第 34 卷　第 1 期　　　　　　发　光　学　报　　　　　　Vol. 34　No. 1
2013 年 1 月　　CHINESE JOURNAL OF LUMINESCENCE　　Jan., 2013

Article ID: 1000-7032(2013)01-0066-07

High Internal Quantum Efficiency Blue Light-emitting Diodes with Triangular Shaped InGaN/GaN Multiple Quantum Wells

ZHAO Fang, ZHANG Yun-yan, SONG Jing-jing,
DING Bin-bin, FAN Guang-han*

(*Institute of Optoelectronic Materials and Technology*, *South China Normal University*, *Guangzhou* 510631, *China*)

* *Corresponding Author*, *E-mail*: *gfan@scnu.edu.cn*

Abstract: The internal quantum efficiency (IQE) of InGaN quantum wells (QWs) light-emitting diodes (LEDs) is numerically investigated, which involved its emission spectra, carrier concentrations, energy band, electrostatic field and internal quantum efficiency. Optical properties of InGaN/GaN LEDs with varied QW numbers are numerically studied. The results reveal that, for the LEDs with conventional rectangular shaped QWs, two quantum wells (2-QWs) units structure has better optical performance than 5-QWs and 7-QWs structures. The advantages of nitride-based LEDs with triangular shaped InGaN/GaN multiple quantum wells (MQWs) are also discussed. The simulation results indicate that the triangular shaped MQW LEDs exhibit a higher electrical luminescence (EL) intensity, higher IQE and a stronger light-output power than the conventional rectangular MQW LEDs. All the advantages are due to the higher carrier injection efficiency and recombination rate which are caused by the higher electron-hole wave function overlap, and small quantum confined stark effect (QCSE).

Key words: light-emitting diodes; triangular shaped quantum well; numerical simulation

CLC number: TM23; O242.1　　**Document code**: A　　**DOI**: 10.3788/fgxb20133401.0066

具有三角形 InGaN/GaN 多量子阱的高内量子效率的蓝光 LED

赵　芳, 张运炎, 宋晶晶, 丁彬彬, 范广涵*

(华南师范大学 光电子材料与技术研究所, 广东 广州　510631)

摘要: 对 InGaN 量子阱 LED 的内量子效率进行了优化研究。分别对发光光谱、量子阱中的载流子浓度、能带分布、静电场和内量子效应进行了理论分析。对具有不同量子阱数量的 InGaN/GaN LED 进行了理论数值比对研究。研究结果表明,对于传统结构的 LED 而言,2 个量子阱的结构相对于 5 个和 7 个量子阱具有更好的光学性能。同时还研究了具有三角形量子阱结构的 LED,研究结果显示,三角形多量子阱结构具有较高的电致发光强度、更高的内量子效率和更好的发光效率,所有的优点都归因于较高的电子-空穴波函数重叠率和低的 Stark 效应所产生的较高的载流子输入效率和复合发光效率。

关　键　词: 发光二极管; 三角形量子阱; 数值模拟

收稿日期: 2012-09-05; **修订日期**: 2012-10-11
基金项目: 国家自然科学基金(61176043); 广东省战略性新兴产业专项资金(2010A081002005,2011A081301003); 广东省教育部产学研结合项目(2010B090400192)资助项目

作者简介: 赵芳(1987 –), 女, 陕西宝鸡人, 主要从事光电子材料的研究。
E-mail: zhaofang1026@yahoo.com.cn

1 Introduction

The visible Ⅲ-Ⅴ nitride material light-emitting diodes (LEDs) have received much attention due to their wide application in full-color display, liquid crystal display back-lighting and illumination[1-3]. The InGaN alloy is especially pivotal because it constitutes active region in quantum well structure and emits light by the recombination of electrons and holes injected into the InGaN QWs[4-6]. However, many problems still prevent InGaN/GaN quantum well based LEDs from acquiring higher efficiency[7-12]. There are two reasons acknowledged widely. One is the poor hole injection efficiency. Due to their relatively high effective mass and very low mobility in nitride-based materials, holes are very difficult to move in the nitride-based materials and the injection efficiency of holes is very low. Furthermore, the electron blocking layer (EBL) is found to act as a potential barrier also for holes to transport into the active region, which results in non-uniform distribution of holes in the MQW region[13]. That seriously affects the radiative recombination in the QWs. The other challenge is the quantum confined stark effect (QCSE)[14-16] which is associated with the strong piezoelectric (PZ) field in the wurtzite III-nitride QW due to the large lattice mismatch between InGaN and GaN. The strong piezoelectric field leads to charge separation effect, which in turn impacts both the radiative recombination rate and carrier dynamics in the QWs.

It has been realized that the effect of QW number does not follow the pattern of "the more the better". Seeing that the correlation between QW numbers and the optical performance of the LEDs is not linear, there should be an optimized value of QW number to achieve the best optical performance of InGaN LEDs.

The most commonly used QW is rectangular shape, in which the indium composition is kept at a constant value. In this case, the PZ fields significantly decreases the electron-hole wave function overlap and accordingly leads to a small radiative recombination rate and poor light emission. Recently, several approaches have been proposed to suppress the charge separation issue by employing novel QWs with improved electron-hole wave function overlap such as non-polar InGaN QWs[17-19], staggered InGaN QW[20-22], InGaN-delta-InN QW[23], dip-shaped QW[24], *etc.* Their results indicate that triangular shaped QWs provide higher electron-hole wave function overlap and exhibit increased optical gain. However, many of the fundamental properties are not yet well understood, because studies based on these structures are at an early development stage. Thus, the study of triangular shaped QW structure is quite necessary to obtain high internal quantum efficiency and output power.

In this paper, an optimized value of QW number for conventional LEDs is discussed, triangular and shaped QWs are proposed to relieve the above issues. The optical and electrical properties of conventional LEDs with rectangular QWs and newly designed LEDs with triangular shaped QWs are investigated numerically with the APSYS (Advance Physical Model of Semiconductor Devices) simulation software, which was developed by the Crosslight Software Inc. APSYS software is capable of dealing with the physical properties of LEDs by solving the Poisson's equation, current continuity equations, carrier transport equation, quantum mechanical wave equation, and photon rate equation.

2 Structure and Parameters

The conventional LED used in this paper was grown on a *c*-plane sapphire substrate. The LED comprises a 20-nm-thick undoped GaN layer, and a 4.5-μm-thick n-type GaN layer (The concentration of n-doping is 5×10^{18} cm^{-3}) and the active region consists of two 3-nm-thick $\mathrm{In_{0.2}Ga_{0.8}N}$ well layers separated by three 15-nm-thick n-type GaN barrier layers (The concentration of n-doping is 1×10^{18} cm^{-3}). On the top of the active region is a 20-nm-thick p-type $\mathrm{Al_{0.15}Ga_{0.85}N}$ EBL and a 0.15-μm-thick p-type GaN cap layer (The concentration of p-doping is 7×10^{17} cm^{-3}). Based on this structure, the QW number is varied to explore an optimized value of QW number for conventional LEDs. The device geometry was designed with a rectangular shape of 300 μm × 300 μm. The operating temperature is assumed to be 300 K. The light extraction efficiency is assumed to be 0.78[25]. The parameters of the newly designed triangular structure are the same as the conventional rectangular LEDs but for the traditional rectangular shaped QWs are replaced by triangular shaped QWs which are formed by modulating the indium composition in the InGaN well. The detail structure of the QWs can be seen in Fig. 1.

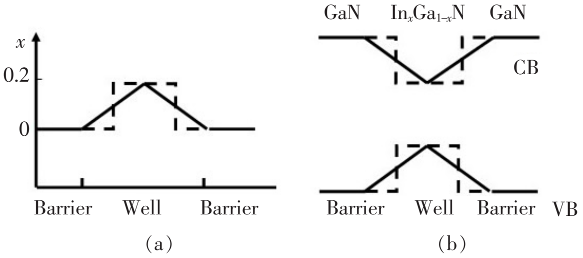

Fig. 1 (a) In composition profile of the well and barrier layer, and (b) energy structure of a triangular quantum well (solid line) compared with rectangular one (dash line).

The band gap energies of InGaN and AlGaN ternary alloys can be expressed, respectively, as[26]

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

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

Where $E_g(InN)$, $E_g(AlN)$, and $E_g(GaN)$ are the band gap energies of InN, AlN, and GaN, with the values of 0.78, 6.25, 3.4 eV, respectively. Most of the parameters in this paper are the same as in Ref. [27]. Other material parameters of the devices used in the simulation can be found in Ref. [28]. Chang Shengxia, *et al.* studied the advantages of blue InGaN light-emitting diodes LEDs with InGaN barriers using these parameters and the same software. The results which were published in *Applied Physics Letters* in 2011 show good agreement between the experimental data and their simulations.

3 Results and Discussion

Fig. 2 illustrates the carrier concentrations of InGaN/GaN LEDs against different QW numbers. The 5-QWs and 7-QWs structure have worse performance because the carriers are distributed non-uniformly in different QWs and the overlap of electrons and holes in the active region is poor. What's more, the hole concentration in the first three QWs near n-type layer can hardly be observed. Whilst the performance of the 2-QWs structure is improved because the carriers distribute more uniformly throughout all QWs and the overlap between the electrons and holes in all QWs increases markedly. As a result, it can be seen from the Fig. 2 that the 2-QWs structure has the most even electron distribution. The total hole concentration in its active region is much larger than that of the other two structure. As a consequence, the radiative recombination rate in the 2-QWs structure is more uniform, and as shown in Fig. 3(a), almost all of the wells can contribute to the emission efficiency which result in a smaller efficiency droop (by 13% shown in Fig. 3). In comparison, the non-uniform carrier distribution means that only last two QWs contribute to radiative recombination in the conventional LEDs. These phenomenon are closely related to results presented in the Fig. 3 (b), which indicates that both 5-QWs and 7-QWs structure show serious efficiency droop when

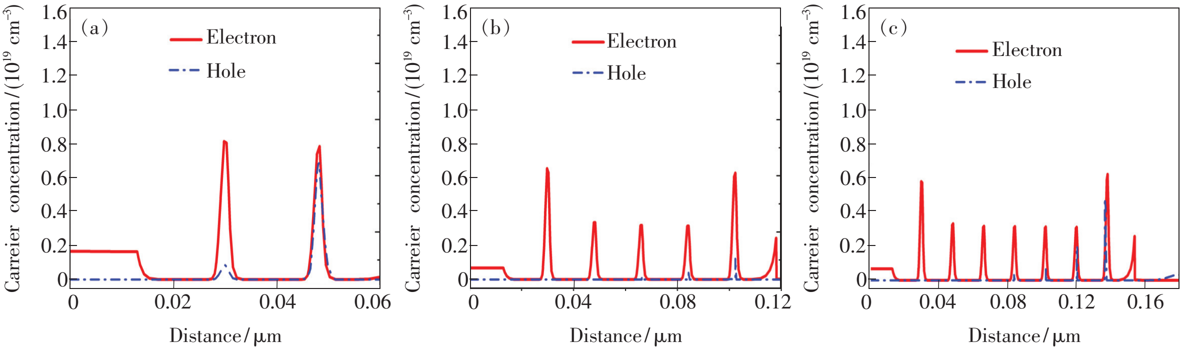

Fig. 2 The carriers distributions of (a) 2-QWs structure, (b) 5-QWs structure and (c) 7-QWs structure.

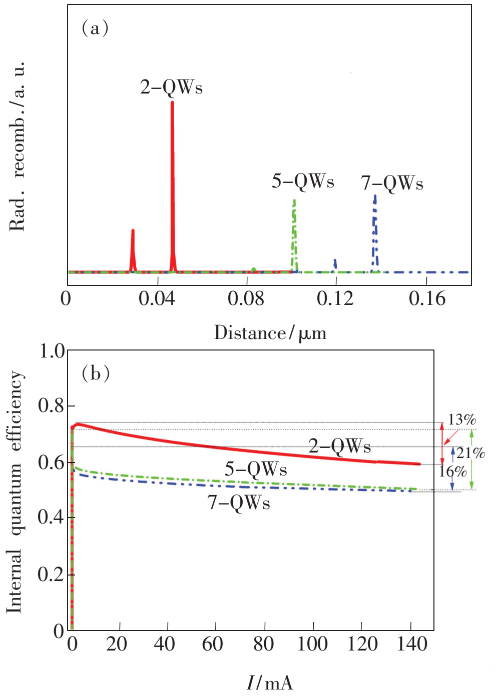

Fig. 3　(a) Radiative recombination rates of 2-QWs, 5-QWs and 7-QWs structure at 20 mA, respectively (There are small location excursions in horizontal axes for better observation). (b) IQE of 2-QWs, 5-QWs and 7-QWs structure.

the current is increasing, by 21% and 16%, respectively. However, the total radiative recombination rate of 2-QWs has not achieved the expected rate yet. Therefore, in the subsequent studies, with the conventional rectangular shaped 2-QWs LEDs as a reference, the merits of nitride-based LEDs with triangular shaped InGaN/GaN MQWs are discussed.

As is shown in Fig. 4, the spectrum intensity of the LED with triangular wells is much stronger than that of the LED with rectangular wells and there is red shift in rectangular structure, which can be ascribed to the potential merits of triangular wells' shape. It is very apparent that the LED with triangular wells has higher IQE and a stronger light-output power. Therefore, it can be found that the optical and electrical performances of the newly designed triangular structure are much better than those of the conventional structure.

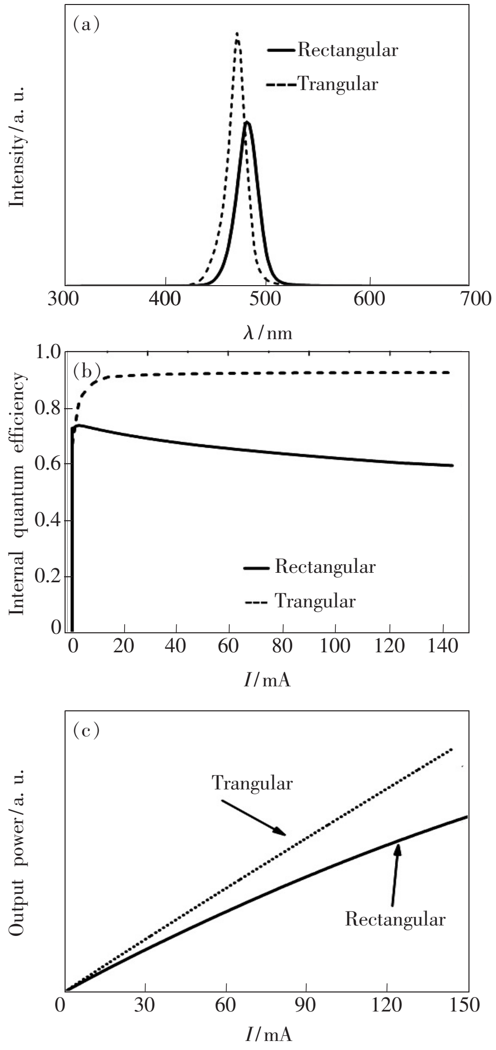

Fig. 4　(a) Spectra at 20 mA, (b) IQE, (c) output power *vs.* injection current of LEDs with triangular and rectangular wells, respectively.

Fig. 5 shows the band structure of the two structures. The lattice mismatch became worse with the increase of In composition in QWs. Therefore, the piezoelectric field in the QWs would be bigger with higher In composition which would cause severe band bending. In rectangular QWs, the In component is much higher than that of triangular ones. Thus, the rectangular ones have much bigger band bending than the triangular ones which can be seen in Fig. 5. In Fig. 5, Ⅰ, Ⅳ are effective potential barrier for electrons and Ⅱ, Ⅲ, Ⅴ, Ⅵare effective potential barrier for holes which are caused by band bending effect. Ⅳ is much higher than Ⅰ. Electrons are easier to inject into the active layer in LEDs with triangular QWs through the lower electron barrier Ⅰ. As can be seen in the ellipse in Fig. 6(b), the electron concentration of the first QW in LEDs with triangular QWs is much bigger than that of the LED

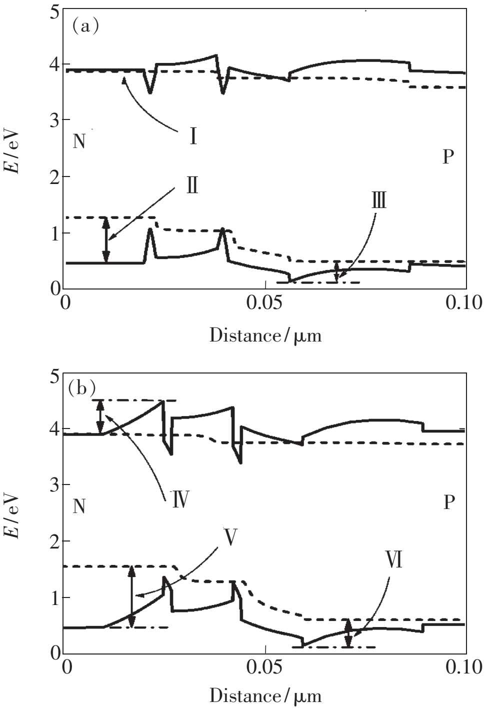

Fig. 5 Energy band diagrams of (a) triangular structure and (b) rectangular structure at 20 mA

with rectangular QWs. Due to the same reason, the band bending of EBL in LEDs with triangular QWs is much smaller than that of with rectangular QWs. Therefore, in Fig. 5, the effective potential barrier Ⅲ is much lower than Ⅵ for holes. Thus, holes are easier to inject into the active layer in LEDs with triangular QWs because of the lower hole barrier Ⅲ.

As can be seen in the ellipse in Fig. 6(a), the hole concentration of the second QW in the new structure is much bigger than that of conventional structure. Electrostatic fields near the active region of the two LEDs are shown in Fig. 6(c). The electrostatic field is suppressed apparently in triangular shaped QWs. It is apparent that because a large electrostatic field around the interface between the last quantum barrier and the p-AlGaN EBL in rectangular QWs, the intense downward conduction banding might cause the severe electron leakage current at a high current injection density. It is one of the reasons why the IQE of the rectangular structure is dropping dramatically with the increase of current.

In Fig. 6(d), the radiative recombination rate of the triangular structure is much bigger than rectangular structure. Rectangular QW structure is generally used with constant In composition in InGaN for the well region. Due to the QCSE, electrons and holes tend to accumulate at opposite sides of the well.

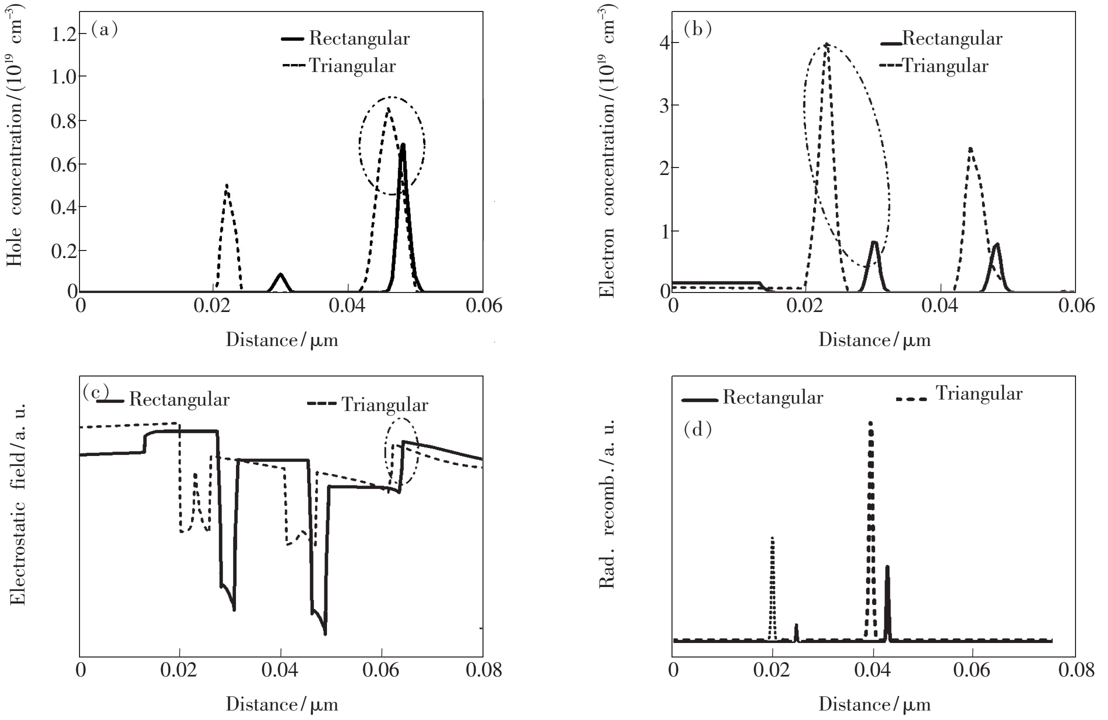

Fig. 6 (a) Distribution of hole concentration, (b) electron concentration, (c) simulated electrostatic fields, and (d) radiative recombination rates of the triangular structure and rectangular structure at 20 mA (there are small location excursion in horizontal axes for better observation).

In this case, indirect recombination is expected and thereby poor light emission is expected due to the high spatial separation of wave function. The low spatial shift in wave function can be explained as follow: the apparent spatial shift in the carriers' wave function is attributed to the potential incline at the edge of the rectangular QW, while triangular structure is realized by changing In concentration linearly to locate the lowest band edge in the middle of QW. Thus, a lower PZ field at the edge significantly influences the triangular QW into reducing the shift in wave functions, increasing in overlap and the band bending. Furthermore, the band bending caused by the PZ field in triangular QW does not stagger the lowest point in the conduction band and the highest point in the valence band. Those are helpful in confining the wave functions in both the conduction band and the valence band to the well center and in maintaining a higher wave function overlap. Therefore, triangular QWs provide higher electron-hole wave function overlap and are less affected by the QCSE. In consequence, it brings about higher efficiency in radiative recombination shown in Fig 6. (d) and higher power output shown in Fig. 4(c). In addition, the stability and reproduction are greatly improved.

4 Conclusion

In summary, for the LEDs with conventional rectangular shaped QWs, the 2-QWs structure has better optical performance than the ones with 5-QWs and 7-QWs, primarily due to the former structure provides more opportunity for electrons and holes to meet which results in relatively even carriers distribution and less severe efficiency droop. The LEDs with triangular wells have better electrical and optical performances than the conventional ones with rectangular QWs such as electrical luminescence, higher IQE and higher output power. All the advantages are mainly due to smaller PZ field and less affection by QCSE. Furthermore, the stability and reproduction are greatly improved. Thus the triangular QW structure is a promising structure for the active region for LEDs and LDs.

References:

[1] Strite S, Morkoc H. GaN, AlN, and InN: A review [J]. *J. Vac. Sci. Technol.* B, 1992, 10(4):1237-1267.

[2] Pearton S J, Zolper J C, Shul R J, *et al.* GaN:Processing, defects, and devices [J]. *J. Appl. Phys.*, 1999, 86(1):1-78.

[3] Jain S C, Willander M, Narayan J, *et al.* Ⅲ-nitrides:Growth, characterization, and properties [J]. *J. Appl. Phys.*, 2000, 87(3):965-1007.

[4] Chen G C, Fan G H. Study on long-wavelength optical phonons in hexagonal InAlGaN crystals [J]. *Chin. J. Lumin.* (发光学报), 2012, 33(8):808-811 (in English).

[5] He T, Chen Y, Li H, *et al.* Optimization of two-step AlN buffer of *a*-plane GaN films grown on *r*-plane sapphire by MOCVD [J]. *Chin. J. Lumin.* (发光学报), 2011, 32(4):363-367 (in English).

[6] Xing B, Cao W Y, Du W M. Temperature dependent PL of InGaN/ GaN multiple quantum wells with variable content of In [J]. *Chin. J. Lumin.* (发光学报), 2010, 31(6):864-869 (in Chinese).

[7] Li Y L, Huang Y R, Lai Y H. Efficiency droop behaviors of InGaN/GaN multiple-quantum-well light-emitting diodes with varying quantum well thickness [J]. *Appl. Phys. Lett.*, 2007, 91(18):181113-1-3.

[8] Ki M H M, Schubert M F, Dai Q, *et al.* Origins of efficiency droop in GaN-based light-emitting diodes. [J]. *Appl. Phys. Lett.*, 2007, 91(13):133507-1-3.

[9] Schubert M F, Xu J, Kim J K, *et al.* Polarization-matched GaInN/AlGaInN multi-quantum-well light-emitting diodes with reduced efficiency droop [J]. *Appl. Phys. Lett.*, 2008, 93(4):041102-1-3.

[10] Rozhansky I V, Zakhei D A M. Analysis of dependence of electroluminescence efficiency of AlInGaN LED heterostructures on pumping [J]. *Phys. Status Solidi* C, 2006, 3(6):2160-2164.

[11] Kim A Y, Goetz W, Steigerwald D A, *et al.* Performance of high-power AlInGaN light emitting diodes [J]. *Phys. Status Solidi* A, 2001, 188(1):15-21.

[12] Rozhansky I V, Zakheim D A. Analysis of processes limiting quantum efficiency of AlGaInN LEDs at high pumping [J]. *Phys. Status Solid* A, 2007, 204(1):227-230.

[13] David A, Grundmann M J, Kaeding J F, *et al.* Carrier distribution in (0001) InGaN/GaN multiple quantum well light-emitting diodes [J]. *Appl. Phys. Lett.*, 2008, 92(5):053502-1-3.

[14] Takeuchi T, Sota S, Katsuragawa M, *et al.* Quantum-confined stark effect due to piezoelectric fields in GaInN strained quantum wells [J]. *Jpn. J. Appl. Phys.*, 1997, 36:L382-L385.

[15] Chichibu S F, Abare A C, Minsky M S, *et al.* Effective band gap inhomogeneity and piezoelectric field in InGaN/GaN multiquantum well structures [J]. *Appl. Phys. Lett.*, 1998, 73(20):2920-2921.

[16] Kuokstis E, Yang J W, Simin G, *et al.* Two mechanisms of blueshift of edge emission in InGaN-based epilayers and multiple quantum wells [J]. *Appl. Phys. Lett.*, 2002, 80(6):977-979.

[17] Park S H, Ahn D, Chuang S L. Electronic and optical properties of *a*-and *m*-plane wurtzite InGaN/GaN quantum wells [J]. *IEEE J. Quantum Electron.*, 2007, 43(12):1175-1182.

[18] Schmidt M C, Kim K C, Farrell R M, *et al.* Demonstration of nonpolar *m*-plane InGaN/GaN laser diodes [J]. *Jpn. J. Appl. Phys.*, 2007, 46(9):L190-L191.

[19] Farrell R M, Feezell D F, Schmidt M C, *et al.* Continuous-wave operation of AlGaN cladding-free nonpolar *m*-plane InGaN/GaN laser diodes [J]. *Jpn. J. Appl. Phys.*, 2007, 46(32):L761-L763.

[20] Liao C T, Tsai M C, Liu B T, *et al.* Improvement in output power of a 460 nm InGaN light-emitting diode using staggered quantum well [J]. *J. Appl. Phys.*, 2010, 108(6):063107-1-6.

[21] Zhao H, Tansu N. Optical gain characteristics of staggered InGaN quantum well lasers [J]. *J. Appl. Phys.*, 2010, 107(11):113110-1-12.

[22] Park S H, Moon Y T, Lee J S, *et al.* Spontaneous emission rate of green strain-compensated InGaN/InGaN LEDs using InGaN substrate [J]. *Phys. Status Solidi* A, 2011, 208(1):195-198.

[23] Zhao H, Liu G, Tansu N. Analysis of InGaN-delta-InN quantum wells for light-emitting diodes [J]. *Appl. Phys. Lett.*, 2010, 97(13):131114-1-3.

[24] Lu T P, Li S T, Zhang K, *et al.* Blue InGaN light-emitting diodes with dip-shaped quantum wells [J]. *Chin. Phys.* B (中国物理 B), 2011, 20(10):491-495 (in English).

[25] Wang T H, Chang J Y, Tsai M C, *et al.* Efficiency enhancement of blue InGaN LEDs with indium composition graded InGaN barriers [J]. *SPIE*, 2011, 7954:79541F.

[26] Stringfellow G B, Craford M G. *High Brightness Light Emitting Diodes* [M]. San Diego: CA Academic, 1997:412-415.

[27] Kuo Y K, Chang J Y, Tsai M C, *et al.* Advantages of blue InGaN multiple-quantum well light-emitting diodes with InGaN barriers [J]. *Appl. Phys. Lett.*, 2009, 95(1):011116-1-3.

[28] Vurgaftman I, Meyer J R. Band parameters for nitrogen-containing semiconductors [J]. *J. Appl. Phys.*, 2003, 94(6):3675-3696.