Improving the efficiency of emission extraction from nitride LED structures with textured interfaces

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Abstract. The light-emitting diode (LED) structures based on gallium nitride (GaN) and grown on sapphire substrates were investigated. The obtained experimental data include the emission spectrum, optical power and current-voltage characteristics. Monte Carlo simulation based on the parameters of the structures was conducted. During the simulation optimal parameters of surface texturing were evaluated, and alternative methods of structure modification were shown.

1. Introduction

Realization of the potential advantages of blue light-emitting diodes (LEDs) based on gallium nitride (GaN) and its solid solutions, as light sources satisfying modern specifications, requires considerable development and improvement efforts. Primarily, significant increase of power and external quantum efficiency (EQE) of the LEDs is required. There are various methods to improve the parameters of the structures based on GaN [1-2].

The main physical effect, which reduces the ratio of the output optical power to the emission power generated inside the crystal, is a total internal reflection [3,4] at the interface of materials with high and low refraction indexes.

The effective way to solve the problem of limiting the light output is to obtain surfaces that scatter light [5-7, 9-13]. When creating a surface texturing forms with predetermined parameters, the impact effect of total internal reflection is reduced, and part of the light output from the device can be increased. At present, the texturing of both substrates and epitaxial layers is used widely [6]. In the LED industry two basic approaches are applied: random texturing technology and patterned sapphire substrate. Random texturing of the top layer of p-GaN is an economical method where additional efforts are not required.

At present, the transition from experimental methods to the analytical prediction and the calculation of the value of the efficiency of the emission output depending on the size and geometry of textures interfaces is of current interest [7]. The aim of the work was to find the optimum variant of texturing interfaces in the Al₂O₃/GaN/InGaN flip-chip LED structure leading to the maximum efficiency of the emission output. To reach this goal, a mathematical model describing the process of the emission output of the nitride LED structures was created, and numerical calculation was carried out by the Monte Carlo method. The results of
calculation are compared with the analytical solution of this problem. The experimental studies of emitting structures have been undertaken, and a more than three-fold increase of the emission output efficiency when using texturing was demonstrated.

2. Numerical simulation Monte Carlo

Below, we call an elementary particle of light propagating according to the laws of geometrical optics a photon.

In the simulation of the emission propagation through the optical semiconductor structure by the Monte Carlo method, two main approaches are used: wave and corpuscular [9]. Since the geometrical dimensions of the roughness greater than the wavelength emission, it is possible to use the Monte Carlo method. For the purpose of increasing the calculation accuracy, absorption in the thicker layers should be taken into account. Since the calculation is carried out in geometrical optics approach, where the absorption in the medium is not considered, the Bouguer-Lambert-Beer law for the light intensity is used for numerical calculations:

\[ I(l) = I_0 e^{-k_\lambda l}, \quad k_\lambda = \frac{4\pi k}{\lambda}. \]

Since the Bouguer-Lambert-Beer law is applicable to the flux intensity consisting of a great number of photons, the corpuscular Monte-Carlo method operates with single photons, the problem in modeling using the Monte-Carlo method is the choice of criterion, according to which one determines whether a particular photon has been absorbed or continues its movement through the material. We suggest a following statistical approach to establishing a relation between a single particle and a flux. The criterion of absorbing a photon on the interface is based on comparison between a randomly chosen number with the intensity calculated according to the Bouguer-Lambert-Beer law, in which the length of the path is substituted with the actual path length of the photon. To find the transmission efficiency using the Monte-Carlo method one has to calculate the ratio of the number of photons that passed through the structure to their total number, i.e. take into account all the possible scenarios of interaction between the photons and the structure with randomly distributed parameters.

As randomly distributed variables the following ones were taken: the initial position of a photon generated in the active region, the vector of its movement (which defines the initial solid angle), and the factor of interaction with the medium (characterizes the photon absorption probability, namely to take into account the absorption of defects, free charge carriers, contacts, and other types of absorption). The angle of its incidence on the phase boundary during traversal of a photon through the structure was calculated. Depending on this angle either a rotation of the photon’s velocity vector or its reflection from the interface occurs. After a series of reflections and refractions the photon can be absorbed by the multilayer structure or it can pass through it. Having a sufficient number of generated photons one can determine the transmission coefficient of the structure according to their statistics, which is what has been done within the framework of our model.

As the basis of parameters modeling the structure type "A" was taken, which is described in Experiment. The superlattice was accounted for as a "mirror" under the active region. Generation occurred only in the active region where the internal quantum efficiency was considered equal to 1. In the neighboring areas it was not considered. The peak emission was at 455 nm, the absorption coefficient was $10^3 \text{ cm}^{-1}$[9].

The computer program was developed in the graphical programming environment of LabVIEW. The grid step was 10 nm, the number of cross-sectional nodes was $8.25 \times 10^{14}$, and the number of generated photons was $10^6$. The choice of these numbers is the result of finding
a compromise between the precision and the speed of calculations as well as finding optimal conditions of interaction between the photon and the structure (with a smaller grid step a photon would be sensitive to too small-scaled roughness and with a larger one the calculation would describe the interaction with the texturing inadequately).

In the course of generation of photons in the active region and their traversal through the LED structure a significant part of radiation is lost due to reflection from the interface. Making pyramids with different refraction coefficients on the surface of semiconductors leads to an observable increase of transmission, which is explained by photons finding optimal trajectories that lead out of the structure as a result of multiple reflections (see Figure 1).

In reality it is impossible to produce identical texturing over the entire area of the interface. In order to take this into account in modeling one has to introduce a statistical distribution of roughness parameters with main variable parameter being the aspect ratio (roughness ratio of base to height) on the interface. Also, the presence or absence of lenses and the width of the semiconductor layer is used as a parameter. The width of the layer was 1.5, 4.5 and 7.5 μm.

Figure 1. Ray diagram of light exiting a textured layer.

Depending on the parameters of the structure different values of shape and size parameters are used for the texturing. The shape has the strongest influence since it defines the process of photon emission. Presently, the sphere-shaped, well-shaped, and pyramid-shaped (both sharp and canted) texturing is used. In the present work we use the well-shaped texturing in the modeling.

The texturing can be created using a variety of methods: the technique of wet etching in combination with the Laser-lift-off technology, creation of microoptic elements on a sapphire substrate [10], micromachining [11], using porous surfaces [12] etc.

The modeling was performed using the parameters of real nanoheterostructures based on solid solutions (Al, Ga, In)N with multiple quantum dots [13] and superlattices [14] created with MOCVD method on a sapphire substrate. The nanoheterostructures had identical structure except for the last p-GaN epitaxial layer. The buffer and contact n-GaN layers with total thickness of 4 microns were grown on a c-Al₂O₃ substrate. The active region contained one 2.5 nm-thick In₀.₁₅Ga₀.₈₅N quantum well. Then a low-doped i-GaN layer with 50 nm thickness was grown. The final p-GaN layer was of 4 following types: a superlattice consisting of 9 pairs of 1.5 nm-thick Al₀.₁₅Ga₀.₈₅N and GaN layers (type A), a p-AlGaN with 15% of aluminum (type B), a p-AlGaN with 10% of aluminum (type C), and a p-GaN layer (type D).
A calculation of transmission coefficient for structures with different values of thickness of GaN (Figure 3) and sapphire layers was performed. It was shown that the increase of the thickness of the semiconductor layer greatly reduces the transmission coefficient. For optimal transmission this layer should be made as thin as possible. The increase of thickness of the sapphire layer does not influence the light emission. Figure 3 also demonstrates the effect of a lens that collects the emitted light, which was placed on the sapphire layer.

The obtained dependencies suggest the possibility to increase the transmission through the structure by decreasing the thickness of the semiconductor layer and adding a lens that gathers incoming light (particularly in absence of texturing).

The first effect is explained by a decrease in the average path length of photons that propagate through the layers with the highest light absorption coefficient. As a result, reduction in the thickness of the GaN layer from 7.5 to 1.5 um increases the transmittance coefficient almost by one third (figure 3). This suggests that the thickness of the semiconductor layer has a determining influence on the efficiency of the optical emission output of the LED. Improving effect is observed for all the aspect ratio texturing, since absorption occurs for all photon paths.

Adding a lens allows to achieve the greatest improvement transmission at low aspect ratio texturing (figure 4), because in this case the effect of texturing is weak. In this case, one can achieve almost doubling the transmission. For large aspect ratio effect is minimized.
3. Experiment

The investigations of nanoheterostructures were carried out using a test-diagnostic system operating parameters of light-emitting nanoheterostructures developed by the authors [2, 15]. The system allows for defining all the main characteristics of solid-state light sources and devices based on them: spectral, watt and volt-ampere characteristics, power and efficiency of emission. In addition, it provides an opportunity to determine the temperature of the active region nanoheterostructures. For this purpose a new rapid non-contact method of determining the temperature of the active region is used [16]. This method is based on a detailed analysis of the electroluminescence spectra and allows us to investigate not only the separated crystals on the plates, but also LEDs including in the LED lamps. In general, the diagnostic system allows the measurement of the most important optical and electrical characteristics of any LED and devices based on them in the following ranges: wavelengths 200 – 1100 nm, forward currents: $10^{-8}$ – 10 A, voltages: 0 – 250 V, temperatures: 10 – 500 K. In this contribution, the samples were a non-separated emitting chips on a sapphire substrate, so the diagnosis was carried out by using probe station. For the test samples all the major parameters were determined: the emission spectra, power, current-voltage and temperature dependence.

Figure 5 shows the dependence of the optical power of the current samples with various finishing layer. It can be seen that the greatest power and other parameters were achieved for the sample "A". Next, this sample used in the simulation as a research object.

![Figure 5. The optical capacity dependency on the current.](image)

![Figure 6. The dependence of the efficiency of the current for different aspect ratios (0 - absence of texturing, characterizing experimental data the sample A).](image)

Figure 6 shows the results of the experiment (graph A) and the expected efficiency, if the surface of the LEDs texturing start. The greatest effect of the semiconductor/sapphire, since the emission passing across the first interface through the roughness comes in sapphire layer at the enough right angles and passes on without problems. Maximum efficiency occurs when the aspect ratio corresponds to the critical angle of the interface GaN/sapphire - for this structure, it is about unity, i.e. facet of the pyramid are arranged at an angle $45^0$ to the interface.

The graph shows the possible efficiency at the various currents and texturing parameters. The main variable parameter is the average statistical aspect ratio obtained roughness. Maximum value on the proposed LED structures may be obtained by texturing with an aspect ratio equal
to one, and a current value of 20 mA. This is due to the choice of the critical angle interface sapphire/semiconductor, in which the middle path of photons from the point of generation to the point where they exit from the structure is minimal.

4. Experiment Conclusion

In this paper LED structures based on GaN grown on sapphire substrates have been investigated (the sample with two SL of InGaN and AlGaN showed the best stability and performance). All the basic characteristics were obtained: the emission spectra, power, voltage and current characteristic. Based on the parameters of the structures numerical simulation of the emission output was made by Monte Carlo method. As a result of simulation of the LED structures, the patterns of the effect of the interface and the input roughness on the part of the emission output from the structure were obtained. Thanks the data obtained during the simulation, the change of the structures, that come as a result of surface texturing, were predicted, as well as other changes - for example the addition of lens or reducing the thickness of the semiconductor layer. It was found that the output of the structure can be increased more than 3 times by creating a pyramid with an aspect ratio equal to 1, by a decreasing the layer of gallium nitride, as well as the creation of the lens on the sapphire interface, and may be more than 30%.

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