Modeling AlGaN p-i-n Photodiodes



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Introduction

III-nitride compound materials that consist of InN, GaN, AIN, and *their alloys* are semiconductors with such interesting physical properties as high electron mobility, high carrier saturation rate, good thermal stability and conductivity, direct and variable width forbidden zone with a high coefficient of optical absorption.

The absorption coefficient of III-nitride materials is over 10^4 cm^{-1} [1]. A significant fraction of light penetrates as deep as several hundred nanometers of the absorbing region. The band gap of the Al_xGa_{1-x}N (AlGaN) material varies from 3.4 eV to 6.2 eV depending on the x proportion of aluminum in the Al_xGa_{1-x}N compound [2, 3]. Due to these physical properties, III-nitride semiconductors are promising materials for numerous optoelectronic devices such as LEDs, laser diodes, solar cells and photodiodes.

Most modern photodiodes are based on a p-i-n structure. Photons absorbed in the region of their own conductivity (i-layer) generate electron-hole pairs which are then separated by an electric field, thus creating a load current. Multiple quantum wells (MQW) [4] or superlattice structures [4] contained in nanometer AlGaN layers can be used as additional factors for bulk structures to improve crystal quality of active layers and increase sensitivity of photodiodes.

In the late 2000s E. Berkman et al. [5] developed a p-i-n-photodiode InGaN which showed a sensitivity of 37 mA / W at a wavelength of 426 nm. Then the sensitivity parameter improved rapidly with each new development. A year later, Su et al. [6] produced a p-i-n photodiode with its own $In_{0.11}Ga_{0.89}N$ active layer and the highest spectral sensitivity of 0.206 A / W at a wavelength of 380 nm. This figure was surpassed by Lu et al. [7] who reported a peak sensitivity of 0.22 A / W at 378 nm in an unbiased p-i-n photodetector.

In this case, the maximum of the watt-ampere characteristic is k = 0.085 A / W in the short-wave part of the range, with x = 0.8, in the long-wave part k = 0.175 A / W, with x = 0.

It is quite obvious that the spectral characteristic decreases as the light wavelength reduces. It happens if the photon flux density decreases while the value of the incident light power is constant and the photon energy increases. Moreover, the applied model of the frequency dependence of the Sellmeier refractive index determines its increase as the light wavelength decreases. An increase in the refractive index results in a decrease in the transition matrix element in the light absorption model and a corresponding decrease in light absorption.



Figure 4. Dispersion graphs of the AlGaN absorption coefficient with different values of aluminum fraction

Figure 4 shows dispersion graphs of the AlGaN absorption coefficient with different values of aluminum fraction. It is surprising that until now there are no generally accepted values of this quantity for AlGaN in the region of its absorption of light power. According to some papers [9], its value α is more than 10⁵ cm⁻¹, but according to the others [10], it is about 1.8 * 10⁴ cm⁻¹. The values of α obtained in our modeling quite confirm the latter value. However, it is not obvious that the applied model of a semiconductor interacting with radiation takes into account all the mechanisms of this process. The intersection of graphs at a wavelength of 0.23 µm is still explained by refractive index dispersion of the material. It affects the value of the transition matrix element more at lower x than at higher ones.

All the achievements mentioned above are related to the region of violet and near ultraviolet range. As the wavelength shortens, the achievable sensitivity index should decrease because an increase in photon energy at a constant value of radiation power means a decrease in the density of photon flux. Therefore, at a wavelength of 200 nm one should expect half the sensitivity indicator, i.e. about 0.1 A/W.

The authors of this work have made an attempt to model p-i-n-photodiodes based on the AlGaN triple compound with the use of COMSOL MULTIPHYSICS-Multiphysics software [8]. Based on the constructed model, they determined dependences of the photodiodes characteristics on such parameters as molar fraction of aluminum and thickness of the layer with intrinsic conductivity (i-layer). The information obtained from the models was used to develop a UV photodetector with a maximum spectral sensitivity at a wavelength of 0.24 μ m. The simulation results presented in this work can be used to optimize AlGaN / GaN photodetectors and develop a new generation of optoelectronic devices.

Photodiode Structure and Numerical Model

$p^+Al_xGa_{l-x}N$ 2.1×10 ¹⁸ cm ⁻³	h5Ĵ
$p - Al_X Ga = N : 2.4 \times 10^{16} \text{ cm}^{-3}$	h4 <u></u>]
$i - Al_x Ga_{1-x}N$	h3Ĵ
$n - Al_x Ga_{1-x}N: 7.2*10^{17} cm^{-3}$	h2‡
$n^+ - Al_x Ga_{1-x}N: 4.1*10^{18} cm^{-3}$	h1

Figure 1. Photodiode structure

The structure shown in Figure 1 is typical of nitride photodiodes. Between the n and p layers which have moderate electron and hole conductivity there is a pretty thick i-layer with its own conductivity where most light is absorbed and converted into free charge carriers. This three-layer structure is complemented with highly doped n⁺ and p⁺ layers at the top and bottom which make it possible to obtain omic contacts with metallic leads shown in thick lines in the figure.

One of the important issues in creating p-i-n photodiodes is choosing a thickness of the absorbing i-layer. There are some physical grounds to expect an optimum of this value according to some criteria. For example, the thicker the i-layer is, the higher the absorption of light power, on the one hand, but, on the other hand, it makes the path of photocarriers longer and increases their losses due to recombination. This allows us to assume that there is an optimum of the maximum conversion coefficient.



Figure 5. Watt-ampere characteristics calculated for GaN

Figure 5 shows graphs of watt-ampere characteristics calculated for x = 0 (pure GaN) with various thicknesses of the i-layer (h3). It can be seen in these graphs that a change in the thickness of the i-layer from 50 to 3200 nm (64 times) increases the maximum photocurrent from 0.07 to 0.23 A (approximately 3 times). In this case, the main increase in the photocurrent falls on the thickness range from 200 to 800 nm. Apparently, this range of i-layer thicknesses is the best to realize the highest conversion coefficient. However, the maximum sensitivity is not detected by the thickness of the i-layer. The graph curve slowly reaches 0.23 A / W and then goes almost horizontally. Volt-ampere characteristic (CVC) of a photodiode can be easily constructed with the COMSOL MULTIPHYSICS software because it is not necessary to take into account any interaction with luminous flux.

The lower n⁺ layer solves some other problems except for contacting the leads. It reduces an intergrowth of dislocations from contact with the substrate into the overlying layers and compensates for errors in the etching depth of the upper layers when separating diodes. Therefore, the lower n⁺ layer is much thicker than the others. It is applied on an AIN buffer layer which, in turn, rests on a sapphire substrate.

Thicknesses of the h1 - h5 layers are parameters that can be easily changed before the model is calculated. The lower n⁺ region is made wider than the rest of the structure and the omic contact is made from above the protruding part.

The applied two-dimensional model is shown in Figure 1. Taking into account the same processes along the horizontal axis, the model is actually one-dimensional, which simplifies calculation. The COMSOL MULTIPHYSICS "optoelectronics" module solves a number of basic semiconductor equations, including the Poisson equation, the continuity equation and the transport equations for electrons and holes. In addition, it offers several modern physical models for the interaction of a semiconductor with EM radiation

Results and Discussion

COMSOL MULTIPHYSICS calculates a number of characteristics of simulated processes and has a very rich toolkit to present the results. The most illustrative one is the graphical form used

below.



Figure 2. Impurity dopants distribution for a 2 µm thickness of depletion layer

Figure 2 shows a graph of impurity dopants distribution for a 2 μ m thickness of depletion layer. Acceptor impurity corresponds to positive values while donor impurity corresponds to the negative ones. There is no doping in the thickness range from 0.15 μ m to 2.15 μ m. We have a layer with its own conductivity that absorbs radiation incident on it.



Figure 6. Straight edge with different values of the x proportion of aluminum in the solid solution

Figure 6 shows graphs of a straight edge with different values of the x proportion of aluminum in the solid solution. The course of the graphs is obvious as an increase in x leads to an increase in the band gap, and this, in turn, decreases the reverse current and shifts the CVC graph to the right. What is of special interest is the value of direct voltage when a noticeable direct current appears. Let's call it U_x . Then $U_0=3.2$ V, $U_{0.2}=3.53$ V, $U_{0.5}=4.51$ V, $U_{0.8}=5.2$ V.

Conclusions

We proposed the new numerical model using COMSOL MULTIPHYSICS software to estimate I– V curve, spectral sensitivity, absorption coefficient, and other parameters as a function of the proportion of aluminum in the AlGaN alloy and the thicknesses of the layers forming p-i-n photodiode based on AlGaN. This model was able to calculate the voltage and current dependency similar to device simulation as a continuous solution and could be useful for device development as a quick calculation. It could be also useful to academical and educational understanding the behavior of the electrical characteristics.

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The main parameters of the photodetector are coefficient of conversion of the incident light power into electric current (watt-ampere characteristic) and dependence of this coefficient on the length of the light wave (spectral characteristic).



Figure 3. The photocurrent value depends on the light wavelength and the molar fraction of aluminum in the i-layer

Figure 3 shows the graphs obtained as a result of calculation. They reveal how the photocurrent value depends on the light wavelength (lambda) and the molar fraction of aluminum in the i-layer (x) at an incident light power of 1 W. The calculation was carried out for a 0.2 μ m i-layer and a reverse voltage applied to the photodiode V_n = 1 V. Depending on x, the maximum of the spectral characteristic falls on the wavelengths from $\lambda = 0.2 \ \mu$ m to 0.32 μ m.

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