Investigation of defects in semiconductor structures based on AlInGaN solid solutions

A S Larchenko, I I Mikhailov, I A Lamkin, A E Degterev and S A Tarasov

Saint Petersburg Electrotechnical University (ETU), 5 Prof. Popov str., Saint Petersburg 197376, Russia

E-mail: larchenko_a@inbox.ru

Abstract. Structures based on AlInGaN solid solutions were studied. The types of defects in them and the corresponding emission bands of photoluminescence (PL) spectra were identified. It is possible to determine the concentration of defects in the structure from the ratio of the intensities of the emission line, corresponding to the width of the forbidden zone in GaN, and the emission lines associated with defects.

1. Introduction

Quantum-sized structures are an integral part of modern electronics. Their use is justified by specific properties that have found application both in the creation of fundamentally new devices (resonant tunneling diode) and in improving the characteristics of existing ones (light emitting diode (LED), transistor) [1].

One of the most promising materials for modern nanoelectronics is gallium nitride. A3-B5 semiconductor nitrides are attractive for use in optoelectronics. It is connected with the opportunity to vary the content of InN or AlN in solid solutions of In$_x$Ga$_{1-x}$N and Al$_x$Ga$_{1-x}$N, that allows controlling the most important material characteristic - the width of the forbidden zone in the range from 0.7 eV (IR spectral region) to 6.4 eV (UV spectral region). There are other positive features such as high carrier mobility, high heat capacity and low sensitivity to ionizing radiation [2]. In addition, these transistors based on nitride structures promise to be useful in microwave devices [3]. It is explained by the advantages of wide-gap structures based on GaN over structures based on narrow-gap semiconductor materials. The most important positive factor due to which GaN-based transistors can be identified is the high power density. This leads to a significant simplification of the topology of integrated circuits of power amplifiers and an increase in efficiency. Also, it becomes possible to reduce the weight and improve the overall device parameters. The development of such technologies based on GaN will led to significant practical results and to the development of high-power microwave transistors and monolithic integrated circuits in industrial production [4].

An important issue is obtaining defect-free, high-quality structures. GaN-based substrates have limited application, because of their small size and high cost. Therefore, when sapphire and silicon carbide are used as substrates during the growth of nitrides, this can lead to increasing defect formation due to the difference in grating periods [5]. This highlights the need to examine the quality of structures in order to develop recommendations for improving the technology of their creation [6]. Another way is the application of measuring systems that can be used to obtain clean surfaces and detect luminescence directly during the growth of structures [7].
2. Experiments

2.1. The device design and fabrication

In this research, structures based on solid solutions of In$_x$Ga$_{1-x}$N and Al$_x$Ga$_{1-x}$N were investigated. Structures based on In$_x$Ga$_{1-x}$N (figure 1) were grown by the MOCVD method on a sapphire substrate and were intended to create LEDs based on them in the blue range of the spectrum.

| GaN          |
|--------------|
| In$_x$Ga$_{1-x}$N/GaN MQW |
| GaN          |
| GaN buffer   |
| Sapphire     |

**Figure 1.** The structure of the In$_x$Ga$_{1-x}$N sample.

A buffer layer of GaN was grown on the substrate after a very thin seed layer. It was necessary to reduce the concentration of defects in the active region of the structure. Defects arise due to the inconsistency between the lattice periods of Al$_2$O$_3$ (sapphire) and semiconductor GaN. Further, a high-alloyed GaN layer was grown on the structure that performs the function of the lower emitter of a double heterostructure (DHS). The thickness of this layer reached 2 $\mu$m, which was necessary to ensure the formation of a lower Ohmic contact. The active region consisted of multiple In$_x$Ga$_{1-x}$N quantum wells separated by GaN barriers. The second factor that influenced the quality of the structure was the change in the number of quantum wells from 5 to 10. Next, the GaN layer of the upper emitter was grown. Thus, in the work, the structures of five types, differing by the parameters of the buffer layer and the active region, were investigated.

**Figure 2.** The structure of the Al$_x$Ga$_{1-x}$N sample.

Heterostructures based on solid solutions of Al$_x$Ga$_{1-x}$N (figure 2) with different AlN concentrations were grown on a sapphire substrate taken in the (0001) direction. The AlN layer formed on the
substrate allows smoothing the stress gradient during the transition to the growth of the Al\textsubscript{x}Ga\textsubscript{1-x}N buffer layer, which leads to a decrease in the dislocation density and deformations in the epitaxial layers. The superlattice was grown on top of the buffer layer. It consists of 6 layers of Al\textsubscript{x}Ga\textsubscript{1-x}N of different composition and thickness.

**Table 1.** The data specification of the structures based on solid solutions of Al\textsubscript{x}Ga\textsubscript{1-x}N.

| Sample            | Type | Thickness of upper layer, um | Dopant | Dopant concentration, cm\textsuperscript{-3} | Substrate  |
|-------------------|------|-----------------------------|--------|-----------------------------------------------|------------|
| Al\textsubscript{0.06}Ga\textsubscript{0.94}N | n    | 0.15                        | Si     | 1e+19                                         | c-Al\textsubscript{2}O\textsubscript{3} |
| Al\textsubscript{0.08}Ga\textsubscript{0.92}N | p    | 0.8                         | Mg     | 7e+18                                         | c-Al\textsubscript{2}O\textsubscript{3} |
| Al\textsubscript{0.1}Ga\textsubscript{0.9}N   | n    | 0.15                        | Si     | 1e+17                                         | c-Al\textsubscript{2}O\textsubscript{3} |
| Al\textsubscript{0.25}Ga\textsubscript{0.75}N | n    | 1.8                         | -      | -                                             | c-Al\textsubscript{2}O\textsubscript{3} |

After that, the upper layer was grown. The thickness of it was also different. The data stated in the specification are presented in table 1.

2.2. Measurements and results

Due to the research of the emission bands of the PL spectra, the presence of certain defects in the structure could be discussed. The PL spectra for the In\textsubscript{x}Ga\textsubscript{1-x}N and Al\textsubscript{x}Ga\textsubscript{1-x}N structures at temperature of 300 K and 77 K are shown in figures 3-6.

The emission bandwidth of the GaN band gap with an energy of 3.41 eV is observed for In\textsubscript{x}Ga\textsubscript{1-x}N samples 1, 2, 4 types at temperatures of 300 K and 77 K, as well as for Al\textsubscript{0.06}Ga\textsubscript{0.94}N with n-doping and Al\textsubscript{0.1}Ga\textsubscript{0.9}N with n-doping only at a temperature of 300 K. With a decrease in temperature, a shift in the region of high energies is observed due to the expansion of the band gap.

![Figure 3](image-url) **Figure 3.** The photoluminescence spectra of In\textsubscript{x}Ga\textsubscript{1-x}N samples at a temperature of 300 K.

A peak in the region of 3.28 – 3.31 eV is typical for the PL spectra of nitride structures. It corresponds to the conduction-to-acceptor (e-A) transition. The acceptors can be either dopant atoms (for example, magnesium) or oxygen atoms embedded in the lattice instead of nitrogen. The e-A transitions are observed especially clearly at low temperature.
This band appears in the type 1 \( \text{In}_x\text{Ga}_{1-x}\text{N} \) sample, in which oxygen atoms act as acceptors in nitrogen vacancies. It is most pronounced in the p-type sample of \( \text{Al}_{0.08}\text{Ga}_{0.92}\text{N} \), which is doped with magnesium. Magnesium is an acceptor in this case. Therefore, the e-A transitions in the structure are predominant. With a decrease in temperature, a shift to the region of high energies is also observed due to the expansion of the forbidden zone.

**Figure 4.** The photoluminescence spectra of \( \text{In}_x\text{Ga}_{1-x}\text{N} \) samples at a temperature of 77 K.

At low temperatures, some samples show 1-LO (3.2 eV) and 2-LO (3.02 eV) emission peaks, which are first and second-order phonon replicas for the e-A band. They are characteristic of the type 1 sample of \( \text{In}_x\text{Ga}_{1-x}\text{N} \). The 1-LO phonon replica was manifested in the n-type \( \text{Al}_{0.06}\text{Ga}_{0.94}\text{N} \) and n-type \( \text{Al}_{0.1}\text{Ga}_{0.9}\text{N} \) samples [9].

**Figure 5.** The photoluminescence spectra of \( \text{Al}_x\text{Ga}_{1-x}\text{N} \) samples at a temperature of 300 K.

The blue luminescence emission band of the BL appears at an energy of 2.9 – 3.05 eV. It occurs during the hydrogenation of gallium vacancies \( \text{V}_{\text{Ga}}\text{H}_n \) (small acceptors), as a result of which the \( \text{V}_{\text{Ga}}\text{H}_n \)
– O\textsubscript{N} complexes appear. The blue band is observed at room temperature but becomes invisible at 77 K. Observed in n-type Al\textsubscript{0.06}Ga\textsubscript{0.94}N and n-type Al\textsubscript{0.1}Ga\textsubscript{0.9}N samples, it has the maximum intensity (\(I/I_{\text{max}} = 1\)), which is an indicator of a large number of dislocations and gallium vacancies localized on them.

Also the defect YL “yellow luminescence” band in the region of 2.2 eV is typical for the PL spectra of nitride structures. The reason for its occurrence is the V\textsubscript{Ga} – O\textsubscript{N} complex formed by a Ga vacancy (deep acceptor) and oxygen atoms in nitrogen vacancies (shallow donor) [10]. This band is the most intense in the In\textsubscript{x}Ga\textsubscript{1-x}N samples of 3 and 5 types, and it is also quite wide (0.4 eV), which together indicates a high concentration of defects. Among Al\textsubscript{x}Ga\textsubscript{1-x}N-based structures, the narrowest peak around 2.2 eV was observed in the n-type Al\textsubscript{0.06}Ga\textsubscript{0.94}N (0.13 eV), whereas the widest one was observed in the n-type Al\textsubscript{0.25}Ga\textsubscript{0.75}N (0.5 eV), which also indicates a high concentration of defects in the sample.

![Figure 6. The photoluminescence spectra of Al\textsubscript{x}Ga\textsubscript{1-x}N samples at a temperature of 77 K.](image)

For the sample of p-type Al\textsubscript{0.08}Ga\textsubscript{0.92}N doped with magnesium, the intensity of the YL band was the lowest in comparison with the other samples. This is due to the fact that Mg, being an element of group II, acts as an acceptor and fills vacancies of Ga, an element of group III.

3. Conclusions

Thus, several types of structures based on solid solutions of In\textsubscript{x}Ga\textsubscript{1-x}N and Al\textsubscript{x}Ga\textsubscript{1-x}N were studied by photoluminescence spectroscopy. The causes of the appearance of the PL bands in the structures and the types of defects were identified.

The emission bandwidth of the forbidden zone of GaN is observed at an energy of 3.41 eV.

The radiation band in the region of 3.28 – 3.31 eV corresponds to the transition from the conduction band to the acceptor (e-A). Also, some samples show phonon replicas of this emission line.

The BL emission band appears at an energy of 2.9 – 3.05 eV. It arises during the hydrogenation of gallium vacancies V\textsubscript{Ga}H\textsubscript{n} (small acceptors), then V\textsubscript{Ga}H\textsubscript{n} – O\textsubscript{N} complexes appear.

The YL emission band appears in the region of 2.2 eV. The cause of its occurrence is the V\textsubscript{Ga} – O\textsubscript{N} complex formed by a Ga vacancy (deep acceptor) and oxygen atoms in nitrogen vacancies (shallow donor).

The degree of how high the concentration of defects in a structure is can be determined from the ratio of the intensities of the emission line to the width of the forbidden zone GaN, and the emission lines associated with defects.
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