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# Influence of rapid thermal annealing on the distribution of nitrogen atoms in GaAsN/GaAs

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The article investigates the effect of rapid thermal annealing of ternary $GaAs_{1-x}N_x$/GaAs solid solutions on the distribution of nitrogen atoms in the crystal lattice. The samples are studied by photoluminescence spectroscopy and high-resolution X-ray diffractometry. Due to the size and electronegativity mismatch of nitrogen and arsenic atoms, nitrogen is incorporated unevenly into the GaAs crystal lattice. Options of the nitrogen atoms arrangement in the GaAs crystal lattice before and after rapid thermal annealing are shown.

**Keywords:** dilute nitrides, heterostructures, molecular-beam epitaxy, GaAs, nitrogen.

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## 1. Introduction

The GaAs is one of the most important and widespread materials in the microelectronics. Presently, there is big interest to enlarging the application field of GaAs. In particular, there is interest to addition of nitrogen to GaAs for producing a $GaAs_{1-x}N_x$ nitrogen-containing solid solution, which is a promising material to be applied in solar elements [1], laser devices [2] and spintronics [3].

Traditional ternary and quaternary $A^{III}B^{V}$ solid solutions can be grown in a wide range of the compositions and their electron properties smoothly change along with the composition. In contrast to them, dilute nitrides, for example, $GaAs_{1-x}N_x$, can be grown only in a narrow range of the compositions, wherein the addition of even small quantity of nitrogen to a matrix crystal results in a significant change of the electron properties of the solid solution produced [4]. That is why the interest is paid to the addition of nitrogen to GaAs, which allows significantly varying the $GaAs_{1-x}N_x$ band gap with a small change of the composition [4,5].

With the epitaxial growth of the $GaAs_{1-x}N_x$ solid solution, the nitrogen atoms replace the arsenic atoms in the crystal lattice. However, the significant difference in the sizes and electronegativity of the atoms of nitrogen and arsenic results in non-uniform incorporation of the nitrogen atoms into the crystal lattice. It result in localized states of nitrogen as well as violation of the translation symmetry of the crystal [4]. In this regard, the most promising concentration of nitrogen in the $GaAs_{1-x}N_x$ compound is $< 2\%$. At higher concentrations, there is sharp degradation of optoelectronic devices of these solid solutions [6].

However, even at the concentrations of nitrogen $< 2\%$ in $GaAs_{1-x}N_x$ there is evidently quite a big number crystal defects, negatively affecting the optical and electron properties of the layers [7].

It is known that the crystal and optical quality of the epitaxial layers is often improved by applying rapid thermal annealing [8].

The present article investigates the influence of the rapid thermal annealing of the GaAsN/GaAs layers on distribution of the nitrogen atoms in the crystal lattice.

## 2. Experiment

The $GaAs_{1-x}N_x$ bulk layers of the thickness of 200 nm have been grown on the GaAs (100) semi-insulating substrates by the molecular beam epitaxy. Atomic nitrogen was produced by using a high-quality plasma source of nitrogen. The nitrogen concentration was determined as per data of high-resolution X-ray diffractometry in the DRON 8 unit by the $\theta-2\theta$-scanning (Fig. 1).

Fig. 1 (left) has evident reflection from the GaAs (100) substrate, while the right part thereof includes reflections from the layer $GaAs_{0.9965}N_{0.0135}$ (red) and $GaAs_{0.9935}N_{0.0165}$ (blue). With increase in the nitrogen concentration in the $GaAs_{1-x}N_x$ layer, the lattice constant decreases and, respectively, the angular difference between the reflection from the GaAs substrate and the $GaAs_{1-x}N_x$ layer increases.

After the epitaxial growth the samples were subjected to the rapid thermal annealing at the temperatures 760,

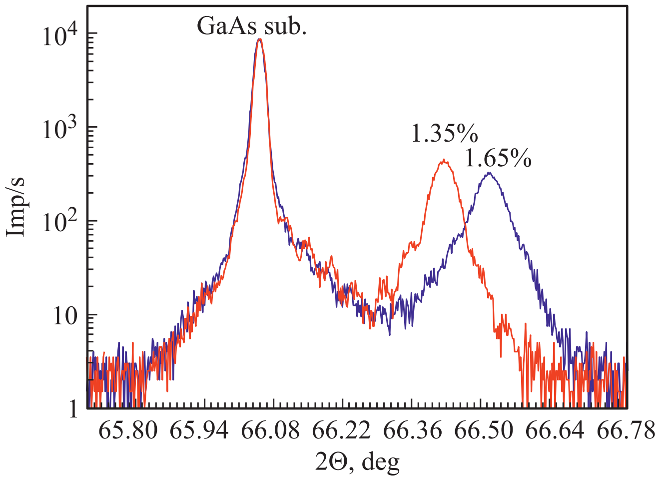


**Figure 1.** X-ray diffraction swinging curves around the symmetrical reflection GaAs (004) from the $GaAs_{0.9965}N_{0.0135}$ (red) and $GaAs_{0.9935}N_{0.0165}$ (blue) layers. (Colored version of the figure is presented in electronic version of the article).

780 and 800°C, the duration was 1 minute.The photoluminescence spectra (PL) of the produced samples were recorded at the room temperature (300 K). The PL is equipped with the Nd:YAG-laser with the wavelength of $\lambda = 532$ nm.

## 3. Results and discussion

There were the photoluminescence spectra at the room temperature of the samples before and after annealing (Fig. 2). There are evidently two peaks on the spectra before annealing — from the GaAs substrate (1.42 eV) and from the $GaAs_{1-x}N_x$ layer. With increase in the annealing temperature, the spectrum shape is changing and the photoluminescence intensity is increasing. The splitting of the photoluminescence spectrum into a series of transitions can be explained by nitrogen clusters of a various configuration in $GaAs_{1-x}N_x$, which occur during the epitaxial growth of $GaAs_{1-x}N_x$ due to a different size and electronegativity of the atoms of nitrogen and arsenic.

The [4] has theoretically determined a position of the nitrogen pairs and other complex clusters of nitrogen in the nitrogen-alloyed GaAs:N and GaP:N. Previously, we have experimentally demonstrated some of these localized states in $GaP_{1-x}N_x$ [9].

Thus, based on the available data, we can suggest various options of the arrangement of the atoms of nitrogen in the GaAs crystal lattice, whose energy positions are below a bottom of the GaAs conductivity band, which is schematically shown on Fig. 3. In a generic form, the possible nitrogen pairs are designated as $NN_i$, whereas at $i = 1$ the atoms of nitrogen are located in the nearest anion positions.

Thus, before annealing, in $GaAs_{1-x}N_x$, there are predominantly optical transitions through the localized states formed by the 3N triplets. As the samples are annealed, the 3N clusters are decomposed and the atoms of nitrogen are redistributed by making the pairs $NN_1$ and $NN_4$. It should be noted that the energy positions of the nitrogen clusters, which are observed on the photoluminescence spectra, coincide with the theoretical calculations [4].

Furthermore, the X-ray diffraction swinging curves have been obtained for the samples after annealing (Fig. 4). For the $GaAs_{1-x}N_x$/GaAs epitaxial structures with a various nitrogen concentration the form of the X-ray diffraction swinging curves was similar.

It is clear that with increase in the annealing temperature the position of the reflection from the $GaAs_{1-x}N_x$ does not change. It is correlated to the fact that the annealing has no nitrogen desorption due to short time of the annealing (1 minute) and quite a strong bond Ga–N [10].

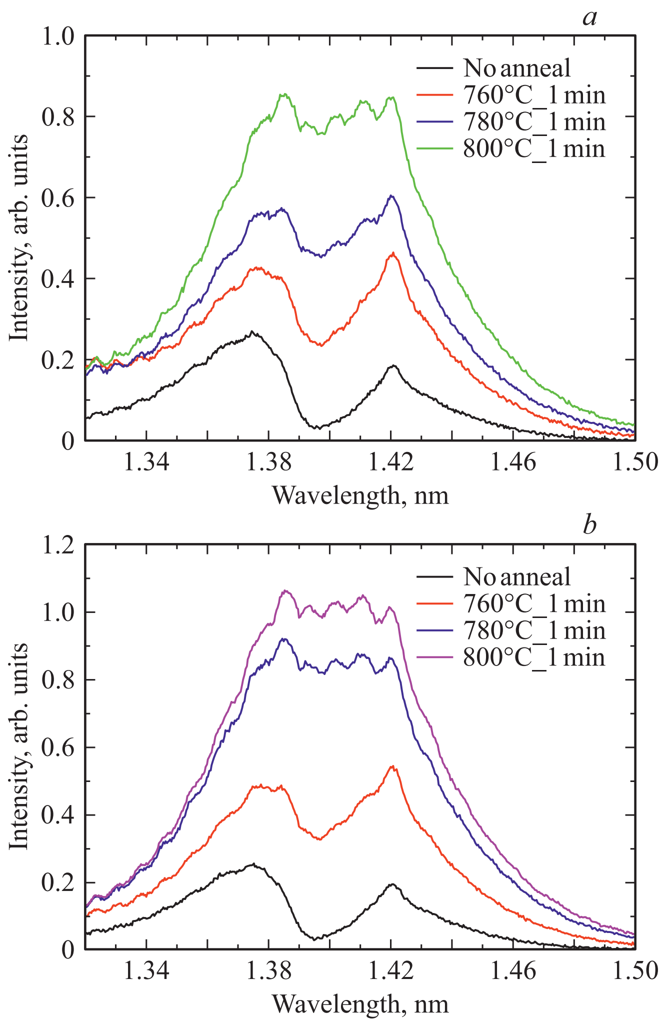


**Figure 2.** Photoluminescence spectra of the (*a*) $GaAs_{0.9965}N_{0.0135}$/GaAs and (*b*) $GaAs_{0.9935}N_{0.0165}$/GaAs heterostructures before annealing and after annealing at the temperatures 760, 780 and 800°C, which are obtained at the room temperature.

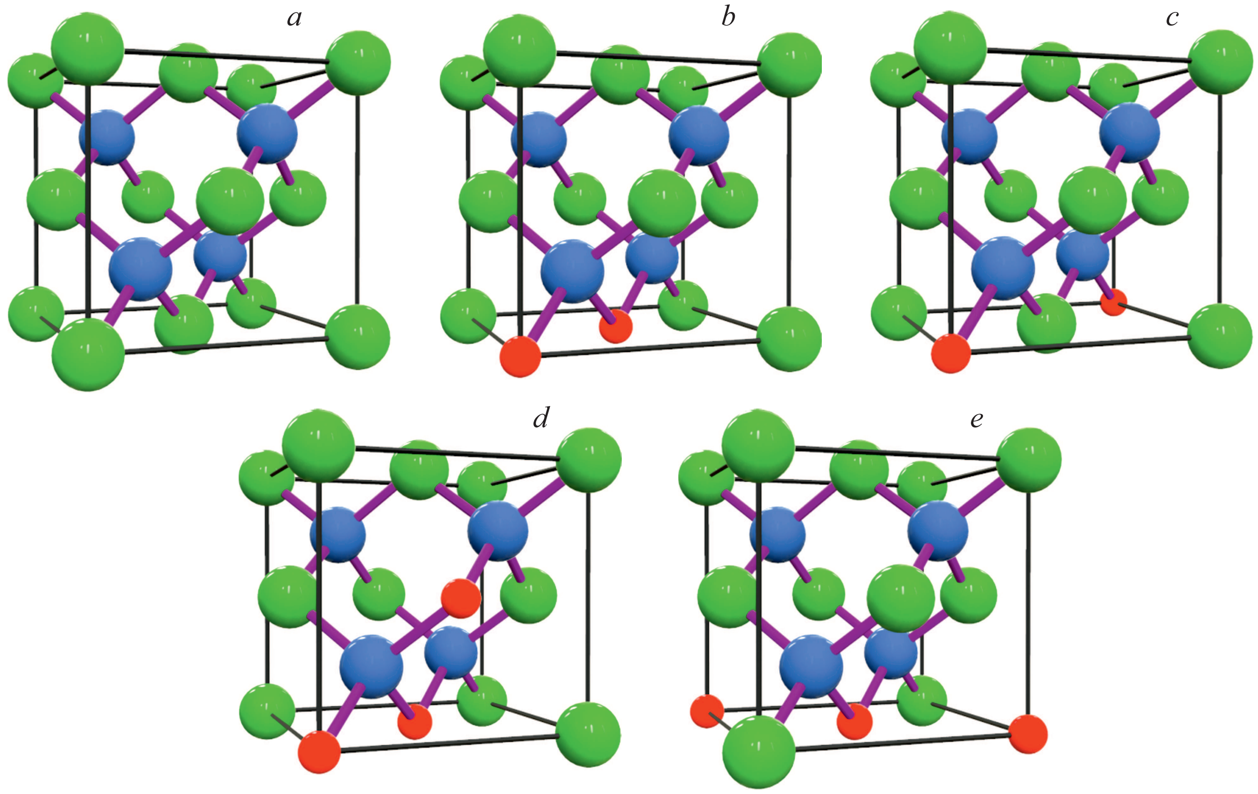


**Figure 3.** Arrangement of the atoms of nitrogen in the GaAs lattice. The green color is used to mark As atoms, so the blue color — Ga, the red color — N. *a* — GaAs without N, *b* — $NN_1$ pair, *c* — $NN_4$ pair, *d* — 3N triplet, *e* — the chain of atoms of nitrogen. (Colored version of the figure is presented in electronic version of the article).

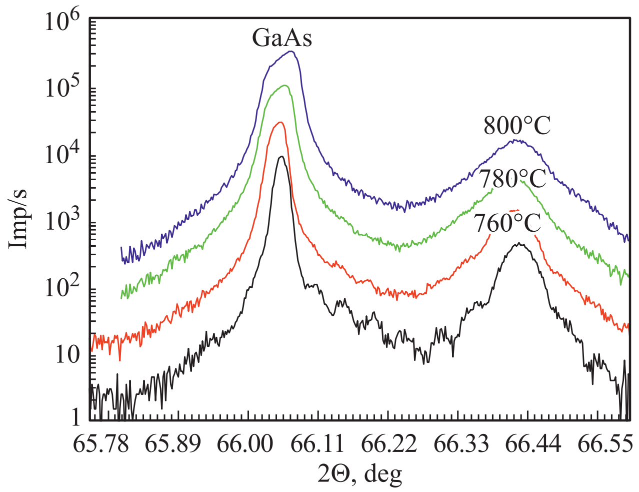


**Figure 4.** X-ray diffraction swinging curves around the symmetrical reflection GaAs (004). The curves were presented for the $GaAs_{0.9965}N_{0.0135}$/GaAs sample before annealing and after annealing at the temperatures 760, 780 and 800°C.

## 4. Conclusion

It has investigated the influence of the rapid thermal annealing of the GaAsN/GaAs ternary solid solutions on the distribution of the atoms of nitrogen in the crystal lattice.

Because of mismatch of the sizes and electronegativity of the atoms of nitrogen and arsenic, the nitrogen incorporates non-uniformly into the GaAs crystal lattice. It has demonstrated the options of arrangement of the atoms of nitrogen in the GaAs crystal lattice.

It is shown that after the rapid thermal annealing the 3N triplets are decomposed to form the pairs $NN_1$ and $NN_4$. It should be also noted that the rapid thermal annealing within the temperature range 780–800°C for the duration of 1 minute does not result in the nitrogen desorption.

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## Conflict of interest

The authors declare that they have no conflict of interest.

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