JOURNAL OF NANO- AND ELECTRONIC PHYSICS
Vol. **7** No 4, 04069(3pp) (2015)

ЖУРНАЛ НАНО- ТА ЕЛЕКТРОННОЇ ФІЗИКИ
Том **7** № 4, 04069(3cc) (2015)

Model of Band Diagram LED White Light in the System of GaN/InGaN

Yu.P. Holovaty[1], V.G. Kosushkin[1], N.A. Khahaev[1], D.A. Romanov[1],
L.M. Chervyakov[2], E.K. Naimi[3], S.L. Kozhitov[3]

[1] *Bauman Moscow State Technical University, 5, 2-ya Baumanskaya St., 105005 Moskow, Russia*
[2] *South-West State University, 94, 50 let Oktyabrya St., 305040 Kursk, Russia*
[3] *National University of Science and Technology «MISiS», 4, Leninsky Pr., 119049 Moscow, Russia*

(Received 01 October 2015; published online 24 December 2015)

The results of the research of semiconductor multilayer nanostructures suitable for making white light LEDs in the GaN/InGaN with red, green and blue emission spectra formed in a single chip. The methodology and the calculation of the energy levels, the wave functions of the carriers, the electric fields caused by the spontaneous polarization and the piezoelectric effect, the spontaneous emission spectrum and chromaticity coordinates of the total radiation.

Keywords: Nitride indium-gallium (InGaN), LED simulation, The band diagram, Semiconductors.

PACS numbers: 61.72.uj, 79.60.Bm

1. INTRODUCTION

Developing nanoelectronics is based on the achievements of physics of quantum systems and the use of nanotechnology, possessing atomic precision in the preparation of nanostructures with the desired chemical composition and configuration. The main direction of the semiconductor nanoelectronics develop is to use the limited movement of charge carriers in one, two or all three dimensions by entering them in the quantum well, quantum thread quantum dots. These principles are base for almost all modern light-emitting devices, photodetectors and high-speed transistors [1-3].

Currently, the basic materials to create white light LEDs are nitrides of elements of the third group. They have a wide band gap that allows you to vary the parameters of radiation and the spectral composition of light. High electron mobility and saturation velocity, high breakdown voltage and thermal conductivity also define the dignity of nitrides of the third group for the manufacture of light-emitting devices.

Objective is to provide a model system in the band structure of GaN / InGaN with red, green and blue emission spectrum in a single chip.

2. THE MODEL OF THE BAND STRUCTURE OF A WHITE LED

The initial structure shown in Fig. 1.

The layers are arranged as follows: an emitter E1, "red" dots W1, barrier B1, «green» dots W2, barrier B2, «blue» dots W3, the emitter E2. Barriers and emitters consist of pure GaN. Quantum wells are composed of a solid solution of $In_xGa_{1-x}N$, where x is the In content in the solid solution. Changing the concentration of indium in the solid solution changes the value of the band gap, which changes the color of the optical emission. The layer thicknesses were chosen according to the desired arrangement of the energy levels and wave functions of the electrons. It was selected wavelengths generated in the "red", "green" and "blue" dots $\lambda_1 = 700$ nm, $\lambda_2 = 540$ nm, $\lambda_3 = 450$ nm respectively. The value of the nominal band gap calculated by the formula:

$$E_{gi} = \frac{2 \cdot \pi \cdot \hbar \cdot c}{\lambda_i \cdot q} \qquad (1)$$

where $\hbar$ – is the reduced Planck constant; c – the velocity of light; λ_i – is the wavelength; q – the charge of the electron.

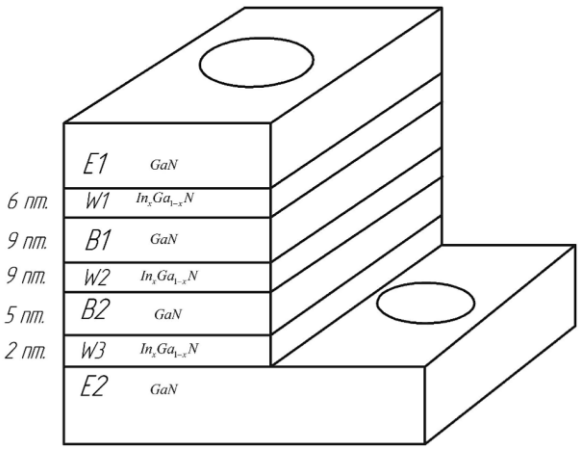

Fig. 1 – The original nanostructure

The obtained values of the restricted areas are summarized in Table 1.

Table 1 – Wavelengths and prohibited zones

The desired wavelength (nm)	700	540	450
The value of the band gap (eV)	1,8	2,3	2,7

Effective" forbidden zone E_{gi} differs from the nominal E_{g0i} amount on the energy levels of quantum electrons E_{en} and holes E_{hn} in the quantum wells,

$$E_{gi} = E_{g0i} + E_{en} + E_{hn} \qquad (2)$$

Each of the three components is dependent on the composition of the respective hole x_i

$$E_{gi} = E_{g\mathrm{InN}} \cdot x_i + E_{g\mathrm{GaN}} \cdot (1-x_i) - B \cdot x_i \cdot (1-x_i) + \\ + \frac{E_0}{M_{p\mathrm{InN}} \cdot x_i + M_{p\mathrm{GaN}} \cdot (1-x_i)} + \\ + \frac{E_0}{M_{n\mathrm{InN}} \cdot x_i + M_{n\mathrm{GaN}} \cdot (1-x_i)} \quad (3)$$

where $M_{n\mathrm{GaN}}$ – is the effective mass of the electron in GaN; $M_{n\mathrm{InN}}$ – the effective mass of an electron in InN; $M_{p\mathrm{GaN}}$ – effective mass of holes in GaN; $M_{p\mathrm{InN}}$ – effective mass of holes in InN; B – parameter slack-forbidden zone GaN; $E_{g\mathrm{GaN}}$ – zone-forbidden InN; E_0 – setting with the dimension of energy.

$$E_0 = \frac{\pi^2 \cdot \hbar^2}{2 \cdot m_0 \cdot d^2 \cdot q} \quad (4)$$

The values of the content of InN in the pits and efficient energy band gaps calculated from equation (3) are shown in Table 2.

Table 2 – Contact indium content in the composition of the epitaxial layer and the band gap energy

The value of the effective energy gap, eV	2,7	2,3	1,8
In content in the solid solution,%	15	28	45

The spontaneous and piezoelectric polarization was considered in modeling. The characteristic features of nitrides of group III is the high value of the degree of ionic character of bonds and deformation caused by the mismatch of lattices. This leads to the spontaneous and piezopolarizationi. The barrier consisting of GaN, was polarize offline. The electric field due to the combined effect of the two polarizations in each of the five layers (wells and barriers), and can be calculated as [4-5] from the formula:

$$E_j = \frac{\sum_k l_k P_k / \varepsilon_k - P_j \sum_k l_k / \varepsilon_k}{\varepsilon_j \sum_k l_k / \varepsilon_k} \quad (5)$$

where k – is the number of layers; l_k – the thickness of the layers; P_k – Complete the total polarization in all sectors; ε_k – The total dielectric constant in all layers; j – Stock No layer; P_j – full total polarization in the layer; ε_j – dielectric constant.

The field values are shown in Table 3. They bend the energy gaps, resulting in the band diagram of the structure takes the form (Fig. 2).

The energy levels of electrons E_{en} and holes E_{hn} in the structure of their wave functions Ψ_{en}, Ψ_{hn} are found numerically from the Schrodinger equation

$$-\frac{\hbar^2}{2 \cdot m} \cdot \frac{d^2 \Psi_n(x)}{dx^2} + V(x)\Psi_n(x) = E\Psi_n(x) \quad (6)$$

where m – the mass of the particle; $V(x)$ – the potential energy; E – total energy; $\Psi_n(x)$ – the wave function.

The resulting wave functions and energy levels are shown in (Fig. 3).

The energy levels of the electron wave functions for each level are showed above. Below shows the energy levels and wave functions of the heavy and light holes.

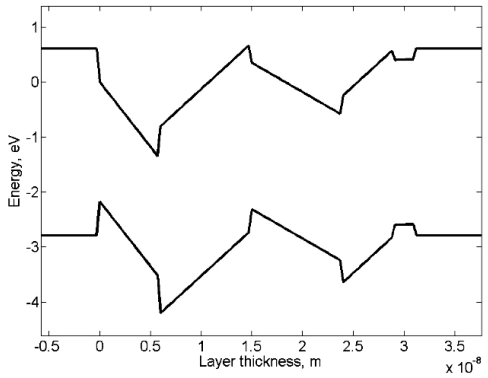

Fig. 2 – The band energy profile and thickness by applying a potential

Table 3 – The values of the electric fields in the layers

Layers	Red dot	Barrier	Green dot	Barrier	Blue dot
E, В/м	$2.4 \cdot 10^8$	$1.7 \cdot 10^8$	$1.1 \cdot 10^8$	$1.7 \cdot 10^8$	$5.1 \cdot 10^6$

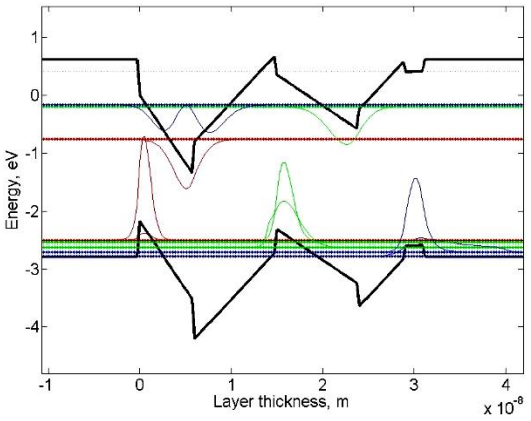

Fig. 3 – Wave functions and energy levels of electrons, light and heavy holes

Optical radiation is generated when the transitions of electrons from the conduction state to the state of heavy and light holes in the valence band. An important parameter in the calculation of the spectrum is the position of the quasi-Fermi levels in the structure. Changing the position of these levels depends on the applied bias to the structure. The emission spectrum is calculated for each hole:

$$r_{sp}(h\upsilon) = \left(\frac{q^2 h}{2m_0 \varepsilon \varepsilon_0}\right)\left(\frac{1}{h\upsilon}\right) D_{opt} D_r |M|^2 f_c (1-f_v), \quad (7)$$

$$D_{opt}(h\upsilon) = \frac{\varepsilon n_r}{\pi^2 \hbar^3 c^3} (h\upsilon)^2, \quad (8)$$

$$D_r = \frac{m_r}{\pi \hbar^2 d_z}, \quad (9)$$

where q – the charge of the electron; m_0 – electron mass; ε – is the relative dielectric constant; ν – is the frequency; $|M|^2$ – the matrix element of the transition; f_c – the distribution function of the electrons in the conduction band; f_v – the distribution function of the holes in the valence band; ε_0 – dielectric constant; h – Planck's con-

stant; D_r – the density of optical modes; n_r – the refractive index of the material; d_z – the thickness of the quantum well; m_r – the reduced mass of the electron and hole.

The calculated emission spectra in the red, green and blue dots for three values of bias shown in Fig. 4, 5, 6, respectively.

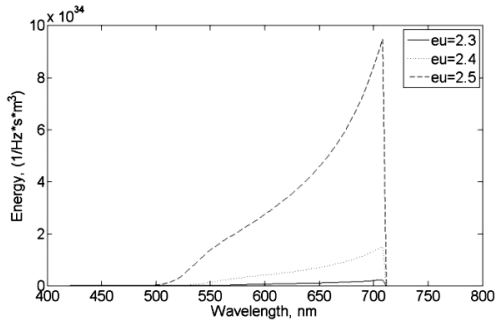

Fig. 4 – The emission spectrum in the red hole

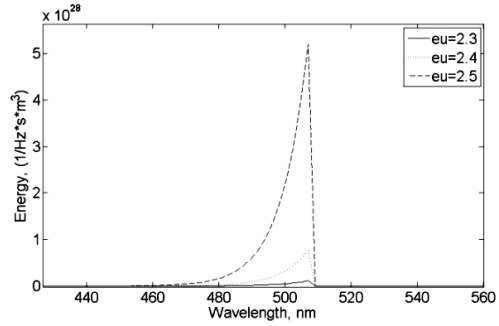

Fig. 5 – The emission spectrum of the green dot

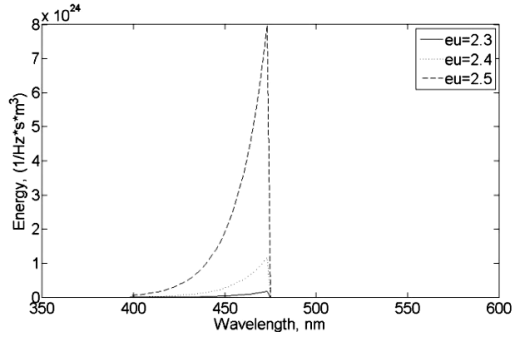

Fig. 6 – The emission spectrum of the blue dot

The chromaticity coordinates of the emitted total spectrum corresponding to transitions $e_1 \to h_1$, $e_2 \to h_2$, $e_3 \to h_3$ for the displacements were calculated in the range 1 B $\le U \le$ 3 B of formulas

$$X = \frac{x'}{x' + y' + z'} \tag{10}$$

$$Y = \frac{y'}{x' + y' + z'} \tag{11}$$

where, x', y', z' – the coordinates of the color.

$$x' = \int_{\lambda\min}^{\lambda\max} I(\lambda) \cdot x(\bar{\lambda}) \cdot d\lambda \tag{12}$$

$$y' = \int_{\lambda\min}^{\lambda\max} I(\lambda) \cdot y(\bar{\lambda}) \cdot d\lambda \tag{13}$$

$$z' = \int_{\lambda\min}^{\lambda\max} I(\lambda) \cdot z(\bar{\lambda}) \cdot d\lambda \tag{14}$$

where $x(\lambda)$, $y(\lambda)$, $z(\lambda)$ – ordinates of the curve addition colorimetric system XYZ, $I(\lambda)$ – the emission spectrum. These points are plotted on the XY plane of the color (Fig. 7).

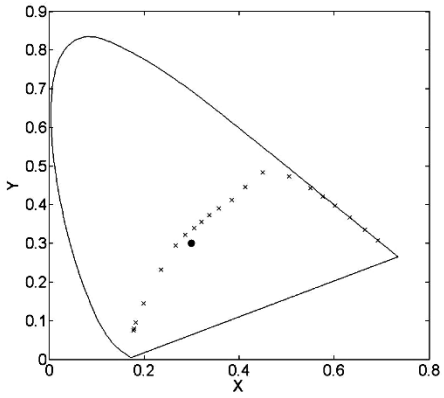

Fig. 7 – The dependence of the total spectrum of the color difference of the Fermi levels in the plane color

3. CONCLUSIONS

As a result of: 1. A physical model of tri-band LEDs based on quantum wells in the GaN/InGaN. 2. The method of mathematical modeling of spontaneous emission spectra calculated in this system. 3. It is shown that the difference between the quasi-Fermi levels in the range of 2.3 V to 2.5 V total spectrum color close to white. Thus, this structure may be promising for producing a monolithic transducer white.

REFERENCES

1. J. Piprek, S. Li, *Optoelectronic Devices: Advanced Simulation and Analysis* (Springer: 2005).
2. L.V. Kozhitov, V.G. Kosushkin, S.G. Emelyanov, S.S. Strel'chenko, Y.N. Parkhomenko, V.V. Kozlov, *Scientific publication. Monograph. South-West University, 2nd Ed. Rev. and Corr.* (Kursk: 2012).
3. V.G. Kosushkin, S.L. Kozhitov, *J. Nano- Electron. Phys.* **5** No 4, 04022 (2013).
4. V. Bashtovoi, A. Reks, S. Klimovich, A. Motsar, P. Ryapolov, A. Storozhenko, L. Shalanjva, *J. Nano-Electron. Phys.* **5** No 4, 04028 (2013).
5. F. Bernardini, V. Fiorentini, *Phys. Rev. B* **56** No 16, R10024 (1997).