to lessen the separation of electron and hole wave functions, such as using the step-like InGaN QWs and the staggered InGaN QWs.[12−14] Choi *et al.*[15] reported on QWs with a triangular indium (In) composition profile and obtained good results with regard to increasing the optical emitting intensity and reducing the operation voltage. Yang *et al.*[16] showed that the InGaN triangular quantum well (TQW) exhibits remarkable increases in both the optical gain and the TE mode com-

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ponent. Zhu *et al.*[17] demonstrated that the quantum efficiency of the LED with triangular wells prevails over that with rectangular quantum wells (RQWs). Wang *et al.*[18] manifested that the spontaneous emission rate of graded QW is higher than that of RQW. Nevertheless, the band profile modulation of the QW is difficult to achieve in metal organic chemical vapor deposition (MOCVD) growth and relies on more precision growth methods such as molecular beam epitaxy (MBE), and few theoretical analyses have been reported about the device performance and the efficiency droop behavior of the GaN-based TQW (triangular quantum well) LED.

In this paper, we investigate the physical characteristics of InGaN/GaN blue TQW LED theoretically. The energy band profile, the carrier concentration, the overlap of electron and hole wave functions at the Brillouin zone center, the radiative recombination rate, and the efficiency droop behavior are discussed and compared with those of a conventional RQW LED.

2. Model and method

We discuss the optical and electrical properties of the TQW LED by using the numerical program APSYS,[19] which was developed by Crosslight Software Inc. The APSYS is capable of dealing with the physical properties of LEDs by solving Poisson's equation, current continuity equations, carrier transport equations, quantum mechanical wave equations, and photon rate equations.[20]

The TQW LED and the conventional RQW LED are both grown on the c plane, and the In composition in the TQWs linearly varies along the growth direction. From bottom to up, the LED structure consists of a 100-μm-thick sapphire substrate, a 3-μm-thick n-type GaN layer with an Si-doping concentration of 3×10^{18} cm^{-3}, three pairs of undoped $In_xGa_{1-x}N$/GaN multiple QWs with 3-nm-thick wells and 10-nm-thick barriers in the active region, a 20-nm-thick p-doped $Al_{0.15}Ga_{0.85}N$ e-blocking layer with a p-doping concentration of 3×10^{17}cm^{-3}, and a 200-nm-thick p-doped GaN layer with a p-doping concentration of 1.2×10^{18} cm^{-3}. As shown in Fig. 1, the In composition is fixed at 0.15 for the conventional RQW LED, and the center In composition of the QWs is fixed at 0.25 for the TQW LED, which is selected to maintain a transition wavelength of 460 nm similar to that in a conventional RQW LED. The device geometry is 300 μm × 300 μm. In our simulation, the polarization charge at the interface is calculated using the non-linear formulas in Ref. [21]. The band offset ratio (ΔE_C:ΔE_V) is 7:3.[22] The percentage of the screening effect due to defects is fixed at 50%. The other parameters used in our simulation can be found in Ref. [23]. We set the first QW close to the n-side, and the last one close to the p-side in our simulation.

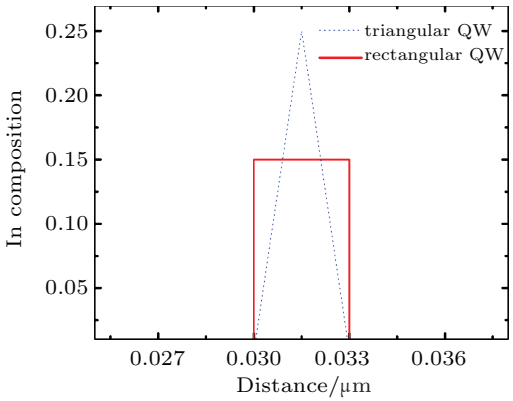


Fig. 1. (colour online) Schematic diagram of the In composition distributions in RQW and TQW.

3. Results and discussion

Figure 2 shows the energy band diagrams and the quasi-Fermi levels of the conventional RQW LED and the TQW LED at 600 mA. It is found that the energy band of the RQW LED has severe tilting due to the existence of a polarization electrostatic field, which is detrimental to the carrier distribution and the overlap of electron and hole wave functions, as seen in Fig. 2(a). For the TQW LED, figure 2(b) shows that the energy band of the quantum barriers is flatter than that of the RQW LED, which suggests that the internal polarization field in the TQWs is much smaller than that in the RQWs at the edge region. Meanwhile, the extreme energy points of the conduction and valance bands are still localized at the center of the triangular wells.

We now discuss the carrier distributions in the three QWs under the polarization conditions. Figure 3(a) shows that the electron concentration in the TQWs is higher than that in the RQWs, which means that the electron leakage in the RQW LED is worse than that in the TQW LED. As shown in Fig. 3(b), the hole concentration in the first RQW is smaller than that in the first TQW, but the hole concentration exhibits the opposite situation in the last two QWs, which corresponds to the quasi-Fermi level closer to the valance band in the last two RQWs, as illustrated

in Fig. 2. Therefore, it is concluded that the TQW LED does not improve the hole concentration distribution.

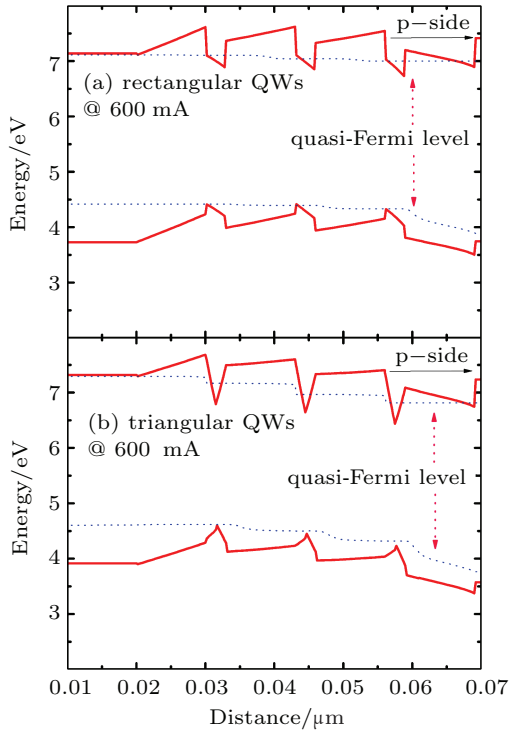


Fig. 2. (colour online) Energy band diagrams near the active regions of (a) RQW and (b) TQW LEDs.

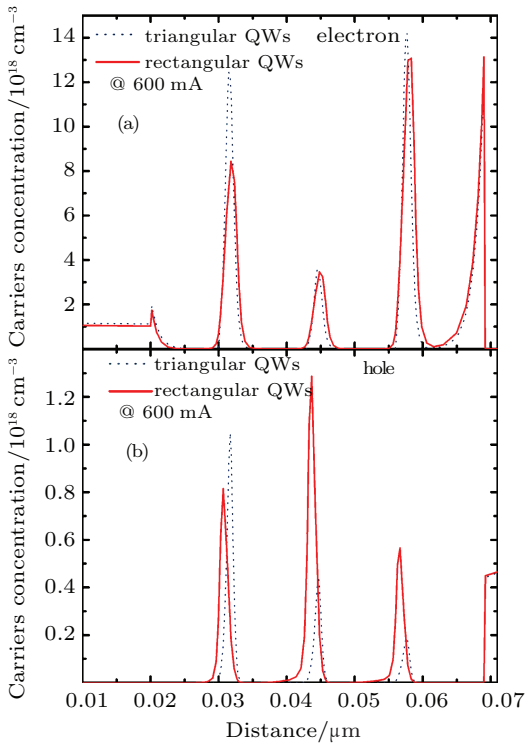


Fig. 3. (colour online) (a) Electron and (b) hole concentrations of RQW and TQW LEDs around the active region at 600 mA.

In addition, the overlap of electron and hole wave functions is also analyzed in the calculation, which is related to the radiative recombination rate. We focus our attention on the TE-mode transition between the lowest conduction subband (C1) and the uppermost valence subband (HH1), which is the dominant component in the radiative recombination. Figures 4(a) and 4(b) show the electron and the hole wave function envelopes of the C1–HH1 transition at the three QWs in both structure models at 600 mA, respectively. In Fig. 4(a), for the conventional RQW LED, it is found that obvious shifts exist in the electron and the hole wave function due to the band bending caused by the strong polarization electrostatic field, and electrons and holes tend to accumulate at different sides of the InGaN wells. The overlap of electron and hole wave functions is 56.17% in the first QW, and 45.64% and 37.29% in the last two QWs, respectively. On the contrary, the overlaps of electron and hole wave functions reach 95.71%, 96.16%, and 94.14% in the corresponding QWs of the TQW LED, which are shown in Fig. 4(b). The higher overlaps of electron and hole wave functions in the TQWs indicate that the spatial shifts of electron and hole are remarkably reduced.

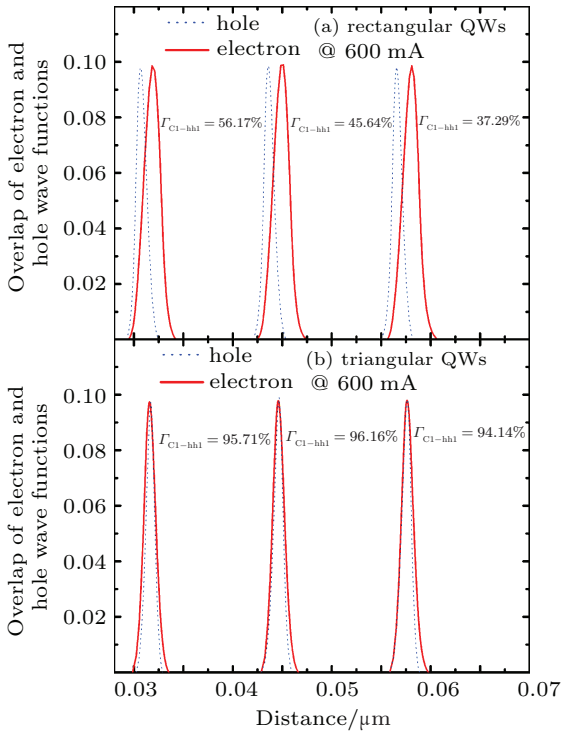


Fig. 4. (colour online) Electron and hole wave function envelopes of C1 and HH1 at the three quantum wells of (a) RQW and (b) TQW LEDs at 600 mA.

Thus the triangular well is beneficial for confining electrons and holes, especially for holes. The result agrees

with the previous report using the $\boldsymbol{k}\cdot\boldsymbol{p}$ method,[16] and it can be interpreted as follows. First of all, the large polarization electrostatic field existing at the edge of the RQW is caused by the large lattice mismatch between the well and the barrier, and the electron and hole are separated to the opposite edge regions of the well. However, the internal polarization electrostatic field is distributed gradually along the TQW due to the graded In composition. Therefore, the distribution of a higher internal electrostatic field at the center of the triangular well and a lower one at the edge of the well can reduce the opposite shifts of electron and hole. Simultaneously, the extreme energy points of valance and conduction bands are positioned at the center of the wells as mentioned above, and it can be found that both the electron wave function of the conduction band and the hole wave function of the valance band are close to the center of the well. As a result, a higher overlap of electron and hole wave functions is obtained in the TQW model. Therefore, a higher radiative recombination rate and a higher internal quantum efficiency for the TQW LED are expected.

Figure 5 shows the radiative recombination rates of the TQW and the RQW LEDs at 600 mA. The result shows higher radiative recombination rates in all quantum wells of the TQW LED. In the first quantum well, the larger carrier concentration and the better carrier confinement lead to the higher radiative recombination rate, which is enhanced by about 4 fold compared with that of the conventional RQW. Although the second and third quantum wells show higher hole concentrations for the RQW LED, the radiative recombination rates of the RQW LED are still lower than those of the TQW LED. Therefore, the lower radiative recombination rate arises from the poor overlap of electron and hole wave functions, and the carrier concentration is not the key factor for the reduction of efficiency in the simulation of the two LED structures with the same parameters as mentioned above.

The higher radiative recombination rate indicates that the internal quantum efficiency can be enhanced in the TQW LED, which is shown in Fig. 6. The output power of the TQW LED is twice that of the RQW LED at 600 mA. Moreover, the maximum output power does not emerge at 600 mA, while the performance of the RQW LED already deteriorates seriously at 600 mA due to the efficiency droop. The efficiency droop is defined as $(\eta_{\rm peak} - \eta_{600\ {\rm mA}})/\eta_{\rm peak}\times 100\%$. The smaller maximum efficiency is seen in the RQW LED due to the QCSE influenced by the internal polarization field, and the efficiency droop behavior (55%) occurred in the conventional RQW LED can be seen in Fig. 6(b). For the TQW LED, the efficiency droop is reduced to 18%, which is significantly improved compared with the RQW LED. We believe that the alleviation of the efficiency droop of the TQW LED is attributed to the higher overlap of electron and hole wave functions under the high injection current.

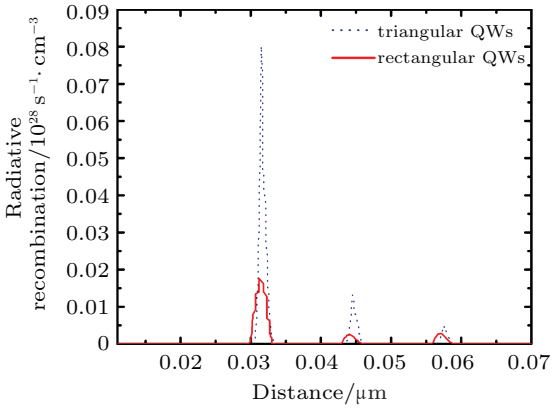


Fig. 5. (colour online) Radiative recombination rates of RQW and TQW LEDs at 600 mA.

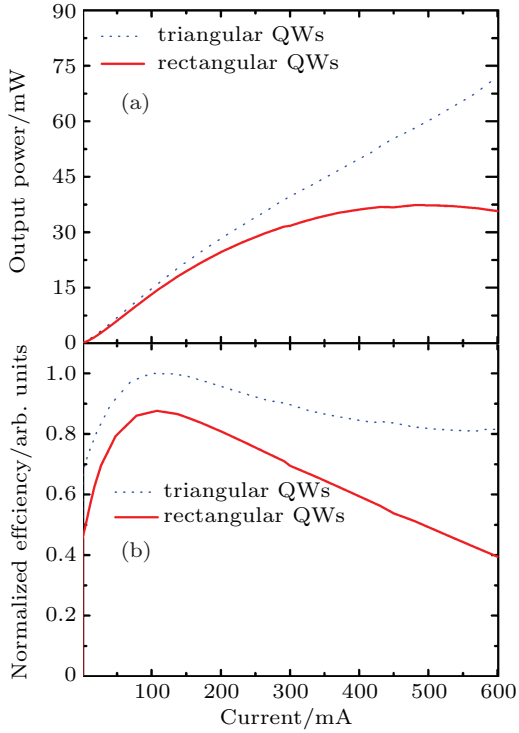


Fig. 6. (colour online) (a) Light output power and (b) internal quantum efficiency each as a function of current for RQW and TQW LEDs.

4. Conclusion

In summary, the physical characteristics of the InGaN/GaN LEDs with TQWs and RQWs are an-

alyzed using theoretical simulations. The simulation results reveal that the InGaN/GaN TQW LED exhibits a higher radiative recombination rate than the conventional RQW LED due to the enhanced overlap of electron and hole wave functions. Furthermore, our simulation shows the efficiency droop is reduced from 55% to 18% at 600 mA compared with the RQW LED. The cause of this should be attributed to the larger overlap of electron and hole wave functions. This result confirms that the TQW design does contribute to the alleviation of the efficiency droop. This TQW LED structure is expected to improve the performance of blue InGaN/GaN LEDs at high injection currents, however further experimental investigations are necessary in the future.

References

[1] Pimputkar S, Speck J, DenBaars S P and Nakamura S 2009 *Nat. Photonics* **3** 180

[2] Schubert E F and Kim J K 2005 *Science* **308** 1274

[3] Kim M H, Schubert M F, Dai Q, Kim J K, Schubert E F, Piprek J and Park Y 2007 *Appl. Phys. Lett.* **91** 183507

[4] David A and Grundmann M J 2010 *Appl. Phys. Lett.* **96** 103504

[5] Chen Y X, Shen G D, Guo W L, Xu C and Li J J 2011 *Chin. Phys.* B **20** 017204

[6] Tao Y B, Chen Z Z, Zhang F F, Jia C Y, Qi S L, Yu T J, Kang X N, Yang Z J, You L P, Yu D P and Zhang G Y 2010 *J. Appl. Phys.* **107** 103529

[7] Bernardini F and Fiorentini V 1997 *Phys. Rev.* B **56** R10024

[8] Rau B, Waltereit P, Brandt O, Ramsteiner M, Ploog K H, Puls J and Henneberger F 2000 *Appl. Phys. Lett.* **77** 3343

[9] Lu T P, Li S T, Zhang K, Liu C, Xiao G W, Zhou Y G, Zheng S W, Yin Y A, Wu L J, Wang H L and Yang X D 2011 *Chin. Phys.* B **20** 098503

[10] Akasaka T, Gotoh H and Kobayashi Y 2006 *Appl. Phys. Lett.* **89** 101110

[11] Kwon S Y, Kim H J, Yoon E, Jang Y, Yee K J, Lee D, Park S H, Park D Y, Cheong H, Roi F and Dang L S 2008 *J. Appl. Phys.* **103** 063509

[12] Yen S H and Kuo Y K 2008 *Opt. Commun.* **281** 4735

[13] Lu T P, Li S T, Zhang K, Liu C, Xiao G W, Zhou Y G, Zheng S W, Yin Y A, Wu L J, Wang H L and Yang X D 2011 *Chin. Phys.* B **20** 108504

[14] Zhao H P, Liu G Y, Zhang J, Poplawsky J D, Dierolf V and Tansu N 2011 *Opt. Express* **19** A991

[15] Choi R J, Hahn Y B and Shim H W 2003 *Appl. Phys. Lett.* **82** 2764

[16] Yang Z W, Wei Q Y, Yu T, Zhang Y Z, Chen W H and Hu X D 2009 *Appl. Phys. Lett.* **94** 061120

[17] Zhu L H, Zheng Q H and Liu B L 2009 *Semicond. Sci. Technol.* **24** 125003

[18] Wang L, Li R, Yang Z W, Li D, Yu T, Liu N Y, Liu L, Chen W H and Hu X D 2009 *Appl. Phys. Lett.* **95** 211104

[19] APSYS by Crosslight Software Inc. Burnaby, Canada, available at http://www.crosslight.com

[20] Zhang Y Y and Yao G R 2011 *J. Appl. Phys.* **110** 093104

[21] Fiorentini V, Bernardini F and Ambacher O 2002 *Appl. Phys. Lett.* **80** 1204

[22] Martin G, Botchkarev A, Rockett A and Mockoc H 1996 *Appl. Phys. Lett.* **68** 2541

[23] Vurgaftman I and Meyer J R 2003 *J. Appl. Phys.* **94** 3675