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# Structural features and surface morphology of $Al_xGa_yIn_{1-x-y}As_zP_{1-z}/GaAs(100)$ heterostructures

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#### ABSTRACT

Epitaxial metal-organic chemical vapor deposition (MOCVD) heterostructures on the basis of the five-component  $Al_xGa_yIn_{1-x-y}As_zP_{1-z}$  alloys (solid solutions) were grown in the range of compositions isoperiodic to GaAs. Using X-ray diffraction technique and atomic force microscopy it was shown that on the surface of heterostructures nanosize objects were present with islets-like shape which can be aligned on the surface of solid solution in the linear direction. On the basis of calculations of the crystal lattice parameters taking into account internal stresses it is possible to assume that the new compound is a phase on the basis of  $Al_xGa_yIn_{1-x-y}As_zP_{1-z}$  alloy.

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#### 1. Introduction

Development of epitaxial methods of growth, in particular MOCVD method, makes it possible (allows) to create unique semiconductor heterostructure on the basis of  $A_3B_5$  alloys (solid solutions). Combinations of binary semiconductor anionic compounds, such as GaAs, AlAs, InAs, GaP, InP, AlP allow to gain heterojunctions with easily controlled electrophysical properties due to the changes in alloys composition (which electrophysical properties are manageable at the expense of changes in composition) [1].

At present it is known that laser diodes excluding necessity of control of their operating temperature up to  $150\,^{\circ}$ C can be gained on the basis of  $Al_xGa_yIn_{1-x-y}As_zP_{1-z}$  [2]. All these factors make optoelectronic systems on the basis of  $Al_xGa_yIn_{1-x-y}As_zP_{1-z}$  extremely in demand [3–5].

It is clear that the semiconductor epitaxial heterostructures involving quantum-size inhomogeneities represent rather difficult objects for investigations. Their structure and properties are in a strong dependence on the technology of growth. Therefore, determination of lattice parameters, frequencies of optical and interface phonons in systems with inhomogeneities, including quantum-size ones are of high practical value and seem to be perspective from the viewpoint of fabricating optoelectronics devices. This is also important for the study of the structure of nanosize objects in a dependence on formation conditions and control of their properties. Therefore, examination of structure and surface morphology,

as well optical properties in the IR-range of MOCVD heterostructures on the basis of  $Al_xGa_yIn_{1-x-y}As_zP_{1-z}$  alloys isoperiodic to GaAs was the purpose of this research.

#### 2. Objects and research methods

Five-component  $Al_xGa_yIn_{1-x-y}As_zP_{1-z}$  alloys were grown using EMCORE GS 3/100 unit by MOCVD epitaxial method in the vertical reactor with high rotation velocity of GaAs(100) substrate holder. The epitaxy temperature was 750 °C, the reactor pressure was 77 Torr and the substrate holder's rotation velocity was 1000 rpm. The epitaxial layer thickness of the alloy was  $\sim$ 1  $\mu$ m. The compositions set by technologists for  $Al_xGa_yIn_{1-x-y}As_zP_{1-z}$  solid solutions are presented in Table 1.

In this work we only show the possibility of five-component solid solutions in the  $Al_xGa_yIn_{1-x-y}As_zP_{1-z}$  with the appearance of inhomogeneities on the surface of the film and we did not obtain the asymmetric reflection and reciprocal space maps for analysis of strain. Therefore structural quality and lattice parameters of the samples were determined by X-ray diffraction (XRD) using DRON-4-07 diffractometer with high angular resolution using  $Co_{K\alpha1,2}$  radiation.

The surface morphology was studied using atomic-force microscope (AFM) NTEGRA Therma (NT MDT).

#### 3. Results of investigations and their discussion

#### 3.1. XRD investigations

Using X-ray microanalysis with the use of JEOL electronic microscope attachment we have refined the values of concentration set by technologists at the stage of growth for five-component

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Sample	Composition of solid solution	
EM2160	$Al_{0.38}Ga_{0.57}In_{0.05}As_{0.90}P_{0.10}$	
EM2170	$Al_{0.392}Ga_{0.588}In_{0.02}As_{0.90}P_{0.10}$	
EM2175	$Al_{0.388}Ga_{0.582}In_{0.03}As_{0.90}P_{0.10}$	
EM2176	$Al_{0.243}Ga_{0.727}In_{0.03}As_{0.90}P_{0.10}$	

 $Al_xGa_yIn_{1-x-y}As_zP_{1-z}$  alloys. Atomic concentrations in solid solutions were determined from homogeneous areas of the surface with an accuracy of  $\sim$ 0.1 at.%. The refined data of X-ray microanalysis are presented in Table 2.

Investigations of the structural quality of heterostructure samples was performed using patterns of (600) diffraction lines in the range of angles  $141-143^{\circ}$ . The accuracy of interplanar spacing and lattice parameters was  $\sim 0.0001$  Å.

Fig. 1a–d the solid line shows the experimental X-ray diffraction profiles from epitaxial  $Al_xGa_yIn_{1-x-y}As_zP_{1-z}/GaAs(100)$  heterostructure.

Separation of the doublets and modeling of diffraction profiles was carried out by the adjusted method [6] using the software package SigmaPlot 10, which allowed to minimize the error using various analytical functions. The results of decomposition are shown in Fig. 1a–d. According to the results of decomposition Bragg diffraction angles and interplanar distances for the components of heterostructures were determined (see Table 2).

During the growth of thin heteroepitaxial layers on a solid substrate the mismatch of lattice constants in some cases does not lead to the generation of mismatch dislocations, but there is a homogeneous elastic deformation of the epitaxial layer in a plane parallel to the heterointerface [7].

The lattice constant of the alloys taking into account  $a_{\nu}$  elastic stresses in the heteroepitaxial layer, in accordance with the linear theory of elasticity can be calculated as [7]:

$$a^{\nu} = a^{\perp} \frac{1 - \nu}{1 + \nu} + a^{\parallel} \frac{2\nu}{1 + \nu}.$$
 (1)

where  $\nu$  – Poisson's ratios for the epitaxial layers, and  $a^{\perp}$ ,  $a^{\parallel}$  – perpendicular and parallel components of the lattice parameter.

To calculate the Vegard's law for the system of  $Al_xGa_yIn_{1-x-y}As_zP_{1-z}$  alloys Vegard's law for ternary compounds was originally taken, and next for the binary compounds can be applied. Just the same approach is used to determine the dependence of  $Ga_xIn_{1-x}As_yP_{1-y}$  lattice parameter on the concentration of atoms [8]. Thus, for a five-component  $Al_xGa_yIn_{1-x-y}As_zP_{1-z}$  alloy we obtain:

$$a_{Al_{x}Ga_{y}ln_{1-x-y}As_{z}P_{1-z}} = 5.8687 - 0.4387 \cdot x - 0.4182 \cdot y$$
  
+ 0.1896 \cdot z + +0.0414 \cdot x \cdot z + 0.01315 \cdot y \cdot z. (2)

Using relations (1) and (2), as well as the results of decomposition for (600) diffraction profiles (see Table 2). It is possible to determine the lattice constants of five-component  $Al_xGa_yIn_{1-x-y}As_zP_{1-z}$  alloys, taking into account the internal stresses.

Making a more detailed study of diffraction from five-component  $Al_xGa_yln_{1-x-y}As_zP_{1-z}$  alloys we have found that for three heterostructures near the main high-intensity (600) diffraction peak (see Fig. 1a–d) additional  $K\alpha_{1,2}$  doublet shown in the insets in Fig. 1a–d, can be observed.

The intensity of the additional diffraction peaks is by 3 orders lower than the diffraction from  $Al_xGa_yIn_{1-x-y}As_zP_{1-z}$  alloy. Moreover, additional diffraction peaks are shifted toward smaller Bragg angles, indicating a greater lattice constant relative to the main diffraction pattern.

It should be noted that for EM2160 ( $Al_{0.38}Ga_{0.57}In_{0.05}As_{0.90}P_{0.10}$ ) heterostructure with a solid solution having a larger lattice parameter than GaAs substrate, the shift of additional  $K\alpha_{1,2}$ -doublet towards to lower angles is not as strong as for the EM2170 (Al<sub>0.392</sub>Ga<sub>0.588</sub>In<sub>0.02</sub>As<sub>0.90</sub>P<sub>0.10</sub>) and EM2175  $(Al_{0.388}Ga_{0.582}In_{0.03}As_{0.90}P_{0.10})$  heterostructures with a solid solution having a smaller lattice parameter than that of GaAs substrate. In accordance with (1) and (2) such a difference in the angular displacement of the diffraction can be explained by a difference in the internal stresses of crystal lattice of the solid solution  $Al_xGa_yIn_{1-x-y}As_zP_{1-z}$  and a new phase, from which there is an additional  $K\alpha_{1,2}$ -doublet. Therefore, the larger lattice mismatch in solid solution, which is the basis for the growth of new phase and the latest phase, the stronger the shift of  $K\alpha_{1,2}$ -doublet toward lower angles. So for EM2176 ( $Al_{0.243}Ga_{0.727}In_{0.03}As_{0.90}P_{0.10}$ ) heterostructure low-intensity additional diffraction from the solid solution may coincide with the diffraction from the substrate.

Crystal lattice parameters of additional phases in the direction of epitaxial growth are presented in Table 2.

In analyzing the atom content of the alloy constituents in the heterostructures, in which the appearance of a new phase is observed, we can state that the basis of the alloys in these heterostructures is constituted by aluminum, gallium, and arsenic (more than 90 at.% in each of the sublattices). The remaining 10-15 at.% corresponds to summarily indium and phosphorus atoms. Thus, we can suppose that the separated-out new phase present a material based on the  $Al_xGa_{1-x}As$  alloy.

#### 3.2. Atomic force microscopy

Assuming that the appearance of additional phase with a lattice parameter greater than that inherent for  $Al_xGa_yIn_{1-x-y}As_zP_{1-z}$  alloy will be presented as a feature in the surface morphology, we carried out studies of heterostructures by atomic force microscopy.

**Table 2**X-ray microanalysis and XRD data for Al<sub>y</sub>Ga<sub>y</sub>In<sub>1-x-y</sub>As<sub>z</sub>P<sub>1-z-y</sub>

Sample	X-ray microanalysis (at.%)	Lattice parameter in compliance with (2) (Å)	Experimental lattice parameter (Å)	Lattice parameter $a^\perp$ o additional phase (Å)
EM2160	x = 0.354	5.6626	5.6617	5.6919
	y = 0.592			
	z = 0.928			
EM2170	x = 0.368	5.6408	5.6408	5.7069
	y = 0.612			
	z = 0.890			
EM2175	x = 0.360	5.6525	5.6443	5.7149
	y = 0.598			
	z = 0.903			
EM2176	x = 0.234	5.6501	5.6463	=
	y = 0.734			
	z=0.914			

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