UNRELAXED InAs_{1-x}Sb_x ALLOYS GROWN ON COMPOSITIONALLY GRADED BUFFERS WITH MOLECULAR-BEAM EPITAXY

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I. INTRODUCTION

InAs_{1-x}Sb_x solid solutions possess unique property, as a wide range of a variation of the band gap width with the concentrationx. As it is known, width of the band gap of InAs semiconductor is E_{g0} =407.4 meV, and for InSbE_{g0}=227.3 meV at temperature 77K [1]. In InAs1-xSbx solid solutions the width of the band gap smoothly varies, decreasing with the increase of Sb atoms concentration. The most interesting is that, at concentration of Sb atoms close to 60 % (x = 0,6) the width of the band gap reaches the minimum value and can be less, than even in InSb, reaching the value 100 meV [2, 3] (Figure 1). This not ordinary property is actively used now for working out and creation of optoelectronic devices (sources and detectors of radiation, etc.) in technologically important range of a spectrum from 8 microns to 12 microns corresponding to a transparency of atmosphere.



Fig. 1. Dependence of the width of the band gap of InAs1-xSbx solid solution on composition x.

The basic deterrent for obtaining and wide application of thin-film photoelectronic devices (in particular, on the base of $InAs_{1-x}Sb_x$ solid solutions) is the absence of substrates with close values of the lattice parameters. Distinction in a lattice parameters of a working layer and a substrate bring to occurrence of pressure and the deformations of the film leading to creation of the large density of defects and dispositions, influencing, in turn, on the main physical parameters and stability of work of photoelectronic devices. Lattice parameters of GaSb and InSb are equal to 6,096 and 6,479 Å, accordingly [1], i.e. discrepancy more than 6 %. We gradually eliminated this discrepancy for epitaxial pseudomorphic $InAs_{1-x}Sb_x$ solid solutions by application of intermediate step buffer layers (Al, Ga, In) (As, Sb). Thus, we obtained unrelaxed and unstrained $InAs_{1-x}Sb_x$ top epi-layers.

Main purpose of this study is to produce and to thoroughly investigate metamorphous $InAs_{1-x}Sb_x$ alloy thin films free from internal strains and dislocations, with a fundamental band gap of 100–350 meV.

II. EXPERIMENTAL AND RESULTS

We here used oriented high-quality GaSb substrates manufactured by WaferTech LLC. Molecularbeam epitaxy (MBE) of the films was conducted with a Gen-930 Veeco solid-source molecular beam epitaxy systems. The composition of the graded AlGaInSb buffer zone was chosen with regard to the principles described in [4]. During growth of the buffer zone, the substrate temperature was varied in the range of 460– 520 C. During epitaxial growth of the InAs_{1-x}Sb_x composition, the substrate temperature was ~415 °C. The growth rate was ~1 m h⁻¹. The Characteristics (the composition and thickness of layers) of obtained multilayered epitaxial InAs1-xSbx heterostructures with x = 0,43 (sample R811) and x = 0,38 (sample R1051), are shown in Figure 2.



Figure 2 – Compositions and thicknesses of layers of heteroepitaxial structures with $InAs_{0.57}Sb_{0.43}$ (sample R811) and $InAs_{0.62}Sb_{0.38}$ (sample R1051) alloys

From the transmission electron microscopy (TEM) data, it follows that misfit dislocations are formed mainly in the lower region of the buffer layer, at the interface with the GaSb substrate, and localized in a region of $1.5-2 \mu m$ [5].

Figure 3 shows the results of X-ray diffraction (rocking curves) studies of samples R811 ($InAs_{0.57}Sb_{0.43}$) and R1051 ($InAs_{0.62}Sb_{0.38}$) for the [004] reflection. In multilayer structures, in which there are several layers with different interplanar spacings, several, closely arranged broad peaks in the angle distribution of the intensity are observed in the rocking curves for a specified reflection. Scanning was conducted with a step of ~7". The narrow diffraction peak is related to the GaSb substrate.



Fig. 3. Rocking curves for the [004] reflection in samples R811 (InAs_{0.57}Sb_{0.43}) and R1051 (InAs_{0.62}Sb_{0.38})

For sample R811, we observe one broadened peak, which is due to the match between the lattice parameters of the upper $In_{38}Al_{0.62}$ buffer layer and the working $InAs_{0.57}Sb_{0.43}$ layer. In the diffraction pattern for sample R1051, we observe two broadened peaks different in angle by ~300", which in turn is due to a small difference between the lattice parameters of the upper $In_{32}Al_{0.68}$ buffer layer and the working $InAs_{0.62}Sb_{0.38}$ layer.

Figure 4 shows the mapped distribution of the diffracted radiation intensity in q space around the symmetric [004] site and the asymmetric [335] site for sample R1051. From the position of the interference maxima on the map of the [004] and [335] sites, we determined the lattice parameters in the growth direction (a⊥) and growth plane (a||) using well-known formulas. In Figure 4 for the case of asymmetric recording around the [335] site, we can clearly see the almost complete relaxation of strains during growth of the epitaxial heterostructure from the GaSb substrate to the upper part of the buffer layer (solid line) and pseudomorphic growth of the upper part of the buffer layer (ashed vertical line).

We carried out Raman studies for heteroepitaxial structures R811 (with an $InAs_{0.57}Sb_{0.43}$ layer) and R1051 (with an $InAs_{0.62}Sb_{0.38}$ layer), using a Nanofinder 30 (Tokyo Instruments, Japan) confocal Raman microspectrometer. The studies were performed in the backscattering geometry of measurements. For the excitation light source, we used a YAG:Nd laser emitting radiation at the wavelength of the second harmonic

-532 nm. A cooled CCD camera (-70 °C) operating in the photon counting mode of measurements served as a detector. The usual exposure time was 5 min; the power of light incident on the sample was 7–9 mW; and the beam diameter was ~4 µm. In the spectrometer, an 1800 line mm⁻¹ diffraction grating was used. The accuracy in determining the spectral positions of the lines was no worse than 0.5 cm⁻¹.



Figure 4 – Maps of reciprocal q space around the [004] and [335] sites for sample R1051

Penetration depth of laser radiation and consequently, effective depth of the analysis at Raman scattering can be defined from a parity $\lambda/2\pi k$, where k–extinction factor. For the laser with the wavelength of λ =532 nm for analysis of InAsSb system, such depth with the account of data of extinction factor for InAs and InSb is approximately 100 nanometers [6]. It permits to say that, using the given wavelength of the laser for Raman scattering, one can obtain the information only from the top layer of an investigated multilayered covering.

It is well known that, for Group-III–V crystals with a cubic lattice, there are two phonons active in Raman scattering. These are the longitudinal optical (LO) and transverse optical (TO) phonons. According to [7], for InAs bulk single crystals, the LO and TO phonon frequencies are 242 and 220 cm⁻¹, respectively; for InSb crystals, the LO and TO phonon frequencies are 193 and 185 cm⁻¹, respectively.

Figure 5 shows the Raman spectra obtained in the backscattering mode of measurements at room temperature.



Fig. 5. Raman spectra of samples (a) R811 and (b) R1051 and (c) the GaSb substrate.

It is obvious that the characteristic feature of $InAs_{1-x}Sb_x$ (Figures 5a and 5b) alloys is the two-mode type of transformation of the phonon spectra. In Fig. 5, we can clearly see several phonon bands. These are a high-intensity phonon band (allowed by selection rules for the geometric layout of Raman experiments in the study) at the frequencies 187 cm⁻¹ (InAs_{0.57}Sb_{0.43}) or 186 cm⁻¹ (InAs_{0.62}Sb_{0.38}) corresponding to the LO phonon in InSb (the InSb-like LO phonon) and an asymmetric broad phonon band at the frequencies 222 cm⁻¹ (InAs_{0.57}Sb_{0.43}) or 223 cm⁻¹ (InAs_{0.62}Sb_{0.38}). The asymmetric band is formed as a superposition of two bands related to LO and TO phonons in InAs (nAs-like LO and InAs-like TO phonons). It seems likely that observation of the TO phonon band forbidden for the backscattering mode of Raman measurements is a consequence of the violation of the crystal-lattice symmetry of the epitaxial film because of disordering of the crystal lattice of the alloy and, in addition, a consequence of some deviation from the backscattering

mode of measurements. It should be noted that the bulk GaSb substrate is of high structural quality, as follows from the narrow lines with half-widths of $\sim 3 \text{ cm}^{-1}$ (Figure 5c). The frequencies correspond to LO (235 cm⁻¹) and TO (226 cm⁻¹) phonons active in the Raman spectra of GaSb [7].

It can be seen that, as the number of Sb atoms in $InAs_{1-x}Sb_x$ decreases (sample R1051), the 222 cm⁻¹ phonon band shifts to higher frequencies, i.e., the frequencies of Raman active phonons characteristic of InAs. The origin of less intense broad bands at ~140 cm⁻¹ is not established and invites further investigation.

High homogeneity of obtained heteroepitaxial structures has been confirmed by results of investigations of mikro-Raman scattering spectra by laser beam scanning of structure surface in a mapping regime. In a mapping regime it is possible to perform operation with each of the allocated spectral lines on variety of characteristics: Peak position of spectral lines, FWHM of a spectral line, intensity of a spectral line, value of integrated intensity of a spectral line, etc. In fig. 6a mapping results of peak position of a spectral line 187 cm⁻¹ on area 50×50 µm are presented, and in Figure 6b results for FWHM mapping (Full width at half maximum) of a spectral line at 187 cm⁻¹ are shown.



Figure 6 – Mapping of peak position of the spectral line 187 cm⁻¹ (a), and Mapping of half-width (FWHM) of the spectral line 187 cm⁻¹ (b)

III. CONCLUSIONS

Combined analysis of the experimental data obtained by high-resolution X-Ray diffraction studies, scanning atomic-force microscopy, and Raman spectroscopy shows that $InAs_{0.57}Sb_{0.43}$ and $InAs_{0.62}Sb_{0.38}$ alloys grow coherently on graded AlGaInSb and GaInSb buffer layers, respectively. The heteroepitaxial structures produced in the study are of high structural quality, as established from the shape of both symmetric and asymmetric reflections in reciprocal space.

The high degree of homogeneity of the heteroepitaxial structures is confirmed by the data on micro-Raman spectra. In addition, the data of confocal Raman spectroscopy suggest the two-mode type of transformation of the phonon spectra of the $InAs_{1-x}Sb_x$ alloys.

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