Design and investigation of GaPAsN/Si light-emitting diode

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Abstract. The heterostructure of light-emitting diode on a silicon substrate with an active region based on A3B5N was synthesized and investigated. Light-emitting diode demonstrates effective electroluminescence at 645 nm up to the 360 K. This indicates the high crystalline and optical quality of the light-emitting structure, as well as the prospects of this approach for the development of silicon integrated photonics.

1. Introduction
Epitaxy of A3B5 materials on a silicon wafer is one of the most promising approaches to creating efficient light-emitting devices for integrated silicon photonics.

GaP is a A3B5 binary semiconductor that has the smallest lattice mismatch with Si (0.37% for GaP/Si). However, with a non-zero mismatch of the crystal lattices, the layer begins to plastically relax when the thickness exceeds the critical thickness. For GaP/Si, this value was estimated in the range from 40 nm to 100 nm [1-3]. The thickness of the laser structure is usually from 1 to 3 microns. Thus, compounds with an even smaller mismatch of the crystal lattices with Si are necessary.

The ideal lattice matching can be achieved by adding a small amount of nitrogen (2.2% in GaP at room temperature); moreover, the addition of nitrogen of only 0.5% leads to the formation of a direct structure of the electron zones of GaP$_{1-x}$N$_x$ solid solutions. Besides the problems associated with the lattice mismatch of the GaP and Si, there are problems caused by different thermal expansion coefficients of A3B5 materials and Si, as well as different numbers of valence electrons. To solve these problems, during the growth of the heterostructure of the light-emitting diode based on A3B5N on Si substrate, the technological approaches described earlier were used [4,5].

2. Experiment
The heterostructure of light-emitting diode (LED) on a silicon substrate with an active region based on A3B5N was synthesized and investigated. The heterostructure was grown by molecular beam epitaxy (MBE) system with solid-state sources of III and V groups of materials and a source of nitrogen with plasma activation. To overcome the problem of formation of anti-phase regions during the epitaxy of III-V compounds on silicon [4], the vicinal silicon substrates, misoriented by 4$^\circ$ relative to the (001) surface in the [110] direction was used.

Before the epitaxial growth, silicon substrates underwent a chemical treatment cycle [6], and then they were heated in a pre-growth chamber to a temperature of 350$^\circ$C, and next to a temperature of 850$^\circ$C in an epitaxial reactor of the MBE.

For the formation of a high-quality GaP initial layer on a Si substrate, the technique of “epitaxy with enhanced migration” (MEE) was used [7]. The MEE technique represents the successive interaction of the substrate with the stream of gallium atoms and phosphorus molecules. The
temporary absence of phosphorus molecules on the epitaxial surface allows gallium atoms adsorbed on the surface to migrate over the surface for a longer time without forming a chemical bond. In practice, the use of MEE technique leads to the suppression of three-dimensional island growth and the formation of a crystal with a smooth surface [8].

Thereafter, on the obtained MEE GaP initial layer, the LED heterostructure was grown by the standard MBE mode, its design and band diagram are presented on figure 1.

Figure 1. a Design and b band diagram of LED GaPAsN/Si heterostructure (black line - conduction band, red line – valence band, blue dotted line – Fermi level)

LED GaPAsN/Si heterostructure consist of active region and contact layers. Bottom contact layer contains GaP and GaPN layers doped by Be.

A quantum-well (QW) heterostructure consisting of 15 periods of GaP$_{0.982}$N$_{0.018}$/GaP$_{0.832}$As$_{0.150}$N$_{0.018}$ layers is used as the active region. The GaP$_{0.982}$N$_{0.018}$ layers play the role of barriers, and the GaP$_{0.832}$As$_{0.150}$N$_{0.018}$ layers - quantum wells. The upper contact layer is doped with silicon to obtain n-type conductivity. Bulk doping of GaP with silicon does not allow obtaining a high concentration of carriers in the GaP:Si layer. Therefore, to obtain a highly doped GaP:Si layer, a periodic structure (20 periods) was used, consisting of a Si (δSi) monolayer and GaP:Si 10 nm thick [9].

In our early paper it was shown that the the dislocation yield density on the surface of the heterostructure consisting of the initial MEE GaP layer and the GaP buffer layer 200 nm thick grown on a Si (100) substrate with a misorientation by 4° relative to the (001) surface in the [110] direction is ~ 2·10$^8$ cm$^{-2}$ [10]. Good morphology of the surface of the grown GaP layer is achieved due to the fact that the sprouting dislocations arising at the Si/GaP heterojunction are bent during the growth of GaP buffer layer and do not reach the surface. However, a large number of dislocations at the GaP / Si heterointerface does not allow making contact through the substrate. Another obstacle for creating a contact through the substrate is the diffusion of Ga and P atoms into the silicon substrate during the epitaxial growth [8]. As a result of this diffusion, an undesirable p – n junction occurs, which can lead to losses during electrical pumping of the LED structure. This problem can be solved by using intra-cavity contacts, which are created by etching and passivating heterostructure layers, electrodes are brought through the active layers to the doped p- and n-type layers [9].
3. Results and discussion

The current-voltage characteristic of investigated GaPAsN/Si-based LED heterostructure is shown in figure 2. The cut-off voltage at room temperature is ~3.2 V.

![Figure 2. Current-voltage characteristic of investigated GaPAsN/Si-based LED heterostructure](image)

Figure 3 shows the electroluminescence (EL) spectra in a wide temperature range, obtained at forward bias U = 5.4 V (at temperatures of 80–260 K (a) and 300–360 K (b)).

![Figure 3. EL spectra observed at temperature 80-260 K (a) and 300-360 K (b) at U = 5.4 V](image)

A visible intensive EL in the region of 645 nm up to a temperature of 360 K is observed. As the temperature increases, the intensity of EL decreases and the wavelength of the EL maximum shifts to the long wavelength region.

As the temperature increases from 80 K to 160 K, a smooth shift of the position of the EL peak to the long wavelength region is observed. With further increase of the temperature of the LED heterostructure, the position of the maximum does not change and remains at the value of 645 nm. This behavior is associated with internal local heating of the heterostructure, which exceeds the external temperature.
The article describes the stages of creating LED on silicon, and also describes the design of the device. Current-voltage characteristic at room temperature, as well as electroluminescence spectra in a wide temperature range (80-360 K) for grown LED heterustructure were obtained. Our LED demonstrates effective electroluminescence at 645 nm up to the 360 K. This indicates the high crystalline and optical quality of the light-emitting structure, as well as the prospects of this approach for the development of silicon integrated photonics.

Acknowledgments
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