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Simulation investigation of dual-wavelength tuning of light emitting diodes with single QW structure

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Abstract In the present study, spectral tuning of dual-wavelength emission in monolithic InGaN/GaN multiple-quantum well light-emitting diodes was investigated based on an experiment. The reference InGaN/GaN QWs are composed of GaN barriers and "three layers" wells containing a "wetting layer", a grading layer and a relatively low indium content InGaN layer, which has been grown in the laboratory. The simulation results show that the short wavelength light-emitting peak rises with the increasing of the grading layer thickness. In the meantime, when the thickness of the low indium content InGaN layer decreases, the long wavelength light-emitting peak falls. Dual-wavelength emissions can be achieved by tuning the grading layer thickness and the low indium content InGaN layer thickness. In addition, as the ratios of grading layer to the low indium content InGaN layer increase, the emission peaks show redshift because the interband transitions energy became smaller.

Keywords Wavelength tuning · Dual-wavelength · Light-emitting diodes · Phosphor-free LED

1 Introduction

As many governments in the world advocate policies for energy-saving and emission reduction purposes, the III-nitride light-emitting diodes (LEDs) is replacing the traditional light sources gradually. It will be the next generation of lighting source since it is efficient,

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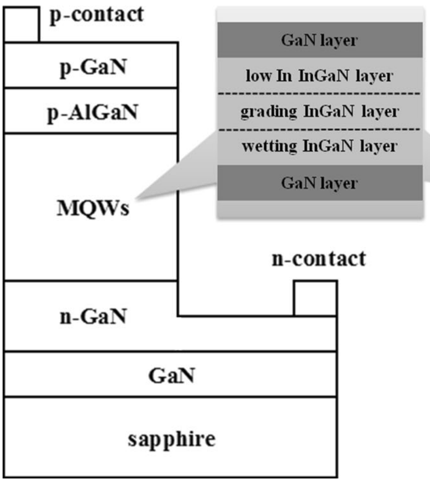
durable and eco-friendly (Damilano et al. 2010; Piprek 2014; Qiaofen et al. 2013; Togtema et al. 2015; Tu et al. 2010). There are three different major types of traditional white-light LED light-emitting mechanisms: blue-light stimulation of YAG phosphor, ultraviolet excitation of mixed fluorescent powder and color-mixing of RGB LED (three-primary-colors LED) (Damilano et al. 2001; Liu et al. 2012; Pimputkar et al. 2009). However, the LED coated with phosphor has poor color rendering index, low efficiency and reduced thermal stability. The costs to produce the three-primary-colors LEDs are relatively expensive (Soh et al. 2008). In order to solve these problems, a new type of LED called fabrication of phosphor-free multi-wavelength is currently being researched and developed (Ozden et al. 2001; Yamada et al. 2002).

Recently, Soh et al. (2008) fabricated phosphor-free broad-band cool white light LEDs which could be realized by growing indium-rich nanostructures in yellow emission wells. By using underlying growth techniques, Lu et al. (2009) manufactured the phosphor-free white light LEDs which combined blue and yellow emissions. Dual-wavelength emission peak was achieved by tailoring the MQW configuration in the active region. In addition, dual-wavelength InGaN/GaN MQW LEDs were made by Liu et al. (2008), which were grown by the metal–organic chemical vapor deposition (MOCVD) with different periods of high and low indium contents. These studies show the existence of variable methods to acquire phosphor-free dual-wavelength LEDs.

By an indium pretreatment after the GaN barrier growth and controlling the growth temperature profile for the InGaN active layers, a new type of quantum well (QW) structure was put forward by Fang et al. (2014). Along with the growth direction, a “wetting layer”, a grading layer and a relatively low indium content InGaN layer constituted a new well structure. Contributing to this structure, a broad-band dual-wavelength emission can be observed. This unique single QW structure provides us with new ways to obtain dual-wavelength LED.

In order to achieve commercial purposes, we need to adjust the emission wavelength of the dual-wavelength LED to different aspects of business applications. However, in the previous work, there should be two active regions to realize the quantum well structure of the dual-wavelength radiation through single chip. What’s more, the regulation of dual-wavelength could only be achieved by regulating the two active regions. In this study, based on the research of Fang et al., by tuning the thickness of the grading layer and the



QWs(InGaN/GaN) configuration

		In%	thickness/nm			
barrier layer		0	10			
well layer	wetting layer	0.22	0.5			
	grading layer	0.22~0.06	1.5	1.8	2.1	2.4
	low In layer	0.06	1.5	1.2	0.9	0.6

Fig. 1 Schematic diagrams of the redesigned LED

low indium content InGaN layer, the LED's luminescence properties and mechanism were characterized and analyzed numerically using advanced physical models of semiconductor devices (APSYS) (APSYS 2013) simulation program. This quantum well structure requires only a single active region to achieve dual-wavelength emission. In addition, the regulation of dual-wavelength can be achieved only by regulating the ratio of the well layer thickness. It provides people with a new way to achieve the regulation of dual-wavelength.

2 Method and parameters

In order to tune the spectrum, as well as referring to the structure investigated by Fang et al. (2014), we redesigned the structure shown in Fig. 1. 3-period InGaN/GaN MQWs are composed of 10-nm-thick barriers and 3-nm-thick wells, while the well layer consists of a 'wetting layer', a grading layer and a low indium content layer. Without changing the other parameters, we set the thickness of the grading layer/the low indium layer as 1.5/1.5, 1.8/1.2, 2.1/0.9 and 2.4/0.6 nm, respectively, as shown in Fig. 1.

Furthermore, we applied APSYS to investigate the optical properties of the LEDs. On account of two-dimensional models containing drift and diffusion of carriers in devices, the APSYS program can work out the Poisson's equation, the current continuity equation, the carries transport equation, the quantum mechanical wave equations and the heat transfer equation. We set the auger recombination coefficient and the Shockley–Read–Hall (SHR) lifetime to be $1 \times 10^{-30} \mathrm{cm}^6/\mathrm{s}$, 100 ns in the simulation procedure (Xia et al. 2013). The band-offset are presumed to be 70:30 for InGaN (Wang et al. 2013). Taking the spontaneous and polarization effects at heterojunction interfaces into consideration, our charge-screening factor is presumed to be 0.3. In the quantum well structure, the heterojunction interface will obtain polarization charge because of the serious polarization effects, hence forming a polarization electric field. Under the influence of an electric field, the spatial distribution and overlapping condition of the electron quantum wells and holes wave functions will change, which makes the band bending bent. This results in a spatial separation between electrons and holes, and the decreased recombination probability.

The spontaneous polarization of ternary nitride alloy scan be calculated as a Vegard interpolation:

$$P_{sp}(In_xGa_{1-x}N) = -0.042x - 0.034x(1-x) + 0.038x(1-x)$$

Strain-dependent piezoelectric polarization of $Al_xGa_{1\text{-}x}N$ can be expressed as:

$$P_{pz}(In_xGa_{1-x}N) = P_{pz}(InN)x + P_{pz}(GaN)(1-x)$$

where

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

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

The basal strain is

$$\varepsilon = \frac{a_{subs} - a(x)}{a(x)}$$

where $a(x)$ and a_{subs} are the lattice constants of the unstrained alloy at composition x and the lattice constants of the substrate.

Finally, the total polarization includes spontaneous and piezoelectric polarization.

$$P_{total} = P_{sp} + P_{pz}$$

3 Result and discussion

The spontaneous emission rates as a function of wavelength for four LEDs under the injection current density of 600 A/m^2 are shown in Fig. 2. As studied in Fang et al.'s (2014) paper, we can see a broad-band dual-wavelength emission consisting of a short wavelength light-emitting peak and a long wavelength light-emitting peak. With the increasing of the grading layer thickness, the radiation rates at the short wavelength light-emitting peak show a tendency to increase, while the radiation rates at the long wavelength light-emitting peak tend to decrease. Another phenomenon can be observed is that the emitting peaks also appear red-shifted.

To explore the origin of the above two phenomena, we compared the energy band diagrams and wave functions of the four QW structures, which are shown in Fig. 3. According to the study of Fang et al., The QW structure could show dual-wavelength emission because of the interband transitions from "e1" to "h1" and "e2" to "h1". It can be found that when the grading layer thickness increases, the emission energy of the interband transitions from "e1" to "h1" and "e2" to "h1" will be smaller. On the basis of the relationship between radiation wavelength and bandgap energy: $\lambda = 1240/E_g(\text{nm})$, the emitting peaks appear red-shifted.

Figure 4 shows the energy band diagrams of the four LEDs. From the figure, we can see that the band bending occurs due to the well-known reason, the polarization effect. Polarization will change the effective band gap, thereby changing the emission wavelength. The stronger the polarization effects are, the greater the energy band bending and the shorter emission the wavelength. In Fig. 4, we learn that with the increasing of the grading layer thickness, the polarization effect weakens. As a result, the band bending becomes smaller, so the emitting peaks appear red-shifted.

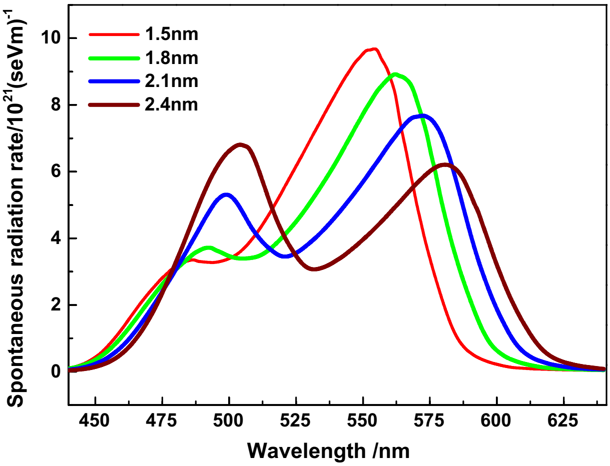


Fig. 2 Spontaneous emission rates as a function of wavelength for four LEDs

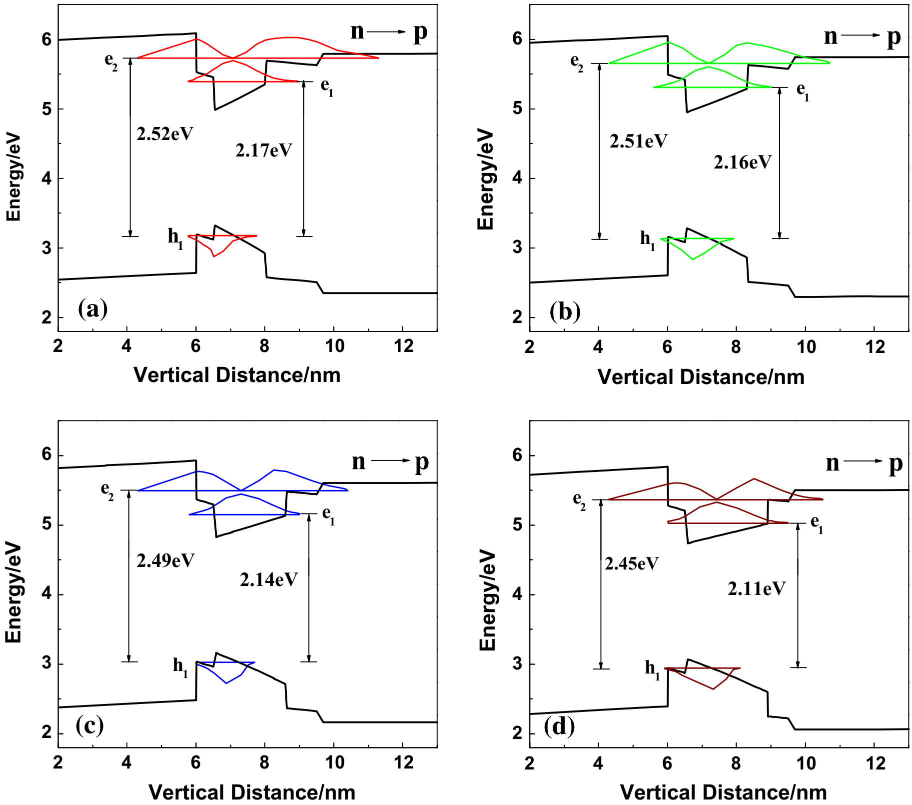
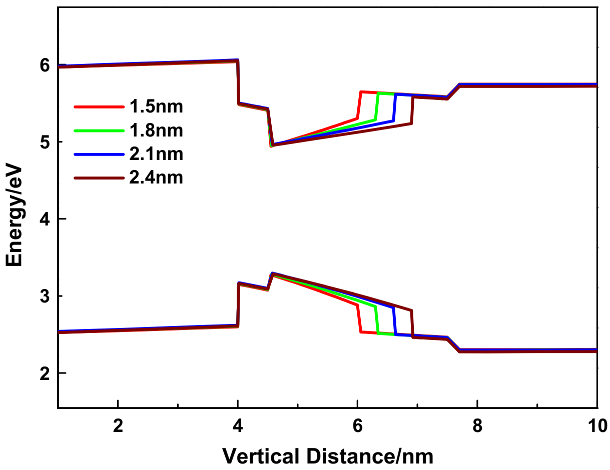


Fig. 3 Energy band diagrams and wave functions of the four QW structures

Fig. 4 energy band diagrams of the four LEDs



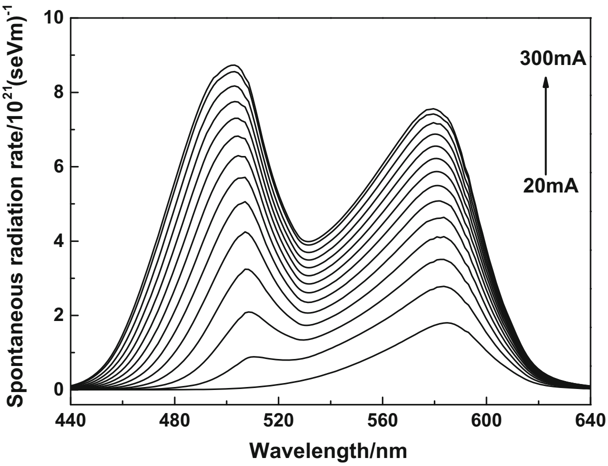


Fig. 5 Spontaneous emission rates of the LEDs with the thickness of the grading layer/the low indium layer as 2.4/0.6 nm at 20 to 300 mA

The asymmetric structure makes the indium content of well layer different. The well layer seems to be divided into two active regions. The "wetting layer" and part of the grading layer form the "high indium content well layer" (HIL), while the rest of the grading layer and the low indium layer form the "low indium content well layer" (LIL). The HIL is the cause of the long wavelength light-emitting peak and the LIL is the cause of the short wavelength light-emitting peak. For the quantum wells that contain the same indium composition, the thickness of the well will affect the luminous intensity. The quantum confined Stark effect causes the narrower quantum well to have a richer electron–hole overlap than that of a wider one, therefore a higher light output can be obtained. The above mentioned phenomenon is because the closer separation between the holes and electrons in the narrower quantum well results in shorter radiative recombination times under the piezoelectric field. In conclusion, with the increasing of the grading layer thickness, the thickness of the HIL increases. The increase of HIL will generate farther separation between the holes and electrons in the wider quantum well, leading to the decrease of the long wavelength light-emitting output. Meanwhile, with the decreasing of the low indium layer thickness, the thickness of the LIL decreases. The decrease of LIL will generate closer separation between the holes and electrons in the narrower quantum well, which causes the increase of the short wavelength light-emitting output.

Figure 5 shows the relationship between the injected current with the spontaneous emission rates. As we can see that with the injection current increasing from 20 to 300 mA, the emission rate also increases, and due to the current injection effect, emission peak appears a slight blue shift. Another phenomenon is that at low current injection, the short-wavelength emission peak is significantly weaker than the long-wavelength emission peak. On the contrary, an inverse relationship appears at high current injection.

4 Conclusions

In summary, in order to realize spectral tuning of dual-wavelength emission in monolithic InGaN/GaN multiple-quantum well (MQW) light-emitting diodes (LEDs), we did the following simulation investigations: (1) the relationship between the thickness of the well layer with the emission spectrum (2) the relationship between the injected current with the spontaneous emission rates numerically on the basis of a new structure which has been grown in the laboratory by Fang et al. Based on the model of "wetting layer" QW, our study referenced the InGaN/GaN QWs which were composed of a grading layer and a relatively low indium content InGaN layer. The results showed that, when the low indium content InGaN layer decreased with the increasing of the grading layer thickness, the short wavelength light-emitting peak rose while the long wavelength light-emitting output fell. In addition, the interband transitions energy became smaller as the ratios of grading layer to the low indium content InGaN layer increased, resulting in the emission peaks red-shifted. Finally, the injection current would effect the spontaneous emission rates of the two"active regions". This work proposes a particular method for the spectral tuning of the single QW structure white LED.

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