Distributions of silicon implanted in GaN epitaxial layers

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Abstract. Ion-doped layers of n⁺-GaN were formed with a high degree of activation of the embedded impurity. Si⁺ ion implantation was performed in GaN epitaxial layers grown by MOCVD. Profiles of embedded silicon in gallium nitride were calculated. The experimental profile obtained by secondary ion mass spectrometry is compared with the calculated one. Optimal implantation modes were determined, the implantation dose is 10¹⁵ cm⁻², and the energy is 50 keV. Activation of the embedded impurity was performed by high-temperature photon annealing in a nitrogen medium using SiO₂ and Si₃N₄ protective coatings. The influence of the annealing temperature on the morphology of protective coatings is considered. The SRIM program was used to simulate the process of ion implantation of silicon at the interface of the AlGaN/GaN heterostructure through SiO₂ dielectric films of different thickness. Ohmic contacts were formed on the ion-doped basis of the Ti/Al/Ni/Au metallization system. The calculation of the contact resistance of ohmic contacts showed that the use of ion doping through a 50 nm thick silicon dioxide film reduces the contact resistance from 1.2 Ω·mm to 0.8 Ω·mm. The use of ion implantation technology in the manufacture of diode structures reduces the direct voltage drop and the minimum voltage drop is achieved when using implantation through a 50 nm SiO₂ mask, this is due to the location of the maximum distribution of the implanted impurity at a depth corresponding to the occurrence of a two-dimensional electron gas.

1. Introduction

In recent years, there has been a growing interest in microelectronic devices based on epitaxial structures of gallium nitride (GaN). The large band gap, high electron saturation drift rate, high breakdown voltage, and high thermal conductivity make this material extremely promising for high-power microwave devices, monolithic integrated circuits, injection lasers, and LEDs.

To further improve the characteristics of devices and fully unlock the potential of the material, it is necessary to use the operation of ion implantation in the manufacturing technology of devices. However, post-implantation annealing and integration of the operation will be a difficult task, and many issues of ion implantation in GaN require further study. In [1, 2], the prospects of using ion implantation for the formation of ohmic contacts on gallium nitride are shown.

When forming n-type ion-doped layers on GaN, silicon ions are most often used as an impurity. Silicon has a smaller atomic radius and higher electronegativity (1.9) compared to gallium (1.8). During Si⁺ ion implantation in GaN, silicon prefers to replace gallium, since the Si – N bond is energetically more advantageous than GaN. Figure 1 shows a scheme for replacing the Ga atom with Si to form covalent bonds with n atoms. The Si atom, which replaces
the Ga atom, gives away a free electron to be embedded in the crystal structure. An electron that moves freely in the crystal lattice increases the electrical conductivity of the substrate.

![Figure 1. The introduction of the implanted Si atoms in the crystal lattice of GaN.](image)

In addition to silicon ions, there are also other donor impurities for GaN, such as O⁺, S⁺, Se⁺, and Te⁺. However, studies on implantation of these impurities in GaN show that the degree of activation of these impurities is small compared to silicon [3]. In table 1 are presented the values of the ionization energy for donor impurities.

| Ion  | Ionization energy, meV |
|------|------------------------|
| Si   | 29                     |
| O    | 78                     |
| S    | 48                     |
| Te   | 50                     |

One of the disadvantages of ion implantation is the damage created during ion bombardment. When an accelerated ion passes through the crystal, point defects occur. Characteristic defects are Frankel defects, which are a combination of a semiconductor atom knocked out of a node in the internode and an empty node formed. Vacancies can move around the crystal, and they can combine and form clusters. Interstitial atoms are also mobile. As a result of combining simple defects, more complex linear and flat defects and packaging defects occur.

During implantation, each moving ion creates a highly disordered area. The size of this disordered region depends on the mass and energy of the ion, the mass of the target atoms, its temperature, and the structure of the crystal. As the size of the disordered region increases, an amorphous region is formed. The dose required for the formation of a homogeneous amorphous layer is called the critical dose. For example, the formation of an amorphous layer in GaN during Si⁺ ion implantation requires a dose of $2.4 \times 10^{16}$ cm⁻² with an energy of 100 keV.

The purpose of the annealing process is to restore the crystal structure of the doped GaN regions and activate the embedded silicon. Defects formed in the implanted area can form localized deep levels that act as traps for free charge carriers and compensate for shallow donors or acceptors. These deep levels can also reduce the efficiency of optical devices by non-radiative recombination. Crystal disordering also provides a high concentration of scattering centers, which significantly reduces mobility. In any case, these defects caused by ion implantation degrade the electrical and optical properties of the semiconductor material. Therefore, after implantation, it is necessary to perform annealing of defects,
and the annealing must be carried out in such a way as to achieve the maximum effect in a minimum period of time at a minimum temperature in order to avoid diffusive blurring of the profile [4].

The annealing temperature for optimal removal of radiation defects in complex semiconductors usually corresponds to 2/3 of the melting temperature of the material.

2. Results and discussion

In previous studies, it has been shown that the necessary temperature to eliminate defects and activate the impurity must be above 1000 °C. Despite the fact that GaN has a high melting point, dissociation of the sample surface begins at 900 °C, which leads to the formation of N₂ and, as a result, to the loss of nitrogen from the GaN crystal lattice. To prevent this phenomenon, it is necessary to apply protective coatings.

To protect the GaN surface, we used SiO₂ and Si₃N₄ dielectric films formed by plasma chemical deposition in inductively coupled plasma at a temperature of 200 °C. The choice of low-temperature SiO₂ and Si₃N₄ films as protective coatings during annealing of ion-doped GaN layers is due to their high reproducibility and wide use in the creation of various microelectronic devices, including structures based on gallium nitride. Table 2 shows how the surface morphology of protective films changes after exposure to high temperatures. Si₃N₄ films, when used as protective coatings, are destroyed at an annealing temperature above 1100 °C.

| Annealing temp., °C | 1100 | 1200 | 1300 |
|---------------------|------|------|------|
| Protective coating  |      |      |      |
| SiO₂                |      |      |      |
| Si₃N₄               |      |      |      |

When the protective film is destroyed, GaN dissociates, nitrogen evaporates from the volume of the semiconductor, and gallium accumulates on the surface. This imposes a restriction on the use of Si₃N₄ films as protective coatings during annealing.

Fast photon annealing in nitrogen was used to activate the embedded impurity. The annealing temperature varied from 1000 to 1300 °C, and the time was fixed at 1 minute. Based on the results of measurements of the electrophysical parameters of ion-doped GaN layers, it was shown that for the implantation dose of Si⁺ 10¹⁵ cm⁻² and the ion energy of 50 keV when using SiO₂ films with a thickness of 0.4 microns as protective coatings, the optimal annealing temperature is 1250 °C, with the impurity activation reaching 100% [5].
The distribution of projection runs of the embedded impurity is described by the Lindhardt-Scharf-Schiott theory (LSS). The deceleration profile has the form of a Gaussian curve and the distribution of embedded ions per unit volume of the target can be written as follows:

\[ N(x) = \frac{\phi}{\sqrt{2\pi \Delta R_p}} \exp \left(-\frac{(x - R_p)^2}{2\Delta R_p^2}\right), \]

where \( \phi \) – the dose of the introduced ions, \( R_p \) – the average projected mileage, \( \Delta R_p \) – average normal deviation of the mileage projection, \( x \) – depth from the target surface.

The maximum concentration of embedded ions is located at a distance of \( R_p \) from the target surface, and its value is equal to:

\[ N_{max}(x) = \frac{\phi}{\sqrt{2\pi \Delta R_p}}. \]

Some parameters of the implantation process can affect the impurity distribution and make changes to the Gaussian profile to more accurately describe the impurity distribution. When falling ions collide with target atoms, they experience a significant degree of backscattering. This leads to the fact that the profiles have a more pronounced asymmetry. In addition, if the trajectory of the incident ion is parallel to the main orientation of the target crystals, an effect called channeling can occur, which can greatly distort the predicted final position of the ion. To eliminate this problem and minimize the channeling effect, the target is positioned at an angle to the incident beam, and most often at an angle of 7°. The distribution of mileage projections is considered Gaussian and is often used to predict the distribution of embedded impurity. However, to predict the runs of embedded ions in targets of complex composition or with a large number of thin epitaxial layers, it is preferable to use simulation programs that offer a more accurate calculation taking into account the influence of large implantation conditions. In this work, we used one of the computer simulation programs with Monte Carlo calculation to model the profiles of implanted ions in GaN epitaxial films.

The main task is to reduce the contact resistance of ohmic contacts of diode structures based on AlGaN/GaN, using ion implantation technology. The AlGaN/GaN heteroepitaxial structure presented in figure 2 was used for the experiments.

**Figure 2.** The initial heteroepitaxial structure.

Heteroepitaxial structures were grown by chemical deposition from the gas phase using organometallic compounds on 2-inch sapphire substrates.

When using ion implantation, it is necessary to form local areas of highly alloyed material. In this case, the maximum impurity distribution should be at the level of a two-dimensional electron gas formed at the interface between AlGaN and GaN, i.e. at a depth of 25 nm.

Using the LSS theory, the Si⁺ distribution in GaN was calculated for implantation with energies of 50, 100 and 150 keV, and the dose used in the calculation was assumed to be \( 10^{15} \text{ cm}^{-2} \) (figure 3).
Figure 3. Calculated profiles of the concentration of silicon atoms embedded in GaN with energies of 50, 100 and 150 keV, implantation dose $10^{15}$ cm$^{-2}$.

Calculations show that at an implantation energy of 50 keV, the maximum Si$^+$ distribution in GaN is at a depth of about 50 nm.

Figure 4 shows the calculated and experimental profiles of implanted silicon ions in gallium nitride. The experimental profile was obtained by secondary ion mass spectrometry for implanted Si$^+$ ions with an energy of 50 keV and a dose of $10^{15}$ cm$^{-2}$.

The maximum concentration value of the calculated profile is close to the experimental value, $2.7 \times 10^{21}$ cm$^{-2}$ and $1.5 \times 10^{21}$ cm$^{-2}$, respectively, and is located at a depth of approximately 50 nm. To determine the depth of the implanted Si$^+$ in the GaN with sufficient accuracy, you can use the LSS calculation method.

The Vesuvius-1 ion implantation unit does not allow implantation of ions with an energy less than 50 keV, so to reduce the depth of the embedded impurity, dielectric films of silicon dioxide of different thickness were used as a mask during the doping process.

Figure 4. Experimental and calculated profiles of implanted silicon ions in gallium nitride.

$E = 50$ keV, $D = 10^{15}$ cm$^{-2}$. 

$1$ - Experiment (SIMS)
$2$ - Calculation (LSS)
The creation of highly alloyed layers was carried out using ion doping of silicon through a pre formed silicon dioxide mask with a thickness of 50 and 100 nm. To determine the thickness of the mask, the average projected run length was calculated in the AlGaN system, performed in the SRIM simulation program. The program allows you to take into account the angle of the incident beam and when modeling the profile, an angle of $7^\circ$ was laid [6].

![Figure 5](image_url)

**Figure 5.** Calculation of the maximum $\text{Si}^+$ distribution in AlGaN/GaN: a) through a 50 nm thick SiO$_2$ film; b) through a 100 nm thick SiO$_2$ film.

According to simulation data, the maximum impurity concentration during ion implantation through a 100 nm thick SiO$_2$ film remains in the silicon dioxide film. With a mask thickness of 50 nm, the maximum $\text{Si}^+$ in AlGaN/GaN is at a depth of 25 nm, and when implantation is performed without the use of a mask, the maximum $\text{Si}^+$ concentration is located at a depth of more than 40 nm (figure 5). Implantation of $\text{Si}^+$ ions in GaN was performed with the energy of the introduced ions-50 keV and a dose of $10^{15}$ cm$^{-2}$. To prevent the channeling effect, the plates were positioned at an angle of $7^\circ$ to the normal of the incident beam. After doping, the structures were subjected to high-temperature photon annealing in a nitrogen medium using a protective coating of SiO$_2$. Annealing was performed for 1 minute at a temperature of 1250 °C.

At the next stage of creating instrument structures, a system of ohmic contacts to doped areas was formed. The Ti/Al/Ni/Au system was used as the metallization of ohmic contacts. For comparison of characteristics, contacts were also created to a semiconductor without the process of ion implantation. The contacts were formed by electron-beam sputtering using explosive photolithography technology. After creating the contact pads, metallization was annealed at a temperature of 800 °C for 30 seconds.

The contact resistance was evaluated using the long line method on test structures with a distance between the contacts of 30, 25, 20, 15, 10 and 5 microns. The calculation of the contact resistance of ohmic contacts showed that the use of ion doping through a 50 nm thick silicon dioxide film reduces the contact resistance from 1.2 Ω mm to 0.8 Ω·mm.

The formation of a Schottky contact with a diameter of 150 microns was performed using electron-beam deposition of the Ni/Au system (0.07/0.3 microns). The contacts were formed using explosive photolithography. The height of the barrier and the coefficient of imperfection were 0.66 and 1.37 eV.

After manufacturing the diode structures (figure 6), the volt-ampere characteristics were analyzed. Direct volt-ampere characteristics of structures are shown in figure 7. When analyzing the characteristics, the values of the direct voltage drop by the direct current level of 100 A/cm$^2$ are determined.
Figure 6. Diode structure with an ion-doped layer.

Figure 7. Direct volt-ampere characteristics of diode structures.

Diode structures doped through a 50 nm mask have a lower direct voltage drop, due to the location of the maximum distribution of the implanted impurity at a depth corresponding to the occurrence of a two-dimensional electron gas.

3. Conclusion
The paper defines the conditions for the formation of ion – doped GaN layers with a high degree of activation of implanted silicon. Calculations of Si+ distribution in GaN during implantation with energies of 50, 100 and 150 keV were performed and the depth of its occurrence was determined. A comparative analysis of the calculated and experimental profiles of embedded silicon in gallium nitride with an energy of 50 keV and a dose of 10¹⁵ cm⁻² was performed. A simulation of the process of ion implantation of silicon at the interface of the AlGaN/GaN heterostructure through SiO₂ dielectric films of different thickness was performed. The paper considers the technology of forming ohmic contacts to diode structures based on the AlGaN/GaN heterojunction. The prospects of using silicon ion implantation for the formation of ohmic contacts are shown. Improved direct volt-ampere characteristics of diode structures formed using ion implantation are presented.

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