

The Study of Doping Concentration in ALYGA1-YN Block Layer Based on Multi Quantum Well of 313m LED

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Abstract

The structure of UVLED with three multi-quantum wells (MQW) of $iAl_yGa_{1-y}N$ barrier - $iAl_{0.20}Ga_{0.80}N$ QW - $iAl_yGa_{1-y}N$ barrier are studied by the SiLENSe software with various doping concentration of Mg in the block layer. This UVLED is emitted the wavelength of 312 nm for sterilization. The IEQ values was found to be stable with $N_d = 5 \times 10^{18} \text{ cm}^{-3}$. The emitting wavelength of this structure is around 313nm. The components of Aluminum material in the block of $Al_yGa_{1-y}N$ layer is test to 45% and 55% to predict the increasing of radiating wavelength over 314nm, which are in good agreement with the recent publication.

Keywords: UVLED, MOCVD, AlGaN, MQWs, sterilization

INTRODUCTION

As recent as last year, the growth rate of III-nitride-based light emitting diode market demands a careful optimization of both fabrication technology and design of these devices. The effort has been made to improve the material quality [T. Mukai (2003), S. Kymiyama (2002)], efficiency of light extraction from LEDs and contact geometry [J. Baur (2002), A. Y. Kim (2001)].

InGaN, AlGaN, and AlInGaN alloys with the wurtzite-crystal structure are now widely studied and developed due to their extremely wide range of emission wavelengths and direct energy band gap. The band gap energy of Alga based materials can be adjusted from 6.2eV (An) to 3.4eV (Gann), the (In) Alga alloys have become promising candidate materials for unless [K. Takahashi (2007)]. Such solid-state light sources are expected to replace the traditional fluorescent and incandescent lamps from the viewpoint of energy saving. Furthermore, the radiation of UVLEDs are useful for application [S. Nakamura (2000)] in the medical and biochemical field, purification equipment, sensing fields, and high density optical recording.

Recently, N.V.Hieu *et al* [N.V. Hieu *et al* (2011)] reported on the lamp of LED with 365nm of ultraviolet wavelength for E. coli and Coliform bacteria sterilization in running water.

In this paper, the UVLED structure with MQW will be studied in the various doping concentrations in

barrier layers to find out their semiconducting and optical properties by simulation.

METHODOLOGY

The modeling study reported in this paper is aimed at better understanding the operation of MQWs UVLED and calculated the physical and optical properties for the structure of UVLED with three MQWs of $iAl_yGa_{1-y}N$ barrier - $iAl_{0.20}Ga_{0.80}N$ QW - $iAl_yGa_{1-y}N$ barrier by the SiLENSe software with various doping concentration of Mg in the block layer. The MQWs UVLED operation based on direct-band gap wurtzite semiconductors were simulated by using the SiLENSe package implementing the 1D model based on the Poisson equation for the electric potential and drift-diffusion transport equations for the electron and hole concentration. This UVLED is emitted the wavelength of 312nm for sterilization

UVLED STRUCTURE

The UVLED used as a reference for subsequent simulation was grown on a (0001) sapphire substrate by low-pressure horizontal-flow metal organic chemical vapor deposition (MOCVD), which had an emission wavelength of approximately 312nm. Figure 1 depicts the structure of the UVLED under study. Firstly, a sapphire substrate was cleaned under H_2 at 1020°C . After, a 500nm-thick n- $Al_yGa_{1-y}N$ layer with a doping concentration of $[Si] = 2 \times 10^{18} \text{ cm}^{-3}$ was grown on a sapphire substrate. The component of Aluminum in un-doped $Al_yGa_{1-y}N$ was checked with 0.45% for below structure.

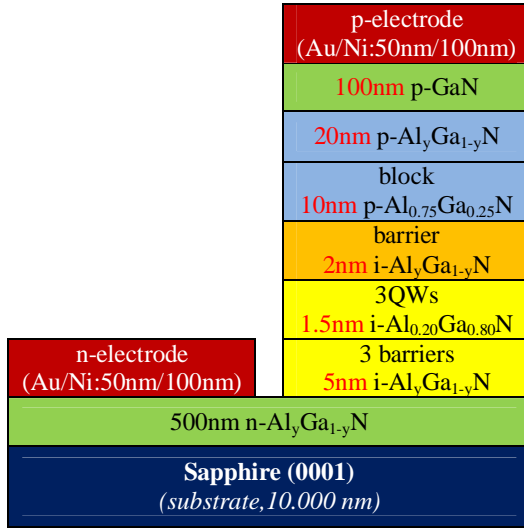


Fig. 1. The modeling structure of UVLED.

The active region consisted of three un-doped $\text{Al}_{0.20}\text{Ga}_{0.80}\text{N}$ quantum wells (QWs) each 1.5nm-thick, separated by the 5nm-thick $\text{Al}_y\text{Ga}_{1-y}\text{N}$ barriers, however, the last $\text{Al}_y\text{Ga}_{1-y}\text{N}$ barrier of MQWs layer with a 2nm-thick. Every barrier is doped with the Mg concentration varied between $1 \times 10^{17}\text{cm}^{-3}$ and $1 \times 10^{19}\text{cm}^{-3}$. On top of the MQWs active region was a 10nm-thick $\text{p-Al}_{0.75}\text{Ga}_{0.25}\text{N}$ electron blocking layer with doping concentration of $[\text{Mg}] = 5 \times 10^{16}\text{cm}^{-3}$. The 20nm-thick $\text{p-Al}_y\text{Ga}_{1-y}\text{N}$ with doping concentration of $[\text{Mg}] = 1 \times 10^{17}\text{cm}^{-3}$ and 100nm-thick p-GaN contact layer were grown with a doping concentration of $[\text{Mg}] = 7 \times 10^{17}\text{cm}^{-3}$ to complete the structure. The total length from n- $\text{Al}_y\text{Ga}_{1-y}\text{N}$ layer to pGaN layer is 651.5nm. However, the active layer or MQW is only 21.5nm, which will be discussed more detail in next section.

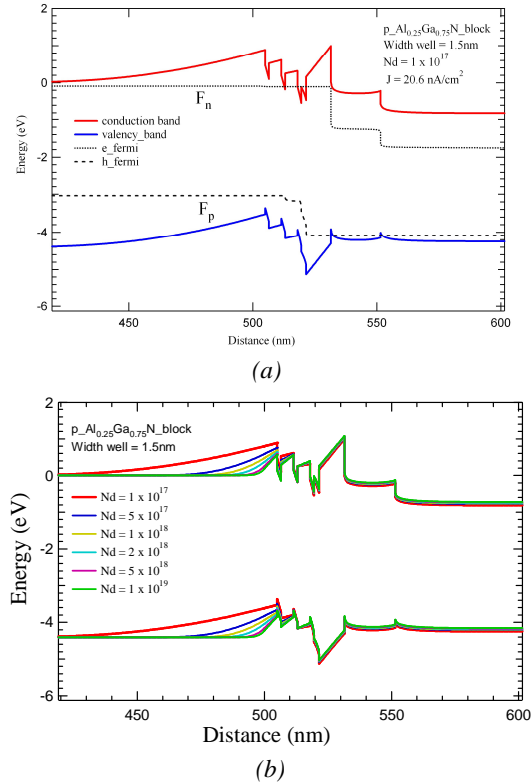
RESULTS AND DISCUSSION

Energy Band Structure and Carrier Concentration

Both the radioactive recombination of the carriers and their non-radioactive recombination on the threading dislocation cores are considered to predict the internal light emission efficiency of the LEDs. The Fermi-Dirac statistics is used, accounting for high non-equilibrium electron and hole concentrations in the active region. To calculate the light emission spectra, we solve self-consistently the Poisson and Schrödinger equations for the carrier wave functions inside each quantum well.

A quantum well (QW) is synthesized from two different semiconductors. Consider two semiconductors with band gap $E_{g, \text{barrier}}$ and $E_{g, \text{well}}$. Band gap energy of the QW will be given by equation [1]:

$$E_{g, \text{QW}} = E_{g, \text{well}} + E_{0, e} + E_{0, h} \quad [1]$$


 Fig. 2. Energy-band diagram in the MQW: (a) with $J=20.6\text{nA/cm}^2$ and (b) with various donor concentrations (N_d) in the barriers.

Where $E_{0, e}$, $E_{0, h}$ are quantized energy of electron and hole, respectively.

The unstrained $\text{Al}_y\text{Ga}_{1-y}\text{N}$ band gap energies are calculated as [S. J. Lee *et al* (2011)]

$$E_g(y) = 6.13y + 3.42(1-y) - y(1-y) \text{ eV} \quad [2]$$

The concentration of ionized donors N_D^+ and acceptors N_A^- are related to total impurity concentrations.

Figure 1 shows the energy of valence band (below) and the energy of conducting band (above) of 3 quantum wells (QW) from 500nm to 521.5nm, which is active area. The well thickness is 1.5nm. Each QW includes 1 un-doped layer of $\text{Al}_y\text{Ga}_{1-y}\text{N}$ barrier and 1 un-doped layer of $\text{Al}_{0.20}\text{Ga}_{0.80}\text{N}$ and is 6.5nm of thickness. With this structure, the energy decreased gradually into 3 wells and increased quickly in the barrier layer.

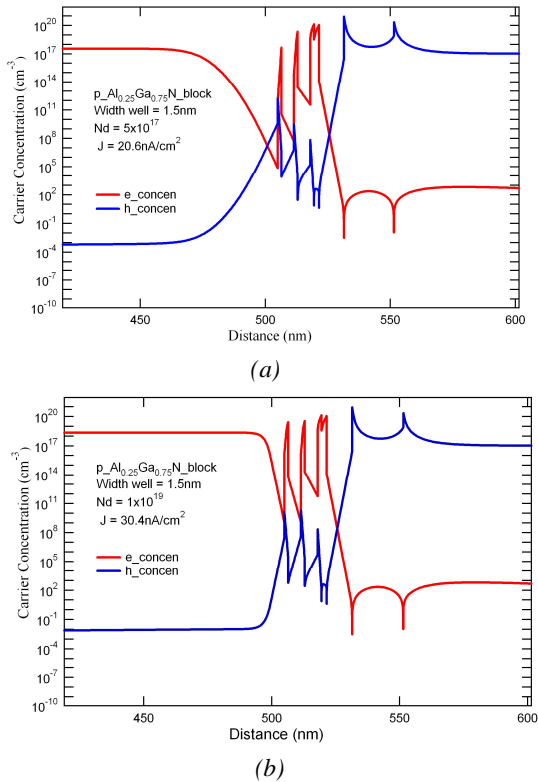


Figure 3. Distribution of carrier concentrations in the MQW LED with two kind of N_d .

The quasi-Fermi levels of electrons (solid line) and holes (dotted line) are denoted as F_n and F_p , respectively, as shown in Fig. 2 (a). There was no more change in band energies of carriers when the increasing of doping concentration in barrier layers (see Fig. 2b). However, the carriers in n-GaN layers were reduced their band energies.

Figure 3 (a, b) show the comparison in carrier distribution as a function of doping concentration in barrier layer. The carriers are equal in n-type layer and also separate clearly in case of the increasing doping concentration N_d . The radioactive recombination of electrons and holes is found to be localized mainly in the QWs. The non-radioactive recombination occurs also in the MQW barriers and p-GaN contact layer where mobile electrons can penetrate these areas.

The latter effect is caused by insufficiently high potential barrier in the p- $Al_yGa_{1-y}N$ emitter which fails to confine electrons at high current densities (see Fig. 1 and Fig.2).

I-V characteristic of MQW layers

Figure 4 indicate the I-V curve in this MQW UVLED structure when the bias voltage was increased from 0 to 10V. Current was linear from the increasing of bias from 2.3V to 5V. The current became saturation above 5V. The oscillation of currents showed higher when the doping concentration N_d was increased too.

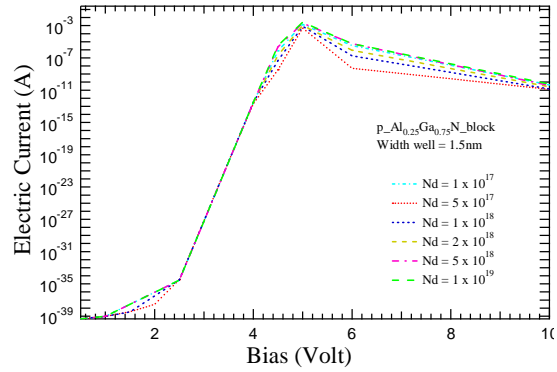


Fig. 4. I-V characteristic of the MQW LED computed for various donor concentrations in the barriers N_d .

Internal Quantum Efficiency (IQE) and Emitting Wavelength

Figure 5 shows the internal quantum efficiency (the ratio of the phonon emission rate of electron-hole pair injection into the LED structure) as the function of current density of the MQW LED computed for various donor concentrations in the barriers. It found IEQ was stable with $N_d = 5 \times 10^{18} \text{ cm}^{-3}$.

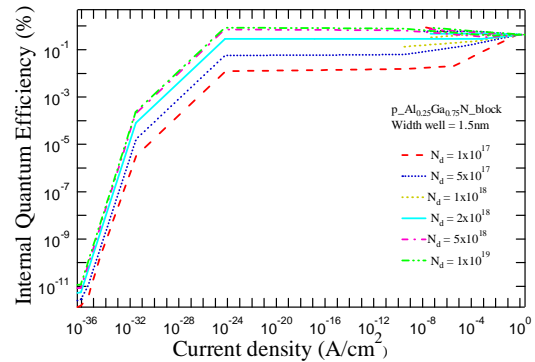


Fig. 5. Internal quantum efficiency versus current density of the MQW LED.

The emission spectra from the UVLED structure plotted with the changing of donor concentrations in the barriers N_d , as shown in Fig. 5. According to the electroluminescence spectra, it is observed that the peak emission wavelength is from 312nm to 314nm as the donor concentrations in the barriers decreases from $1 \times 10^{17} \text{ cm}^{-3}$ to $1 \times 10^{19} \text{ cm}^{-3}$. The emission wavelength is designed depending on the donor concentrations in the barriers of MQWs LED.

At value of bias 4 voltage, when the donor concentration N_d in the barriers changes, an increase from $[Mg] = 1 \times 10^{17} \text{ cm}^{-3}$ to $[Mg] = 1 \times 10^{19} \text{ cm}^{-3}$, the internal emission efficiency increased. In contrast, the wavelength was nearly stable, as shown in Fig. 6.

Internal emission efficiency (IQE) is the function of the donor concentrations in the barriers. Higher donor concentration, increasing performance.

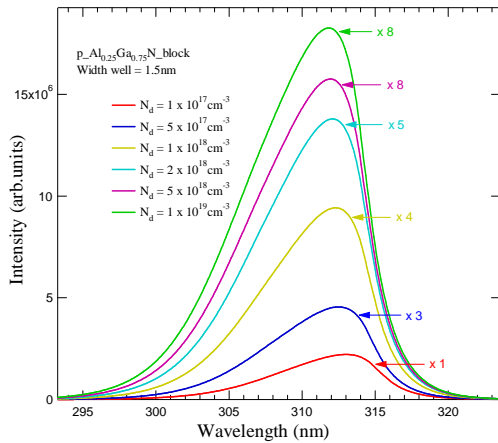


Fig. 6. Emission spectra from the LED structure with $[Mg] = 10^{17} \text{ cm}^{-3}$ to 10^{19} cm^{-3} in the barriers [N.V.Hieu *et al* (2011)].

Internal emission efficiency reaches the highest value was 90% in the donor concentrations $[Mg] = 1 \times 10^{19} \text{ cm}^{-3}$, $2 \times 10^{18} \text{ cm}^{-3}$, and $5 \times 10^{18} \text{ cm}^{-3}$, internal emission efficiency is high value and stability.

4. The change of Al components in barrier block

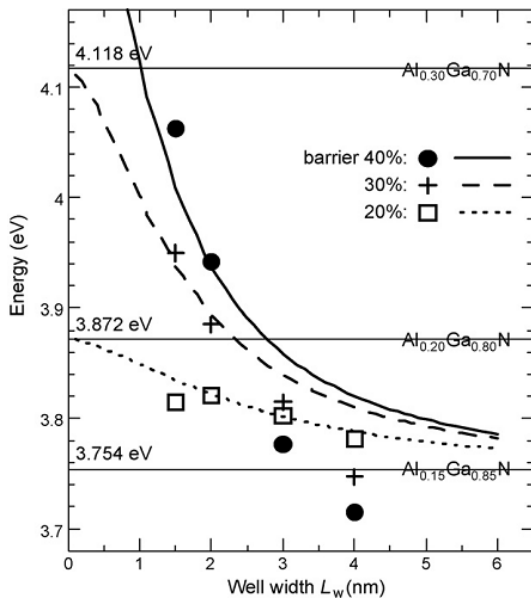


Fig. 7. Well-width dependence of the PL peak energies in three barrier composition cases with $y=0.20;0.30$ and 0.40 [M. Takeuchi *et al* (2007)].

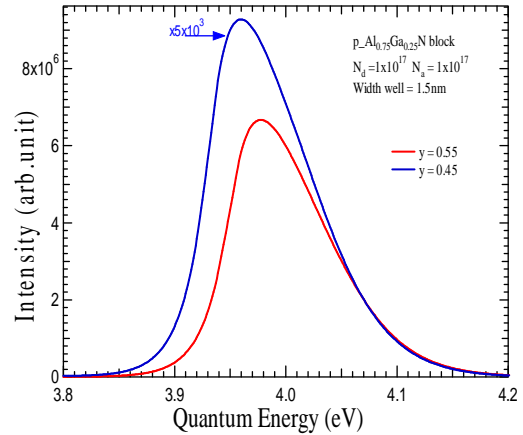


Fig. 8. PL peak energies in two barrier composition cases with $y=0.45$ and 0.55 .

The PL peak energies in two barrier composition cases with $y=0.45$ and 0.55 was estimated around 3.97 eV and 3.96 (see Fig.8), which is similar with the experimental result of M. Takeuchi, 4.04 eV for $y=0.40$. The component of Al in our study is smaller than M. Takeuchi, which is no far different in components. Therefore, it is clearly to inform that these works were in good agreement with measurement.

CONCLUSION

In this paper, we report on the modeling study of a MQW LED hetero-structure with doped barriers of the 45% of Al component in un-doped $\text{Al}_y\text{Ga}_{1-y}\text{N}$ layers. The device operates in the injection-current mode in the practically important range of current density variation, which is derived from the comparison of the computed and measured I-V characteristics of the LED.

The intensity of emission spectra from the UVLED structure will be proportional with the doping concentration of Mg in the $\text{Al}_y\text{Ga}_{1-y}\text{N}$ barrier layers. The IEQ values was found to be stable with $N_d = 5 \times 10^{18} \text{ cm}^{-3}$. The emitting wavelength of this structure is around 313 nm . Based on these results, the fabricating process will be done in next time for the deep-UVLED.

ACKNOWLEDGMENTS

This work is supported in part by the Grant-in-Aid for Scientific Research (78/HD-SKHCN, B2011-18-33) from the government of HCMC and Vietnam National University-HCMC. Author specially thank Aoyagi Laboratory (Ritsumeikan Univ., Japan) for SiLENSe software and and the visiting scholar for MOCVD technology.

The authors also thank the Technical Committee for fruitful comments and suggestion which help to improve the quality of this paper.

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