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Original paper

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MODELING AlGaN *P-I-N* PHOTODIODES

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Abstract. Ternary AlGaN alloys with a band gap of 3.4 to 6.2 eV are very promising for photodetectors in the UV wavelength range. Using the COMSOL MULTIPHYSICS software based on AlGaN, a *p-i-n* photodiode model was developed, including its *I–V* characteristic, spectral sensitivity of the received radiation, absorption coefficient as a function of the aluminum fraction and the depletion layer thickness. To calculate the process of interaction of a semiconductor with EM radiation, we used a model based on the use of an element of the transition matrix through the carrier lifetime during spontaneous recombination. In this case, the peak sensitivity of the photodiode is from 0.08 to 0.18 A/W at wavelengths of 0.2–0.33 μm. This is in line with experimental results taken from the relevant literature.

Keywords: photodetector, two-dimensional model, *p-i-n* structure, numerical simulation.

Conflict of interests. The authors declare no conflict of interests.

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Introduction

III-nitride compound materials that consist of InN, GaN, AlN, and their alloys are semiconductors with interesting physical properties such 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 into 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 to implement 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 the 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 Y., Zhang Y., Li X.Y. [7] who reported a peak sensitivity of 0.22 A/W at 378 nm in an unbiased *p-i-n* photodetector.

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 the 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 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 the wavelength of 0.24 μm. 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

The structure shown in Fig. 1 is typical of nitride photodiodes.

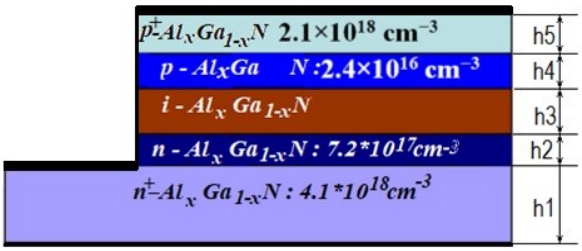

Fig. 1. Photodiode structure

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.

The lower *n*+ layer solves some other problems except for contacting the leads. It reduces an intergrowth of dislocations from a 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 AlN 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 Fig. 1. Taking into account the same processes along the horizontal axis, the model is actually one-dimensional, which simplifies the 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.

The band gap E_g for $Al_xGa_{1-x}N$ at room temperature is calculated by using the well-known formula [9] which approximates the actual dependence of E_g on *x* molar fraction of aluminum by the quadratic dependence:

$$E_g^{AlGaN} = xE_g^{AlN} + (1 - x)\,E_g^{GaN} - 1.1x(1 - x). \quad (1)$$

The values of the AlN and GaN band gap are: $E_g^{AlN} = 6.2$ eV [11] and $E_g^{GaN} = 3.42$ eV [10].

It is known that electronic affinity potential of AlGaN decreases as the fraction of aluminum increases and the band gap increases according to a law close to a linear one. The calculation is based on the following formula from [11]

$$\chi = 4.1 + 0.7\left(Eg^{GaN} - Eg^{AlGaN}\right). \quad (2)$$

Effective densities of the states in the conduction and valence bands are approximated by linear dependences on the fraction of aluminum [11]:

$$N_c^{AlGaN} = \left(\frac{T}{1K}\right)^{3/2} \left(1.8x + 4.6(1-x)\right)\cdot 10^{14}\,\text{cm}^{-3};$$
$$N_v^{AlGaN} = \left(\frac{T}{1K}\right)^{3/2} \left(10.6x + 9.2(1-x)\right)\cdot 10^{15}\,\text{cm}^{-3}. \quad (3)$$

The permittivity constant ε and the relative effective masses of electrons (holes), m_e (m_h), are also assumed to depend linearly on the fraction of aluminum and determined as [11]:

$$\varepsilon^{AlGaN} = 10.1x + 10.4\ (1 - x);$$
$$m_e^{AlGaN} = 0.314x + 0.2\ (1 - x); \quad (4)$$
$$m_h^{AlGaN} = 0.417x + 1.0\ (1 - x).$$

There are temperature-dependent models of carrier mobility in nitride materials in weak and strong fields. However, since the calculation was carried out only at room temperature (293 K), the temperature dependence was excluded from the formulas. This makes it possible to use a simpler expression for the electron mobility:

$$\mu_e(N,x) = \mu(x)_{\min} + \frac{\mu(x)_{\max} - \mu(x)_{\min}}{1 + \left(\frac{N_{tot}}{N_{ref}}\right)^{\alpha(x)}}, \quad (5)$$

where x is fraction of aluminum, $N_{ref} = 10^{17}$ cm^{-3} is reference impurity concentration, N_{tot} is total concentration of impurities in a given area of the crystal. The values of the $\mu(x)_{max}$, $\mu(x)_{min}$ and $\alpha(x)$ parameters obtained experimentally in [11] are presented in the following Tab. 1.

Table 1. The values of the $\mu(x)_{max}$, $\mu(x)_{min}$ and α

Material	μ_{min} cm^2/(V.s)	μ_{max} cm^2/(V.s)	α
GaN	295.0	1460.7	0.66
$Al_{0.2}Ga_{0.8}N$	132.0	306.1	0.29
$Al_{0.5}Ga_{0.5}N$	41.7	208.3	0.12
$Al_{0.8}Ga_{0.2}N$	47.8	199.6	0.17
AlN	297.8	683.8	1.16

In the region with intrinsic conductivity $N_{tot} = 0$, the electron mobility coincides with the maximum value: $\mu_e = \mu_{max}$. This value was calculated using the approximating formula, which provides an exact match at the five points given in the table: $\mu_e = 18475x^4 - 40696x^3 + 32168x^2 - 10723x + 1460$.

The hole mobility is taken equal to 5 cm^2 V^{-1} s^{-1} [10]. As the band gap of AlGaN is quite wide, the main mechanism of carrier loss in AlGaN is defect-mediated recombination. The calculations take into account two recombination models. The first one is a simplified Shockley–Read–Hall (SRH) model of recombination on defects (traps) where one energy level is assigned to the traps while other characteristics, including the concentration of defects, are expressed by the lifetimes of electrons and holes. This time is assumed as equal to 1 ns, and the energy level of defects is taken near the middle of the band gap. The second type taken into account is direct recombination with the parameter C = 10^{-8}cm^{-3}s^{-1} [8].

COMSOL MULTIPHYSICS offers several models of optical generation and carrier recombination. We applied a model based on the calculation of a transition matrix element using the carrier lifetime with spontaneous recombination, which was taken equal to τ_{spon} = 1 ns. The element of the transition matrix is also highly dependent on the n refractive index of the material. The value of the latter, in turn, is a function of the wavelength λ. This dependence can be approximately described by the Sellmeier dispersion equation:

$$n^2(\lambda) = 1 + \frac{A_0}{1 - \left(\frac{\lambda_0}{\lambda}\right)^2}, \tag{6}$$

where the A_0 and λ_0 constants are determined by the band gap and approximated for nitride compounds by the following expressions [1]:

$$\begin{aligned} A_0 &= 6.626 - 0.934E_g + 0.0598E_g^2; \\ \lambda_0 &= (396.8 - 84.12E_g + 6.758E_g^2)\left[\text{nm}\right]. \end{aligned} \tag{7}$$

The band gap in these formulas is in eV and the wavelength is in nm.

COMSOL MULTIPHYSICS calculates many quantities, including the magnitude of the absorption coefficient and its spectral behavior α(λ) which can be easily recalculated into the extinction coefficient:

$$k(\lambda) = \frac{a(\lambda)\lambda}{4\pi}. \tag{8}$$

Numerical modeling was carried out for the AlGaN *p-i-n* photodiode at 293 K. The width of the diode was assumed to be 20 μm, its thickness is the depth size of 1 m. The thickness is chosen taking into account that the absolute value of electromagnetic power in a two-dimensional problem is considered to be distributed in depth per unit of length, i. e. at 1 m.

Results and discussion

COMSOL MULTIPHYSICS calculates a number of characteristics of simulated processes and has a very rich toolkit to represent the results. The most illustrative one is the graphical form used below. Fig. 2 shows a graph of impurity dopants distribution for 2 μm 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 to 2.15 μm. We have a layer with its own conductivity that absorbs radiation incident on it.

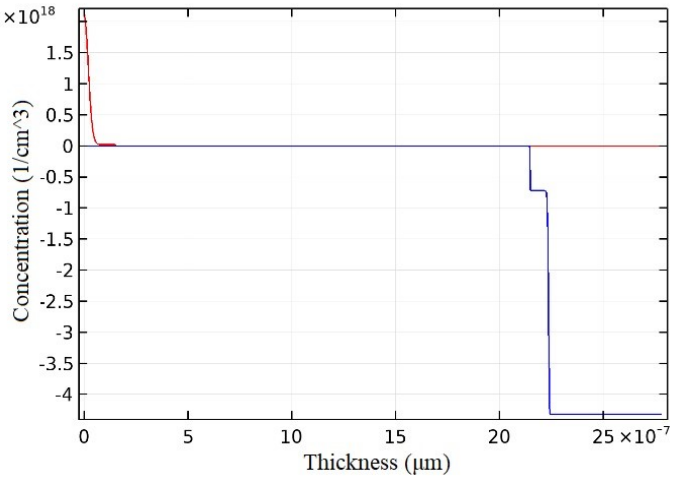

Fig. 2. Impurity dopants distribution for a 2 μm thickness of depletion layer

The main parameters of the photodetector are a 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).

Fig. 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 (x) in the i-layer at an incident light power of 1 W. The calculation was carried out for the 0.2 μm i-layer and the reverse voltage applied to the photodiode $V_n = 1$ V. Depending on x, the maximum of the spectral characteristic falls on the wavelengths from $\lambda = 0.2$ μm to 0.32 μm. 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 $x = 0$.

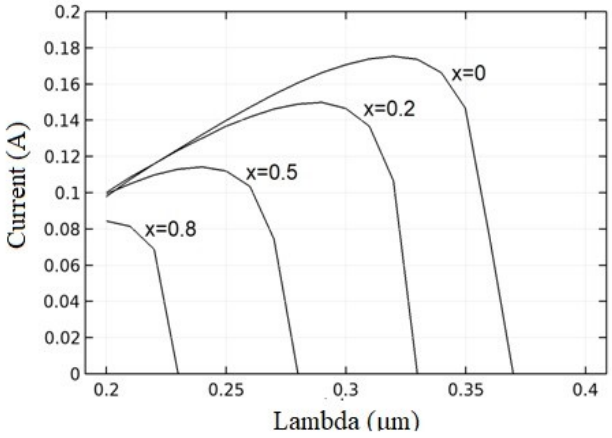

Fig. 3. The photocurrent as function of light wavelength for different x of aluminum in the i-layer

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 the light absorption.

Fig. 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 the light power. According to some papers [12], its value α is more than 10^5 cm^{-1}, but according to other [13], it is about $1.8 \cdot 10^4$ 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.

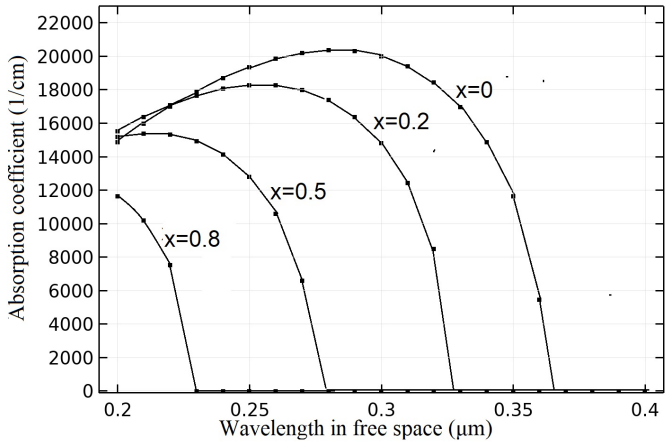

Fig. 4. Dispersion graphs of the AlGaN absorption coefficient with different values x of aluminum fraction

The intersection of graphs at the wavelength of 0.23 μm is still explained by the refractive index dispersion of the material. It affects the value of the transition matrix element more at the lower x than at the higher ones. 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, on one hand the thicker the *i*-layer is, the higher the absorption of light power, 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. Fig. 5 shows graphs of the 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.

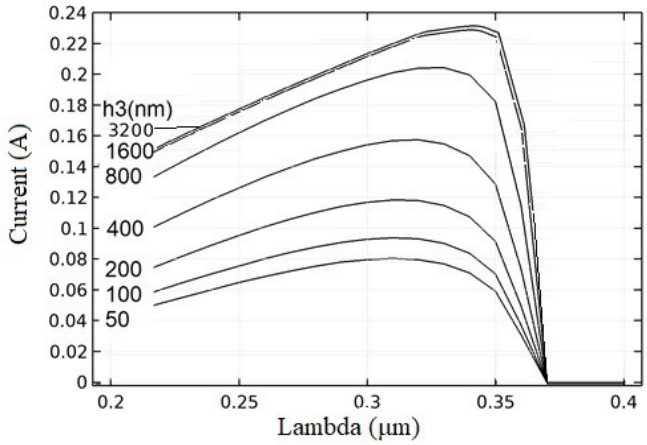

Fig. 5. Watt-ampere characteristics calculated for GaN

A 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 graphs of a straight edge with different values of the x proportion of aluminum in the solid solution are shown at Fig. 6.

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.

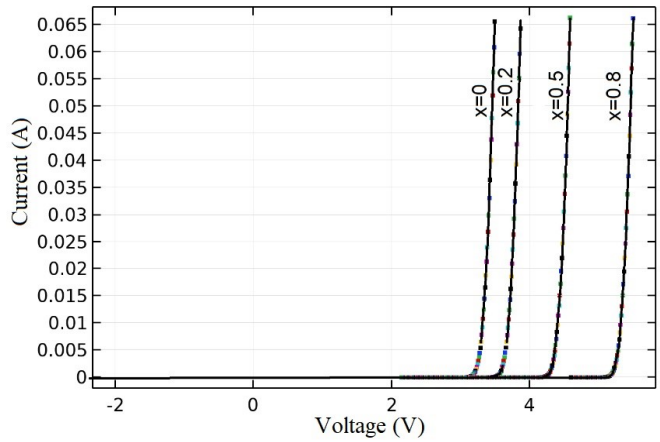

Fig. 6. Straight edge with different values of the x proportion of aluminum in the solid solution

Conclusion

The new numerical model using the 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 [14, 15] is proposed in the article. This model was able to calculate the voltage and current dependency similar to a 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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Authors' contribution

Vorsin N.N. performed the task for the study, contributed to creating the models and discussing the research results, as well as prepared the manuscript of the article.

Gladyshchuk A.A. performed the task for the study, contributed to discussing the research results.

Kushner T.L. did the literature review, contributed to the research results discussion, and prepared the manuscript of the article.

Tarasiuk N.P. contributed to modeling the photodiodes structure, solving math models, and discussing the research results, prepared the manuscript of the article.

Chugunov S.V. contributed to modeling the photodiodes structure, solving math models, and discussing the research results.

Borushko M.V. did the literature review and prepared the manuscript of the article.

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