The efficiency of GaN/AlGaN p-n heterostructures in UV spectral range

S Yu Kurin\textsuperscript{1}, A S Usikov\textsuperscript{2,3}, B P Papchenko\textsuperscript{2}, H Helava\textsuperscript{3}, Yu N Makarov\textsuperscript{1,3}, A S Evseenkov\textsuperscript{4}, S A Tarasov\textsuperscript{4} and A V Solomonov\textsuperscript{4}

\textsuperscript{1}Nitride Crystals –AlN Ltd., pr. Engel’sa 27, St. Petersburg 194156, Russia
\textsuperscript{2}University ITMO, Kronverkskiy pr. 49, St. Petersburg 197101, Russia
\textsuperscript{3}Nitride Crystals Inc., 181 E Industry Court, Suite B, Deer Park, NY 11729, USA
\textsuperscript{4}Saint-Petersburg Electrotechnical University “LETI”, 5 Prof. Popov Str., 197376 St. Petersburg, Russia

E-mail: sergey.kurin@nitride-crystals.com

Abstract. GaN/AlGaN p-n heterostructures emitting in UV spectral range obtained by HVPE approach were investigated. It was shown that the peak wavelength of UV LEDs was in the range of 360 - 380 nm with FWHM of 10 - 13 nm. At operating current of 20 mA, the active region temperature $T_j$ was 43°C, the output optical power and efficiency - 1.14 mW and 1.46%, respectively. The model based on corpuscular Monte Carlo method for calculation of the light extraction index was presented. The simulation results allow us to propose the ways to increase the efficiency of UV LEDs: surface interfaces texturing, optimization of the design of heterostructures, and the use of lenses.

1. Introduction

In modern optoelectronic industry in order to create LED structures, the compositions based on solid solutions of semiconductor nitrides are used. Their most important characteristic is the conversion efficiency of electrical energy into optical radiation. The main problems of UV LEDs are low quality of epitaxial heterostructures [1, 2], low light extraction index [3], and self-heating effect. Addressing these problems will allow us to create high-quality GaN/AlGaN heterostructures for such promising areas as photoelectrochemical hydrogen generation, photopolymerization, medicine. Note also that GaN/AlGaN heterostructures can be used for other application like transistor modules and water electrolysis systems.

The main factor limiting the light extraction from the chip and reducing the efficiency of LEDs is total internal reflection [4, 5] at the interface of materials with high and low optical density. The effective way to solve this issue is introducing into the structure the surfaces that scatter light. When creating a specific shape roughness the light extraction index increases due to a significant increase in the critical angle. At present time, the texturing of the substrates and epitaxial layers is widely used [6]. The texturing can be created using a variety of methods: the technique of wet etching in combination with the Laser-lift-off technology [7], creation of microoptical elements on a sapphire substrate [8], micromachining [9] etc.
The experimental study of the optical and electrical properties of UV LEDs based on GaN/AlGaN [10-12] heterostructures has been carried out. Special attention was paid to investigation of the electroluminescence spectra at different forward currents and temperatures and determination of optical power and luminescence efficiency. In addition, in order to optimize parameters of the emitters a method based on corpuscular Monte Carlo method to simulate light extraction from the LED structures had developed. This approach allows us to not only predict the optical properties of the test structures and describe in detail the processes that lead to the loss of the output radiation, but also to make recommendations in order to improve the luminescence efficiency of LED heterostructures.

2. Experimental results

The main objective of the experiment was to investigate the structural perfection and features of the distribution of impurities in the GaN/AlGaN p-n heterostructures grown by HVPE [13], and determine their most important operating parameters, including output optical power, the temperature of the active region and efficiency [14, 15].

The design of GaN/AlGaN p-n heterostructures emitting in UV spectral range is shown in figure 1. Counting from the surface of the sapphire substrate (0001), the heterostructure includes the following epitaxial layers: nucleation layer, stress control layers, electron emitter, undoped active region, electron-blocking layer, p-contact layer. The total thickness of the above-mentioned layers is about 5 μm. Planar chips were fabricated with dimensions of 0.31 × 0.31 mm² and then packaged. The Ti/Al and Ni/Au metal compositions were used as n-and p-type electrodes, respectively.

Good quality of the structures was confirmed [16] by XRD method. The FWHM of the active layer peak on XRD rocking curve obtained in a symmetric reflection (0002) was less than 400 arcsec. The threading dislocation density measured by AFM varied from 8·10⁷ to 9·10⁸ cm⁻², which is typical for thin epitaxial nitride layers grown on sapphire substrates. The wavelength of PL maximum was in the range of 359.5–362 nm, the average PL FWHM was 11 nm. The position of the PL peak wavelength and FWHM of the main peak were almost identical for different areas on the wafer surface. The results showed that the use of rapid and low-cost HVPE method allowed us to achieve a high degree of structural perfection of epitaxial structures.

When studying the operating parameters of LEDs we focused on the investigation of spectral (figure 2), power-current (P-I) (figure 3) and I-V characteristics, the measurement of power and efficiency of the luminescence, as well as the study of the impact on them of the direct current and ambient temperature. The investigated structures demonstrated high enough output optical power. At 20 mA current it was 1.15 mW and reached a maximum of 4.2 mW at 120 mA. A deviation of the P-I characteristics from the linear dependence was observed at current values above 30 mA. The LEDs showed a working capacity in the continuous operation mode up to the values of the direct current of 140 mA.

Figure 1. The design of GaN/AlGaN p-n heterostructure.

Figure 2. Electroluminescence spectra of UV LEDs at different values of direct current.
Depending on the wavelength of the maximum of the luminescence spectrum on the current value (figure 2) one can see that the shift of the spectral characteristics to long-wave region accelerates with an increase in current. This effect is due to a rapid increase in the temperature of the crystal. In general, the peak wavelength is seen to shift by 20 nm with increasing of the current from 2 mA to 140 mA (figure 4). Special attention was paid to the influence of direct current on the temperature of the active region of the structure (figure 5). The experimental data indicate that the p-n-junction temperature $T_j$ at 20 mA is 43°C, which is higher than the values of blue emitters based on InGaN. At the current of 60 mA $T_j$ exceeded 100°C and then the temperature continued to increase significantly. A comparison dependencies of wavelength and temperature on the current leads to a conclusion that self-heating is one of the main process that reduces the output optical power of the structures. It was determined that the thermal resistance of the samples at $I_f$ was equal to 250°C/W.

![Figure 3. The power-current characteristics of UV LEDs.](image3)

![Figure 4. The dependence of the wavelength at the maximum of the spectral characteristics on the direct current.](image4)

Maximum wall-plug efficiency of packaged UV LED chips was equal to 1.5% at $I_f$ (figure 6). At 100 mA the efficiency decreased by about 2 times.

![Figure 5. The dependence of the temperature of the UV LED active region on the direct current.](image5)

![Figure 6. The dependence of the efficiency of the UV LED on the direct current active region on the direct current.](image6)
3. Numerical simulation by Monte Carlo method

In order to calculate the efficiency of transmission by Monte Carlo method [17] it is necessary to find the ratio of photons passing through the structure to their total number, i.e. one should take into account all possible variants of interaction of photons with the structure through randomly distributed parameters.

The random variables are the initial position of a photon generated in the active layer, its propagation vector (it sets the initial solid angle), as well as the factor that characterizes the probability of absorption of a photon. When photon passes through the structure its incidence angle on the surface of the phase boundary can be found. Depending on this angle either a rotation of the vector of a photon or its reflection from the interface occurs. As a result of consecutive reflections and refractions photon can be either absorbed by multilayer structure or passed through it. For a sufficiently large number of photons one can determine the transmittance of the structure that was actually done in the framework of the established model.

For simulation, the grid step was chosen to be 10 nm, the number of cross-sectional nodes was $8.25 \times 10^{14}$, the number of generated photons $− 10^6$ (per one point). The choice of these parameters is explained by a compromise between accuracy and computational speed, as well as finding the optimal interaction of the photon with the structure (with too small step a photon will “feel” too small irregularities, with too large step – not adequately describe the interaction with the roughness).

The light extraction index was calculated for structures with different thicknesses of the GaN layers and sapphire. The dependencies obtained indicate significant improvement of transmission of the structure with decreasing the thickness of semiconductor layer and small influence of varying the thickness of the sapphire substrate. The first effect is explained by a decrease in the average path length of photons, which accounts for the layers with the highest light absorption. As a result, a decrease in the thickness of the GaN layer from 5.5 to 1.5 μm causes an increase in transmittance more than two times (figure 7). In the case of pyramidal roughness aspect ratio is the ratio between the height of the pyramid and its base. The improvement is observed for all the aspect ratios of texturing, because absorption occurs for all photon trajectories. The decrease in the thickness of the sapphire has very little effect on the transmission of the structure (figure 8), since the absorption therein is very small. This indicates a decisive impact of the thickness of the semiconductor layer on the efficiency of the light extraction from LED.

Adding a lens allows us to achieve maximum improvement of transmission at low aspect ratios of texturing (figure 8), since in this case the influence of texturing is weak. In this case, one can double the transmittance. For higher aspect ratio the effect is minimized.

![Figure 7](image1.png)  **Figure 7.** The dependence of transmittance on the aspect ratio for different thicknesses of the semiconductor layer.

![Figure 8](image2.png)  **Figure 8.** The dependence of transmittance on the aspect ratio for samples with various modifications: (a) thinned sapphire layer, (b) without modifications, (c) use of the lens.
Figure 9 shows the experimental dependence of the efficiency on the direct current in comparison with the simulation results for different aspect ratios of texturing relief – 0.5, 1 and 1.5. The semiconductor/sapphire interface has the greatest impact, since the radiation passing through the first interface through roughness comes in sapphire layer at small angles to the normal. Maximum efficiency is observed when the aspect ratio corresponds to the critical angle of total internal reflection for the GaN/sapphire interface – in the studied structure it was equal to one, i.e. the faces of the pyramid should be placed at the angle of 45° to the interface.

![Figure 9. The dependence of the efficiency on the current. A - experimental data, B - theoretical dependence with aspect ratio equal to 0.5, C - 1, D - 1.5.](image)

4. Conclusions
The GaN/AlGaN p-n heterostructures emitting in UV spectral range were grown by HVPE approach. The FWHM of the active layer peak on XRD rocking curve obtained in a symmetric reflection (0002) was less than 400 arcsec. The threading dislocation density measured by AFM varied from $8 \times 10^7$ to $9 \times 10^8$ cm$^{-2}$. PL measurements revealed a uniform distribution of peak wavelength and FWHM across the wafer. The results showed that the use of HVPE method allowed us to achieve a high degree of structural perfection of epitaxial structures.

The experiment showed that the peak wavelength of UV LEDs was in the range of 360-380 nm with FWHM of 10-13 nm. At operating current of 20 mA the active region temperature $T_j$ is 43°C, the output optical power - 1.14 mW. At 100 mA the efficiency decreased by about 2 times.

It was developed a model based on Monte Carlo numerical method to calculate the light extraction index. The calculated data suggest the possibility of increasing the efficiency of appliances by 3-4 times due to texturing surface interfaces, optimization of the design of heterostructures, and the use of lenses. According to the simulation, the interface that mainly influences the light extraction index is the first interface – GaN/sapphire. This is due to the fact that the main absorption layer is GaN and the rays that have passed through the first layer, leave the roughness at right angles (i.e. almost all the photons reaching the second layer leave the structure). In order to increase the efficiency of light extraction the texturing parameters at the interfaces GaN/Al$_2$O$_3$ and Al$_2$O$_3$/air need to be different. It is shown that the aspect ratio for the texturing relief should tend to cotangents of critical angles of total internal reflection at the interface of respective environments.
Acknowledgments
Work at University ITMO was supported by the Ministry of Education and Science of Russian Federation (grant agreement 14.575.21.0054, unique identifier of research activities is RFMEFI57514X0054).

References
[1] J.E.F. Schubert 2006 Light Emitting Diodes New York, Cambridge University Press
[2] M Kneissl et al 2011. Semicond. Sci. Technol 26 01403
[3] F I Manyakhin et al, 2010 Izv. Vyshh. Uchebn. Zaved 50 54
[4] J K Kim et al 2008 Appl Phys Lett 93 221111
[5] J H Son et al 2012 Advanced Materials 24 2259-2262
[6] C Rooman et al 2005 Photonics Technology Letters 2649-2651
[7] A Deinega et al 2011 J.Opt.Soc. Am. A 28 5
[8] V Osincky et al 2003 FIP 1 94.
[9] K D Lee et al 2010 Semiconductor lighting 5 22.
[10] E A Menkovich, S A Tarasov, I A Lamkin 2012 Functional Materials 19 233-237.
[11] I Lamkin, S Tarasov 2013 Journal of Physics: Conference Series 461 012025
[12] E A Menkovich, A V Solomonov, S A Tarasov, P A Yurgin 2014 Functional materials 21 186-189
[13] S Kurin, A Antipov, I Barash, A Roenkov, H Helava, S Tarasov, E Menkovich, I Lamkin, Yu Makarov 2013 Physica status solidi (c) 10 289–293
[14] E A Menkovich, S A Tarasov, I A Lamkin, S Yu Kurin, A A Antipov, et al 2013 Journal of Physics: Conference Series 461 012027
[15] A V Solomonov, S A Tarasov, E A Men'kovich, I A Lamkin, S Yu Kurin, A A Antipov et al 2014 Semiconductors 48 245–250
[16] E A Menkovich, S A Tarasov, I A Lamkin, A V Solomonov, S Yu Kurin, A A Antipov, I S Barash, A D Roenkov, A S Usikov, H I Helava and Yu N Makarov 2014 Journal of Physics: Conference Series 541 012054
[17] V Kandidatov et al 2006 Quantum Electronics 36 1003-1008