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Simulation Study on Optical Properties of GaN-based Blue LED

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Abstract

The optical properties of GaN-based blue light-emitting diodes (LEDs) are extremely important to study as these LEDs are utilized in a great many industries due to their excellent qualities, including high brightness, high energy efficiency, low energy consumption, and rapid reaction time. In this paper, Silvaco TCAD simulation software is used to do two-dimensional modeling and simulation of a GaN-based blue single quantum well vertical structure LED, with an emphasis on varied forward voltages, In components in InGaN, and quantum well thickness. The volt-ampere characteristic curve is compared and evaluated, as well as the energy band structure, carrier concentration, radiation recombination efficiency, electroluminescence spectrum, and internal current density distribution. The results show that when the forward voltage is 3.5V and the thickness of the quantum well is constant, the luminescence spectrum will show a red shift with the increase of the In content in the quantum well, and the luminescence spectrum will also show a red shift when the thickness of the quantum well is increased. However, when the quantum well thickness and In component are kept constant, the luminescence spectrum appears a red shift with increasing forward voltage.

Keywords: *GaN-based; Blue light; LED; Spectrum; Silvaco TCAD*

1 Introduction

Light-emitting diode (LED) is a kind of semiconductor optoelectronic device that can convert electrical energy into light energy[1]. LED as a new energy-saving light source has many advantages: First, it has high efficiency and a long life; its power consumption is less than 10 times that of an incandescent lamp, and its service life can reach 100000 hours. Second, small size, fast response and rich colors (ultraviolet to infrared). Third, green environmental protection, free of mercury, lead and other heavy metal pollution. According to the relevant parameters, the forbidden band width of InN is 0.7 eV and that of GaN is 3.4 eV [2]. Different forbidden band thicknesses can be obtained by controlling different InN and GaN alloy components, and the forbidden band thicknesses range from 0.7eV to 3.4eV, and their wavelengths range from 365 nm to 1770 nm. By combining a blue LED light source with an already existing red LED light source and a green LED light source, the trichromatic idea may be used to generate a more realistic and practical white light[3-5]. InGaN-series materials used to make blue LEDs are widely employed in a variety of industries. Consequently, there has been a lot of interest in the research into the characteristics of blue GaN-based LEDs. The quantum wells formed in the energy band by InGaN and GaN materials, their thickness, and the amount of In components present will determine their luminous properties. Furthermore, the forward voltage, the amount of Al in the p-type AlGaN layer, the kind of substrate material, and the doping concentration all have a substantial impact on its optoelectronic properties[6]. In this study, a two-dimensional simulation model of a blue single quantum well LED based on GaN is created using the SilvacoTCAD simulation software's Atlas module, and the effects of forward voltage,In component in InGaN and quantum well thickness on a GaN-based blue single quantum well LED are explained and examined.

2 Simulation and Analysis

2.1 GaN-based LED structure

The typical structure of a GaN-based single quantum well LED is a diode composed of p-type semiconductors and n-type semiconductors, which are composed of direct energy gap semiconductors. In p-type semiconductors, holes are the most abundant carriers, and in N-type semiconductors, free electrons are the most abundant carriers[7-8]. The GaN layer is usually used as the electron barrier layer and the InGaN layer as the electron potential well layer. In the actual production process, sapphire is

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commonly employed as the substrate material for GaN-based blue LEDs due to its high temperature resistance, high strength, good stability, and outstanding device quality. An InGaN/GaN single quantum well vertical structure LED on a sapphire substrate is used in this investigation. To simplify the model, a 300nm n-type GaN layer with a doping concentration of 1×1018 cm-3 is formed on a 600nm sapphire substrate, followed by a 3nm thick InGaN layer, as shown in figure 1. A 100 nm thick p-type AlGaN layer with a doping concentration of 1×1019 cm-3 is then created as an electron barrier layer (EBL), confining free electrons in the quantum well area and preventing free electrons from exiting the active region. After the inclusion of suitable Al components, EBL may limit the diffusion of Mg-doped in the p-type GaN layer to the quantum well region, enhancing the luminous efficiency and optical decay characteristics of LED. Finally, a 500 nm thick p-type GaN layer was produced with a doping concentration of 1×1019 cm-3. P-electrodes are made of the metal Ni, whereas N-electrodes are made of the metal Ti. Figure 2 depicts the quantum well band diagram. The energy band in the quantum well is tilted when the input voltage is applied, holes and free electrons accumulate in the quantum well region, and the accumulated holes and free electrons transition in the barrier layer, resulting in a recombination phenomenon that causes LEDs to emit light [9-13].

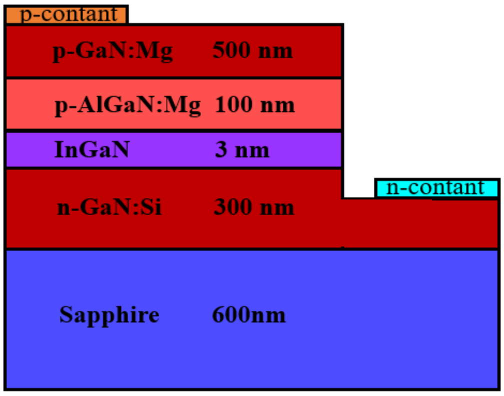

Figure 1 Schematic diagram of the basic structure of a GaN-based single quantum well LED

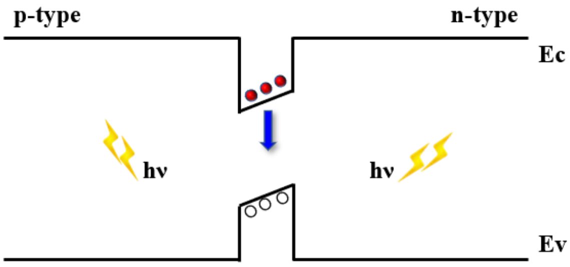

Figure 2 Energy band diagram of the quantum well

2.2 The influence of forward bias voltage

LED volt-ampere characteristics are also known as current-voltage characteristics. When the forward voltage applied to the LED is less than the turn-on voltage, it is difficult to overcome the potential barrier caused by the PN junction's built-in electric field, which hinders the diffusion movement of most carriers and produces high resistance and low current, which are insufficient to make the LED glow. The potential barrier created by the PN junction's internal electric field is completely offset when the forward bias voltage is higher than the turn-on voltage. As a result, the current increases quickly, most carriers' diffusion motion is obviously accelerated, and the LED is turned on [14]. According to the simulation findings, the opening voltage of the model's LED is around 3.2V, which corresponds to the real opening voltage range, as shown in figure 3.

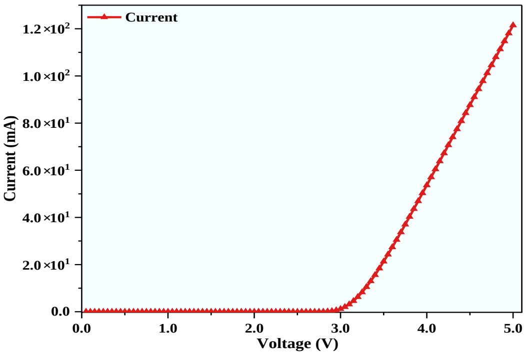

Figure 3 Volt-ampere characteristic curve of a GaN-based single quantum well LED

At forward voltages of 3.0V, 3.5V, 4.0V, 4.5V, and 5.0V, respectively, the electroluminescence spectra of an InGaN/GaN single quantum well vertical structure LED are shown in Figure 4. The LED light-emitting spectrum gains power density when the applied forward voltage is greater than the turn-on voltage, as shown in the figure. As the forward voltage rises, the peak wavelength gradually decreases, and the spectrum exhibits clear blue shift phenomena. Due to the carrier relaxation time in the conduction band (or valence band) being much shorter than the carrier lifetime, the carrier in the quantum well increases, shielding part of the built-in electric field, weakening the quantum-confined stark effect (QCSE), and the ground state in the well increases, so that the LED peak wavelength shifts to the short wave direction [15-16].

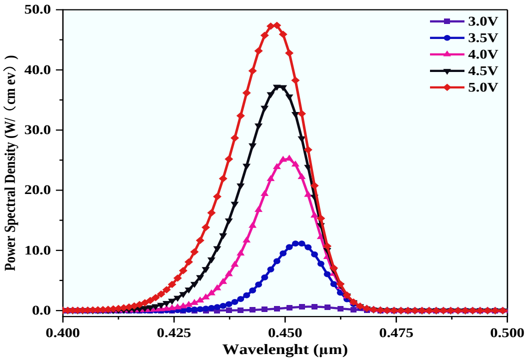

Figure 4 Electroluminescence spectra of GaN-based single quantum well LED structures change with forward voltage

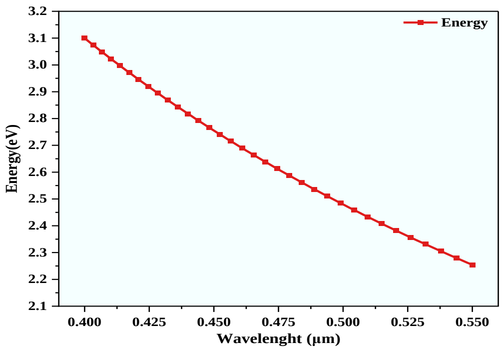

Figure 5 Relationship between the electroluminescence spectrum and energy of a GaN-based single quantum well LED structure

In figure 4, when the forward voltage increases to 3.5 V, the peak wavelength is 0.453 μm (453 nm). The simulation findings in figure 5 demonstrate that the energy is 2.73 eV, which is compatible with the theoretical estimates for the blue light peak wavelength range of 450 nm–490 nm and energy range of 2.53-2.76 eV. When the forward voltage reaches 5.0V, the current density progressively increases, the luminescence spectrum shifts toward the blue, the purple luminescence peak occurs at 0.44 μm, and the peak wavelength shortens. Figures 6(a)-(b) depict the flow direction of the device's internal current at 3.5 V and 5.0 V forward voltages, respectively. By enlarging the current cloud distribution map, it becomes clear that the current flows laterally in the lower portion of the n-type GaN layer and vertically downward in the p-type layer and well layer of the quantum well [17]. The current also flows vertically downward in the upper part of the p-type layer of the quantum well [18].

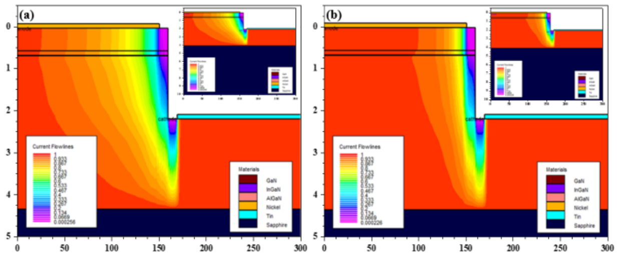

Figure 6 (a) Current density distribution cloud diagram of the LED model at forward voltage 3.5 V. (b) Current density distribution cloud diagram of the LED model at forward voltage 5.0 V

2.3 The influence of In component content

Figure 7 depicts the VI characteristic curve of a GaN-based LED with varied In components. The simulation results show that when the In content grows, the turn-on voltage fluctuates little, indicating that the In component has little impact on the turn-on voltage of the LED. In the case of keeping other parameters and the thickness of the quantum well constant, by varying the concentration of the In component, the effect of the In component on the performance of the GaN-based blue LED was investigated.

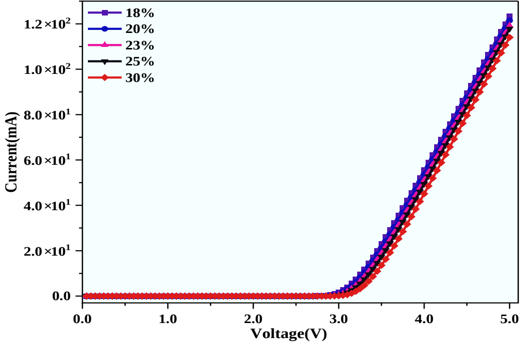

Figure 7 VI Characteristics of GaN-based LEDs with various In components

Figure 8 shows the energy band structures of different In components, which are affected by the piezoelectric effect and spontaneous polarization effect in LEDs, resulting in a polarized electric field. In addition, the lattice constant of InGaN/GaN does not match, and the increase of In content will increase the interface stress of the InGaN/GaN layer and enhance the polarization electric field, this causes the energy band in the quantum well structure to tilt [19]. The top of the valence band moves up, the bottom of the conduction band moves down, and the band gap width of the quantum well decreases. At the same time, the depth of the quantum well increases, thus increasing the relative barrier height, which increases the difficulty of carrier injection. Therefore, as the free electron and hole concentrations decline, so does radiation recombination efficiency, which in turn impacts LED luminous performance.

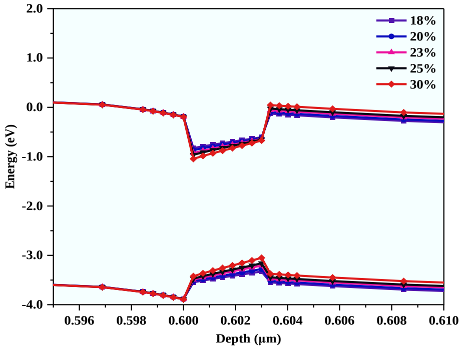

Figure 8 Energy band structure of quantum wells with different In components

Figure 9 shows the free electron and hole concentrations in GaN-based LED quantum wells with different In components. It can be seen from the simulation results that with the increase ofIn component, the free electron concentration near the n-type region decreases gradually and the hole concentration near the p-type region decreases gradually, which further confirms the results in figure 8, that is, as the free electron and hole concentrations in the quantum well decrease, the recombination efficiency is affected by the carrier concentration [20]. Figure 10 shows the radiation recombination efficiency in quantum wells with different In components. With the increase of In components, the radiation recombination efficiency decreases obviously, so the output efficiency is reduced, thus the quantum efficiency of LED is reduced[21].

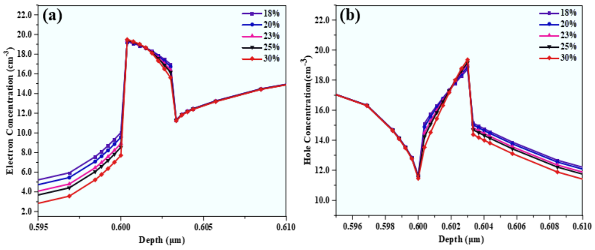

Figure 9 (a) Free electron concentration with different In components; (b) Hole concentration with different In components

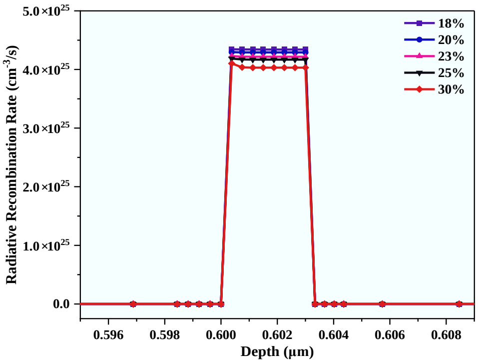

Figure 10 Radiation recombination efficiency with different In components

Figure 11 shows the relationship between optical power and current of LED with different In components. With the increase of In content, the corresponding optical power at the same current decreases. At the same time, with the increase of In content, the lattice matching of InGaN and GaN increases, the radiative recombination efficiency decreases, and the non-radiative recombination efficiency increases, which also leads to a decrease in optical output power.[22] As shown in figure 12, with the increase of the In component, the intensity of the power density decreases, the wavelength of the emitted photon increases gradually, and the peak wavelength shows a red shift to the long wave direction.

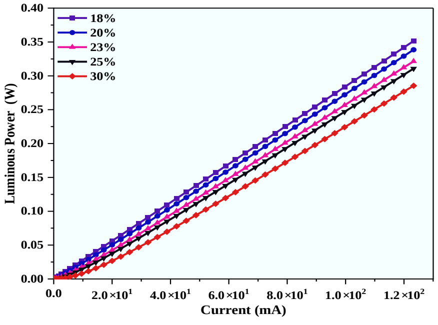

Figure 11 Relationship between optical power and current of LED with different In components

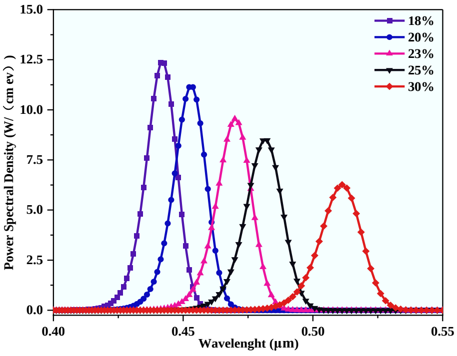

Figure 12 Changes of luminescence Spectra under different In components

2.4 The influence of the thickness of the quantum well

In the manufacturing process of LEDs, the thickness of the quantum well also affects their optoelectronic properties. The thickness range of a quantum well is generally 1－5 nm. The thickness of LED quantum dots well designed in this paper is 2nm, 3nm and 4nm. The thickness of the quantum well will affect the polarization electric field. Due to the existence of the polarization electric field, the energy band, radiation recombination efficiency and other parameters are affected. In the simulation, the working voltage of the LED is set to 3.5 V. Figure 13 shows the VI characteristic curve of GaN-based LEDs with different quantum well thicknesses. It can be seen from the figure that there is little difference in the turn-on voltage of the three structures, but from the illustration in figure 13, the LED turn-on voltage of the 2nm structure is the smallest and the LED turn-on voltage of the 4nm structure is the largest. The turn-on voltage increases with the thickness of the quantum well. Through the analysis, we believe that the main reason why the turn-on voltage of the device increases with the increase in the thickness of the quantum well is that with the increase of the thickness of the quantum well, the series resistance also increases, increasing the required opening voltage. When the thickness of the quantum well decreases, the greater the current obtained at the same voltage [23]. It can be seen from figure 14 that with the increase in the thickness of the quantum well, the tilt of the energy band increases.

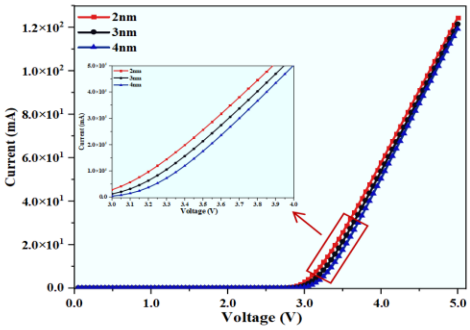

Figure 13 VI characteristic Curve of GaN-based LED with different Quantum well thickness

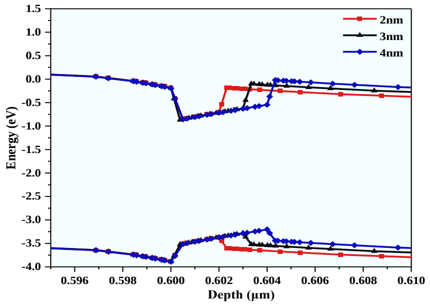

Figure 14 Energy band structure of quantum wells with different thickness

This is due to the increase in the thickness of the quantum well, the enhancement of the polarization effect, the intensification of the QCSE and the decrease of the quantum efficiency of LED [24-26]. Figure 15 shows the variation of LED luminous power with injection current at different quantum well thicknesses. When the quantum well thickness decreases, the LED's luminous power increases.

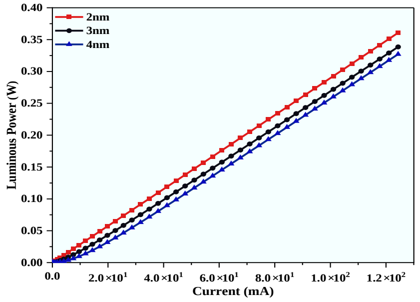

Figure 15 Variation of LED luminous Power with injection current under different Quantum well thickness

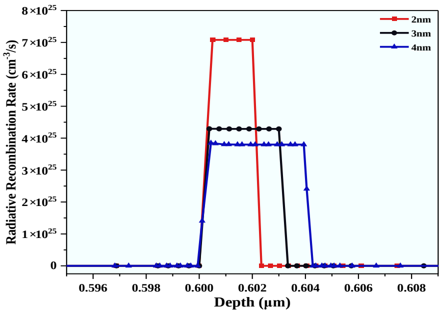

Figure 16 The curve of the radiative recombination efficiency of LED with the thickness of the quantum well

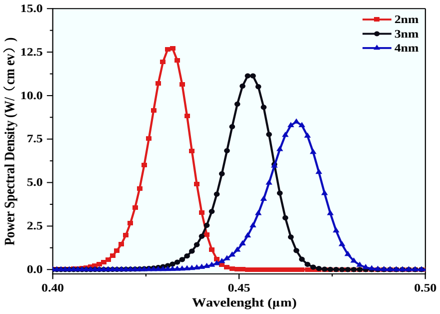

Figure 17 Optical Power density of GaN-based LED with different Quantum well thickness

Figure 16 shows the variation of the radiation recombination efficiency of LEDs with the thickness of the quantum well. The internal quantum efficiency declines as the quantum well's thickness increases due to a reduction in radiation recombination efficiency, this also validates the results in figure 17. The luminous power of LEDs decreases with the increase in thickness of the quantum well, and the peak wavelength shifts to the long wavelength, which leads to the red shift [27]. We think that properly reducing the thickness of the quantum well will increase the luminous intensity of the device, the electric field formed by the carriers in the quantum well weakens the polarization electric field, reduces the influence of the QCSE, and the effective band gap of the quantum well expands obviously, which leads to the blue shift of the LED spectrum [28-29].

3 Conclusion

This article primarily simulates the forward voltage, the content of In in the quantum well, and the quantum well thickness. The results show that with the increase in voltage, the influence of QCSE is weakened, the peak wavelength of LEDs decreases gradually, and the luminescence spectrum shows an obvious blue shift. The range of In components set is 18% to 30%. the increase of the content of in will aggravate the polarization effect, cause the energy band to tilt, the injection of carriers is blocked, and the radiation recombination efficiency is reduced, so the luminous efficiency decreases, and the peak value of the spectrum shifts to the long wave, that is, the redshift occurs. As the thickness of the quantum well is reduced, the electric field created by the carrier weakens the polarization electric field, increasing the effective band gap of the quantum well, shifting the peak wavelength to the short wave, and resulting in a blue shift in the luminescence spectrum.To sum up, for the GaN-based blue LED with this structure, when the well thickness of the InGaN/GaN quantum well is set to 3 nm and the In content is 20%, the device shows good optoelectronic properties. This paper has a basic reference value for the actual design, optimization and related research of GaN-based blue LEDs.

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