

# INFLUENCE OF AN ULTRA-THIN BUFFER LAYER ON THE GROWTH AND PROPERTIES OF PSEUDOMORPHIC GaAsBi LAYERS

S. Pūkienė<sup>a</sup>, A. Jasinskas<sup>a</sup>, A. Zelioli<sup>a</sup>, S. Stanionytė<sup>a, b</sup>, V. Bukauskas<sup>c</sup>, B. Čechavičius<sup>a</sup>,  
E. Dudutienė<sup>a</sup>, and R. Butkutė<sup>a, d</sup>

<sup>a</sup> Department of Optoelectronics, Center for Physical Sciences and Technology, Saulėtekio 3, 10257 Vilnius, Lithuania

<sup>b</sup> Department of Characterisation of Materials Structure, Center for Physical Sciences and Technology, Saulėtekio 3, 10257 Vilnius, Lithuania

<sup>c</sup> Department of Physical Technologies, Center for Physical Sciences and Technology, Saulėtekio 3, 10257 Vilnius, Lithuania

<sup>d</sup> Photonics and Nanotechnology Institute, Faculty of Physics, Vilnius University, Saulėtekio 3, 10257 Vilnius, Lithuania  
Email: renata.butkute@ftmc.lt

Received 23 June 2022; revised 1 July; accepted 1 July 2022

A series of 100 nm-thick pseudomorphic GaAsBi layers with the Bi content varying from 0.97 to 11.2% have been grown by molecular beam epitaxy (MBE) on the semi-insulating GaAs(100) substrates buffered with an ultra-thin up to 20 nm thick GaAs layer. The main attention in this work was focused on the investigation of relaxation in the Bi induced compressively-strained GaAsBi layers containing a various content of Bi. The lattice parameters of GaAs-Bi compound and the Bi concentration have been evaluated from high resolution X-ray diffraction measurements. The relaxation values of GaAsBi layers ranging from 0.4 to 3.5% were obtained analyzing the symmetric and asymmetric reciprocal space maps of (004) and (115) planes, respectively. Also, the complex study was performed to clarify the relaxation effect on structural, morphological and optical properties of bismide layers. Optical measurements revealed a significant reduction of the energy band gap from 1.34 to 0.92 eV for the layers containing 0.97–8.6% of Bi in the GaAs lattice.

**Keywords:** GaAsBi, molecular beam epitaxy, X-ray diffraction, photoluminescence, atomic force microscopy

## 1. Introduction

GaAsBi alloy is well known as a prospective material for application in various optoelectronic devices. Due to the large band gap reduction (by up to 88 meV per Bi %) [1, 2] induced by the substitution of As atoms by Bi in the GaAs host lattice, and the lower temperature dependence of energy band gap (0.1–0.3 meV/K) [2] this compound is very promising as an active layer of lasers operating in the near-infrared (NIR) spectrum range [3–8]. It was demonstrated that GaAsBi thick layers and quantum structures could be applied as a 1.0 eV-subcell photovoltaic material in tandem solar cells [9–11], and THz photodetectors sensitive in a spectral range of (1000–1500 nm) [12–13]. According to the band anti-crossing model, bismuth

affects an electronic structure strongly (mainly valence band) by inducing the energy levels close to the valence band and by increasing the spin-orbit splitting energy between the valence band and the spin-orbit split-off band [14–15]. Polak et al. in Ref. 16 demonstrated that the Bi incorporation also affects slightly the conduction band. Furthermore, the introduction of more than 10% Bi to the GaAs lattice allows the spin-orbit splitting energy to pass the energy of band gap. This behaviour could have an application especially in the infrared lasers, where the optical loss processes are caused by the Auger recombination of emitted photons in the active region. The reduction of non-radiative Auger recombination leads to the enhancement of the lasing feature of sources. Moreover, the temperature sensitivity of small bismide energy band gap will

open a possibility to develop laser modules without cooling.

Despite these advantages, the progress in applications is held back by the challenges of bismide growth technology. Since bismuth is much larger than arsenic and exhibits the strong feature to surface segregate at high temperatures, the incorporation of Bi to GaAs lattice under usual A3-B5 growth conditions is impossible. The reduced growth temperature (lower than 400°C) and the low arsenic overpressure (pressure ratio of As and Ga close to 1) are required for the incorporation of a significant concentration of Bi into the GaAs host lattice [14–16]. The increased Bi solubility under these growth conditions leads to the raised compressive strain in GaAsBi alloy due to the replacement of smaller As atoms by larger Bi. The thickness beyond which the relaxation of strained layers is expected to occur is the critical thickness. Increasing the bismide layer thickness due to the tensile or compressive strain the plastic deformation starts to occur leading to the inhomogeneous strain associated with misfit dislocations. According to Matthews and Blakeslee [17], for any given strain there will be a critical thickness of heteroepitaxial growth at which it will become energetically favourable for dislocations in the material to propagate to the sample surface. On the other hand, Drigo et al. in Ref. 18 investigating  $\text{In}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}$  heterostructures showed that the strain driven dislocation propagation does not result in a significant relaxation of strain. It was shown that the generation of dislocations occurs at greater thicknesses than the Matthews–Blakeslee critical thickness. Many experimental studies depending on the method (XRD, PL, etc.) used to evaluate the critical thickness of bismide layers have demonstrated various results. Tixier et al. using XRD measurements supposed that the critical thickness for GaAsBi containing 3.1% of Bi could exceed even ~270 nm [2], this being significantly higher than the critical thickness reported for the formation of misfit dislocations of InGaAs on GaAs with a similar lattice mismatch (0.37%) – 60 nm.

Since most GaAsBi applications in laser diodes and solar cells tend to avoid the relaxation of layers or multi-quantum well structures, the knowledge about the relaxation level depending on the bismuth content is necessary, and the ability to control the strain is still very important. Moreover, the second crucial factor for epitaxial heterostructures is

surface roughness, since the active area in most of devices or components (for example, LED and LD) is inserted between hundred nanometres or micrometres – thick p and n waveguide cladding layers.

In this work, we present the complex study of a series of 100 nm-thick GaAsBi layers grown by molecular beam epitaxy (MBE) on semi-insulating GaAs(100) substrates with a different Bi content varying from 0.97 to 11.2%. Otherwise than in the referred works, an ultra-thin GaAs buffer layer was used. It was supposed that the ultra-thin (up to 20 nm) GaAs buffer layer could serve as an equivalent of the cladding layer exhibiting the typical surface roughness of about 0.5 nm. The main attention in this work was focused on the investigation of relaxation in the compressively-strained GaAsBi layers induced by a higher surface roughness and different Bi content.

## 2. Materials and methods

GaAsBi samples were grown using two solid source molecular beam epitaxy (MBE) systems: Veeco GENxplor (samples marked with VGA) and SVT-A (samples marked with B). Both MBE reactors were equipped with conventional Knudsen effusion cells for metallic Ga and Bi and an As cracker. After the deoxidation of substrate, an ultra-thin up to 20 nm in thickness GaAs buffer layer was grown at 650°C temperature with 300–500 nm/h growth rate. The thickness of the buffer layer was defined by the change of reflection high energy diffraction (RHEED) image from the bulky substrate pattern ( $1 \times 1$ ) to the clearly determined surface reconstruction of ( $2 \times 4$ ). To introduce different bismuth content epitaxial GaAsBi layers were grown on semi-insulating GaAs(100) substrates at different substrate temperatures 360–425°C and a significantly reduced As/Ga flux ratio varying from 1 to 1.1. The growth temperature was monitored by thermocouple readings. The surface quality and growth mode layer by layer was monitored and evaluated *in situ* during the growth using RHEED. Bismuth flux varied in the wide range from  $10^{-8}$  Torr to  $5 \times 10^{-7}$  Torr by changing Bi source temperature. To enhance Bi incorporation, before the bismide growth the buffered substrates were exposed in the pure Bi flux for 10 s (it allows one to cover the buffer partially by a Bi wetting layer, which acts as a surfactant). The complex investigation of grown GaAsBi layers revealed the narrow enough

window of optimum technological conditions with three crucial parameters: substrate temperature, As/Ga ratio and bismuth flux. It is worth noting that the optimum conditions for the introduction of different concentration of Bi slightly varied: for a lower bismuth concentration higher temperatures, a lower Bi flux and a higher As to Ga ratio are more appropriate, while lower temperatures, As/Ga values closer to 1 and a higher bismuth flux are more favourable for the growth of GaAsBi with more than 6% Bi. This fact well illustrates the sample B839, where the Bi content reaches only 3.1%: i. e. a small Bi flux and a higher As to Ga ratio are bismuth concentration limiting factors though the substrate temperature is very low (320°C). The technological parameters of GaAsBi layers growth are presented in Table 1.

Table 1. Main technological parameters of the GaAsBi layers: the Bi content (%) established from XRD measurements, the thickness (nm) evaluated from MBE RHEED intensity oscillations and the growth temperature (°C) monitored by thermocouple readings.

| Sample No. | Bi content, % | Thickness, nm | Growth temperature, °C |
|------------|---------------|---------------|------------------------|
| VGA0099    | 0.97          | 100           | 425                    |
| VGA0101    | 1             | 100           | 425                    |
| VGA0102    | 1             | 100           | 425                    |
| VGA0108    | 2.5           | 100           | 370                    |
| VGA0109    | 1             | 100           | 370                    |
| B838       | 11.2          | 100           | 320                    |
| B839       | 3.1           | 100           | 320                    |
| B846       | 8.6           | 100           | 350                    |
| B847       | 6.6           | 100           | 360                    |

The crystalline structure and surface morphology of samples *ex situ* were characterized by atomic force microscopy (AFM) measurements using a Dimension 3100 SPM system with a Nanoscope IVa controller (Veeco Instruments Inc., USA). To establish the Bi content in 100 nm-thick GaAsBi layers, XRD measurements were carried out with a SmartLab diffractometer (Rigaku, Japan), by monitoring shifts of the (004) diffraction peak with respect to its position to GaAs. The compressive strain relaxation was defined from the symmetric reciprocal space maps (RSM) of the (004) plane and the asymmetric RSM measured using grazing exit angle geometry for the (115) plane.

Photoluminescence (PL) measurements were carried out using a 500 mm focal length monochromator (Andor SR-500i) along with a liquid nitrogen/thermoelectrically cooled InGaAs photodetector. A diode-pumped solid-state laser emitting at the wavelength of 532 nm was used as an excitation source at different excitation powers (ranging from several tens to several hundred mW). The samples were mounted on the cold finger of a closed-cycle helium cryostat coupled with a temperature controller, allowing for measurements in the temperature range of 3–300 K.

### 3. Results and discussion

#### 3.1. Structure analysis

The lattice parameters of GaAsBi compound and the Bi concentration have been evaluated from high resolution X-ray diffraction  $\omega/2\theta$  measurements (see Fig. 1). The Bi content in the samples determined from XRD varied from 0.97 to ~11.2% depending on the substrate temperature and  $As_2/Ga$  ratio and bismuth flux. The XRD scans measured from the (004) planes for the 100 nm-thick epitaxial GaAsBi layers with a various Bi content grown on GaAs (100) are shown in Fig. 1. The peaks at  $2\theta = 66.055^\circ$  correspond to the GaAs substrate, while the peaks on the left are attributed to the epitaxial GaAsBi layers. Each sample scan is presented by a different colour line (see the legend). The perpendicular lines marking the Bi concentration in the strained GaAsBi compound are shown as guides for the eye. The separation of these two peaks corresponds to the mismatch between the GaAsBi layer and GaAs substrate out-of-plane lattice. The dynamical simulations of XRD scans made by assuming the absence of tetragonal distortion were used for the determination of the layer composition. Evaluating the Bi content (presented in Table 1), the Vegard's law was assumed, and the values for the GaBi and GaAs lattice constants were taken 6.234 and 5.653 Å, respectively. It was revealed from the investigation that the layers are pseudomorphic to the GaAs substrate. In the scans of the samples with a higher Bi concentration the peak corresponding to GaAsBi was significantly wider, what is an indication that Bi is distributed inhomogeneously. The relaxation values of GaAsBi layers were obtained from the symmetric and asymmetric scans of reciprocal space maps of (004) and (115) planes, respectively, shown in Fig. 2.

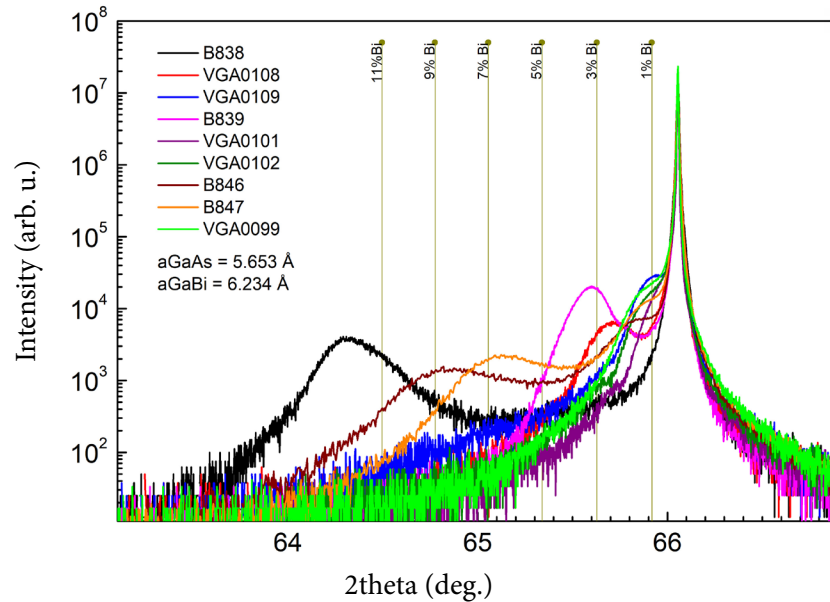


Fig. 1. XRD rocking curves of the (004) diffraction peak of 100 nm-thick GaAsBi layers grown onto the GaAs substrate. Bi content in the layers was calculated taking into account the data obtained from reciprocal space maps showing that GaAsBi layers are almost fully strained even containing the largest bismuth concentration 11.2%. The vertical lines mark the fully strained GaAsBi bulk compound reflex containing Bi content from 0.97 to 11.2%.

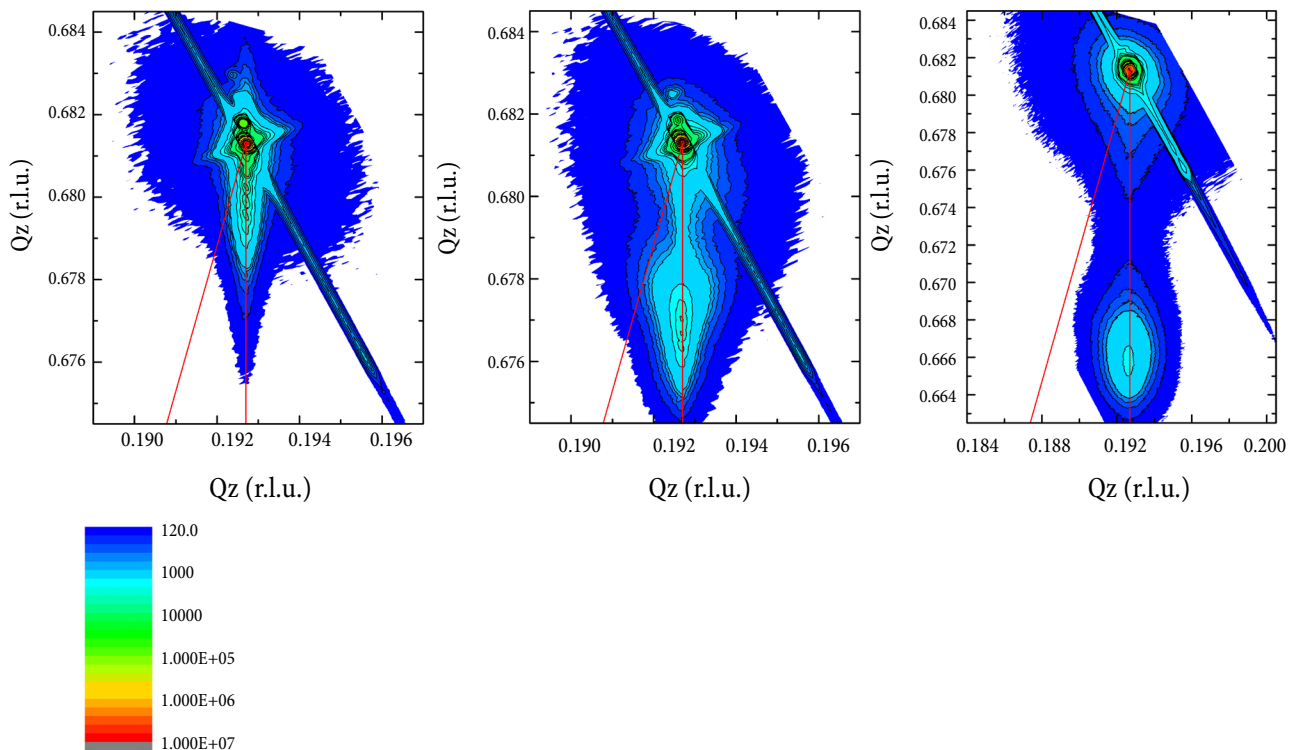


Fig. 2. High-resolution XRD reciprocal space maps of the (115) plane measured for three GaAsBi layers with 0.97, 3.1 and 11.2% bismuth content. The perpendicular and tilted solid red lines on this plot correspond to the fully strained and fully relaxed states, respectively. An insignificant shift of the layer peak from vertical lines is due to low relaxation.

The visible vertical red line starting from the GaAs reflex indicates that the compound is fully strained and has the same in-plane lattice parameter as GaAs. The tilted red line is attributed to the fully relaxed layer. The established relaxation level was very low for all grown samples and reached only tenths or few percents – from 0.4 to 3.5%, respectively, for the GaAsBi layers with the lowest and largest Bi concentration.

The analysis of the shape of RSM peaks attributed to GaAsBi (Fig. 2) suggested that the relaxation of 100 nm-thick GaAsBi layers could be caused by a rough enough ultra-thin GaAs buffer layer. Moreover, the GaAsBi reflexes on RSM are symmetric, so the assumption that the compound started to relax due to the incorporation of larger radius Bi atoms can be refused.

The growth mechanism and surface roughness of 100 nm-thick GaAsBi layers have been characterized *ex situ* by atomic force microscopy (AFM) measurements. The representative AFM images of GaAsBi epitaxial layers with 0.97% (VGA0099) and 6.6% (B847) of Bi, grown using the same As/Ga pressure ratio of about 1.077 and substrate temperature of 425 and 350°C, respectively, are shown in Fig. 3. The AFM investigations revealed that the surface roughness of GaAsBi layers varied from 10 to 18 nm depending on the As to Ga flux ratio and the Bi flux as well as the growth temperature. A smoother surface was registered for lower growth temperatures (320–350°C) used for

the growth of GaAsBi with a larger Bi content, while 18 nm roughness was measured for the 100 nm thick GaAsBi layers grown at 425°C temperature. It should be noted that the pits observed in Fig. 3(a) are caused by the lack of arsenic in the lattice.

### 3.2. Optical characteristics

Firstly, the PL spectra of all investigated 100 nm-thick GaAsBi layers were measured at room temperature. The selected room temperature PL spectra are presented in Fig. 4(a). It can be seen that the PL spectra of the samples of B series, grown into a SVT-A MBE reactor, consist of two PL bands. A higher energy band centred at 1.42 eV is related with the optical transition in the bulk GaAs substrate. A lower energy band was assigned to the optical transitions within the GaAsBi layer. There was no room temperature PL signal at low energies from the GaAsBi layer containing 3.1% of Bi (sample B839). It can be related to a higher concentration of non-radiative recombination centres due to a significantly lower growth temperature of 320°C than the optimal one even if the As to Ga ratio was almost 1.1 and the bismuth flux did not exceed  $10^{-7}$  Torr. Nevertheless, the room temperature GaAsBi related emission was observed at 0.99 and 0.92 eV for the GaAsBi layers with higher Bi concentrations of 6.6% (sample B847) and 8% (sample B846), respectively. A higher PL intensity from the GaAsBi

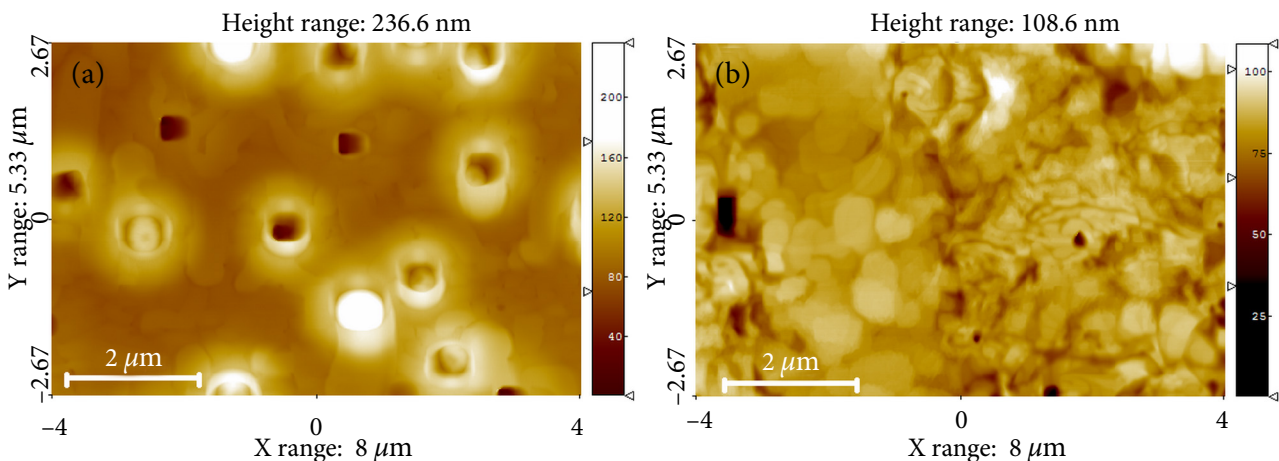


Fig. 3. The surface morphology images of two GaAsBi epitaxial layers with 0.97% (VGA0099) and 6.6% (B847) of Bi, grown using the same As/Ga pressure ratio of about 1.077 and the substrate temperature of 425 and 350°C, respectively, for (a) and (b). The scanned area is  $8.0 \times 5.3 \mu\text{m}^2$ . The right colour code shows a scale bar for the height in the images. Z scale is 236.6 and 108.6 nm for (a) and (b), respectively.



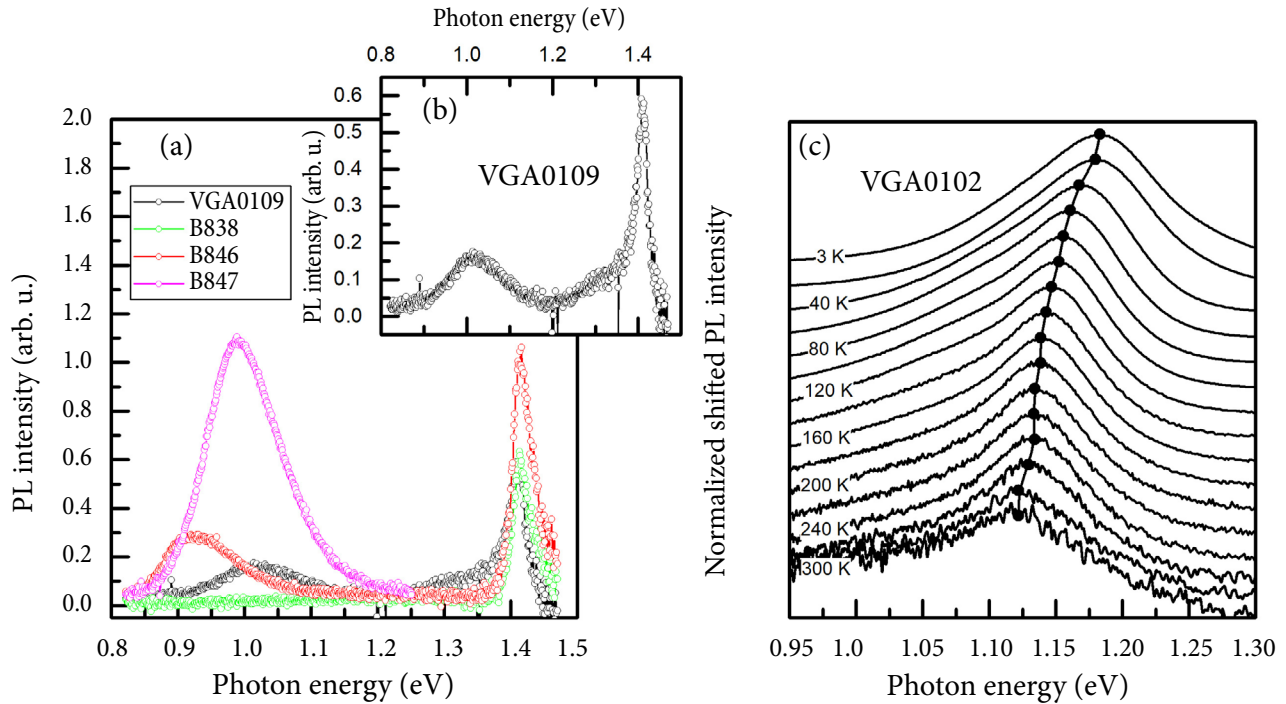


Fig. 4. Room temperature PL spectra of all grown GaAsBi layers with different Bi concentrations (a) and a separated view of the GaAsBi layer with 1% of Bi (sample VGA0109) (b). Temperature-dependent PL spectra of the GaAsBi layer with 1% of Bi (sample VGA0102) measured at the temperatures ranging from 3 to 300 K (c).

layer containing 6.6% of Bi is related with a possibly lower concentration of non-radiative centres due to a higher growth temperature and a lower Bi concentration.

Unexpectedly, the room temperature PL spectra of VGA series GaAsBi layers containing 1% of Bi consisted of three PL components (see Fig. 4(b)). As for B-series samples the PL band at 1.42 eV was assigned to GaAs, a low energy shoulder of the 1.42 eV PL band was assigned to the GaAsBi layer with 1% of Bi. A very low PL intensity of the GaAsBi layer could be explained by the thermal escape of photoexcited carriers from GaAsBi due to a small conduction band offset between GaAsBi and GaAs. The origin of PL band at 1 eV is not so clear. It could be related to the Bi-rich GaAsBi regions due to the prior to bismide growth introduced Bi wetting layer.

The temperature-dependent PL spectra of the GaAsBi layer containing 1% of Bi (sample VGA0102) at a low energy region are depicted in Fig. 4(c). It can be seen that the PL band maximum position change with temperature is small. It changes from 1.185 eV at 3 K to 1.122 eV at 300 K. Therefore, the thermal band gap change value of  $0.21 \text{ meVK}^{-1}$  is much smaller than that reported

for GaAs ( $0.52 \text{ meVK}^{-1}$  [19]) and other conventional semiconductors. Moreover, that supports the assumption that a low energy PL band is associated with optical transitions in Bi-rich GaAsBi regions.

#### 4. Conclusions

Summarizing, the main technological aspects could be pointed out. Thick pseudomorphic 100 nm GaAsBi layers with the Bi content ranging from 0.97 to 11.2% were grown by MBE at the substrate temperature of about 320–425°C using the growth rate of 300–500 nm/h range. The ultra-thin GaAs buffer was used to mimic the possible roughness of cladding layers. The analysis of the shape of RSM reflexes attributed to GaAsBi suggested that the relaxation of 100 nm-thick GaAsBi layers could be mainly caused by a rough enough (of about 0.5 nm) thin GaAs buffer layer. Moreover, this investigation explored that 100 nm thick GaAsBi layers with the Bi content varying from 0.97 to 8.6% and emitting in the spectral range from 925 up to 1350 nm are almost compressively strained. The symmetrical GaAsBi reflexes on RSM plots support the message that the relaxation of 0.4–3.5%, respectively,

for the GaAsBi layers with the lowest and largest Bi concentration is originating from an ultrathin buffer layer, and the assumption that the compound started to relax due to the incorporation of larger radius Bi atoms can be refused. Two different trends of optical features were observed in the GaAsBi layers. PL spectra of the samples of B series, grown into a SVT-A MBE reactor, consist of two PL bands. Higher energy band centred at 1.42 eV was related with the optical transition in the bulk GaAs substrate. Lower energy band was assigned to optical transitions within the GaAsBi layer. On the other hand, the RT PL spectra of VGA series consisted of three PL components: a band at 1.42 eV assigned to GaAs, its low energy shoulder PL to the GaAsBi layer with 1% of Bi and emission at 1 eV, which require more investigation to clarify the origin.

### Acknowledgements

This work was supported by the Research Council of Lithuania under Grant Agreement P-MIP-22-309 (LMTLT).

### References

- [1] K. Oe and H. Okamoto, New semiconductor alloy GaAs<sub>1-x</sub>Bi<sub>x</sub> grown by metal organic vapor phase epitaxy, *Jpn. J. Appl. Phys.* **37**, L1283 (1998), <https://doi.org/10.1143/JJAP.37.L1283>
- [2] S. Tixier, M. Adamczyk, and T. Tiedje, Molecular beam epitaxy growth of GaAs<sub>1-x</sub>Bi<sub>x</sub>, *Appl. Phys. Lett.* **82**, 2245 (2003), <https://doi.org/10.1063/1.1565499>
- [3] T. Fuyuki, R. Yoshioka, K. Yoshida, and M. Yoshimoto, in: *Proceedings of CLEO 2014, JTu4A.122* (OSA, Washington, D.C., 2014).
- [4] R. Butkutė, A. Geizutis, V. Pačebutas, B. Čechavičius, V. Bukauskas, R. Kundrotas, P. Ludewig, K. Volz, and A. Krotkus, Multi-quantum well Ga(AsBi)/GaAs laser diodes with more than 6% of bismuth, *Electron. Lett.* **50**(16), 1155–1157 (2014), <https://doi.org/10.1049/el.2014.1741>
- [5] I.P. Marko, S.R. Jin, K. Hild, Z. Batool, Z.L. Bushell, P. Ludewig, W. Stolz, K. Volz, R. Butkutė, V. Pačebutas, A. Geizutis, A. Krotkus, and S.J. Sweeney, Properties of hybrid MOVPE/MBE grown GaAsBi/GaAs based near-infrared emitting quantum well lasers, *Semicond. Sci. Technol.* **30**, 1–10 (2015), <https://doi.org/10.1088/0268-1242/30/9/094008>
- [6] P.K. Patil, E. Luna, T. Matsuda, K. Yamada, K. Kamiya, F. Ishikawa, and S. Shimomura, GaAsBi/GaAs multi-quantum well LED grown by molecular beam epitaxy using a two-substrate-temperature technique, *Nanotechnology* **28**, 105702 (2017), <https://doi.org/10.1088/1361-6528/aa596c>
- [7] I.P. Marko and S.J. Sweeney, Progress toward III–V bismide alloys for near- and midinfrared laser diodes, *IEEE J. Sel. Top. Quantum Electron.* **23**(6), 1501512 (2017), <https://doi.org/10.1109/JSTQE.2017.2719403>
- [8] C.A. Broderick, S. Jin, I.P. Marko, K. Hild, P. Ludewig, Z.L. Bushell, W. Stolz, J.M. Rorison, E.P. O'Reilly, K. Volz, and S.J. Sweeney, GaAs<sub>1-x</sub>Bi<sub>x</sub>/GaNyAs<sub>1-y</sub> type-II quantum wells: novel strain-balanced heterostructures for GaAs-based near- and mid-infrared photonics, *Sci. Rep.* **7**, 46371 (2017), <https://doi.org/10.1038/srep46371>
- [9] A. Zayan, M. Stevens, and T.E. Vandervelde, in: *Proceedings of 2016 IEEE 43rd Photovoltaic Specialists Conference (PVSC)* (Portland, OR, 2016) pp. 2839–2843, <https://ieeexplore.ieee.org/document/7750172/>
- [10] T. Tomas, A. Mellor, N.P. Hylton, M. Führer, D. Alonso-Álvarez, A. Braun, N.J. Ekins-Daukes, J.P.R. David, and S.J. Sweeney, Requirements for a GaAsBi 1 eV sub-cell in a GaAs-based multi-junction solar cell, *Semicond. Sci. Technol.* **30**, 1–6 (2015), <https://doi.org/10.1088/0268-1242/30/9/094010>
- [11] R.D. Richards, A. Mellor, F. Haruna, J.S. Cheonga, N.P. Hylton, T. Wilson, T. Thomas, J.S. Roberts, N.J. Ekins-Daukes, and J.P.R. David, Photovoltaic characterisation of GaAsBi/GaAs multiple quantum well devices, *Sol. Energy Mater. Sol. Cells* **172**, 238–243 (2017), <https://doi.org/10.1016/j.solmat.2017.07.029>
- [12] V. Pačebutas, A. Bičiūnas, S. Balakauskas, A. Krotkus, G. Andriukaitis, D. Lorenc, A. Pugžlys, and A. Baltuška, Terahertz time-domain-spectroscopy system based on femtosecond Yb: fiber laser and GaBiAs photoconducting components,

- Appl. Phys. Lett. **97**, 031111 (2010), <https://doi.org/10.1063/1.4942819>
- [13] K. Bertulis, A. Krotkus, G. Aleksejenko, V. Pačebutas, R. Adomavičius, G. Molis, and S. Marcinkevičius, GaBiAs: a material for optoelectronic terahertz devices, Appl. Phys. Lett. **88**, 201112 (2006).
- [14] K. Alberi, J. Wu, W. Walukiewicz, K.M. Yu, O.D. Dubon, S.P. Watkins, C.X. Wang, X. Liu, Y.-J. Cho, and J. Furdyna, Valence-band anticrossing in mismatched III–V semiconductor alloys, Phys. Rev. B **75**, 045203 (2007).
- [15] B. Fluegel, S. Francoeur, A. Mascarenhas, S. Tixier, E.C. Young, and T. Tiedje, Giant spin-orbit bowing in GaAs<sub>1-x</sub>Bi<sub>x</sub>, Phys. Rev. Lett. **97**, 067205 (2006).
- [16] M.P. Polak, P. Scharoch, and R. Kudrawiec, First-principles calculations of bismuth induced changes in the band structure of dilute Ga-V-Bi and In-V-Bi alloys: chemical trends versus experimental data, Semicond. Sci. Technol. **30**, 1–10 (2015), <http://iopscience.iop.org/0268-1242/30/9/094001>
- [17] J.W. Matthews and A.E. Blakeslee, Defects in epitaxial multilayers: I. Misfit dislocations, J. Cryst. Growth **27**, 118–125 (1974).
- [18] A.V. Drigo, A. Aydinli, A. Carnera, F. Genova, C. Rigo, C. Ferrari, P. Franzosi, and G. Salviati, On the mechanisms of strain release in molecular-beam-epitaxy-grown In<sub>x</sub>Ga<sub>1-x</sub>As/GaAs single heterostructures, J. Appl. Phys. **66**(5): 1975–1983 (1989).
- [19] I. Vurgaftman, J.R. Meyer, and L.R. Ram-Mohan, Band parameters for III–V compound semiconductors and their alloys, J. Appl. Phys. **89**(11): 5815–5875 (2001), <https://doi.org/10.1063/1.1368156>

## PLONOJO BUFERINIO SLUOKSNIO ĮTAKA PSEUDOMORFINIŲ GaAsBi SLUOKSNIŲ AUGINIMUI IR SAVYBĖMS

S. Pūkienė<sup>a</sup>, A. Jasinskas<sup>a</sup>, A. Zelioli<sup>a</sup>, S. Stanionytė<sup>a, b</sup>, V. Bukauskas<sup>c</sup>, B. Čechavičius<sup>a</sup>, E. Dudutienė<sup>a</sup>, R. Butkutė<sup>a, d</sup>

<sup>a</sup> Fizinių ir technologijos mokslų centro Optoelektronikos skyrius, Vilnius, Lietuva

<sup>b</sup> Fizinių ir technologijos mokslų centro Medžiagų struktūrinės analizės skyrius, Vilnius, Lietuva

<sup>c</sup> Fizinių ir technologijos mokslų centro Fizikinių technologijų skyrius, Vilnius, Lietuva

<sup>d</sup> Vilniaus universiteto Fizikos fakulteto Fotonikos ir nanotechnologijų institutas, Vilnius, Lietuva

### Santrauka

Darbe buvo tiriama 100 nm storio pseudomorfinių GaAsBi sluoksnių, kuriuose Bi kiekis kito nuo 0,97 iki 11,2 %, serija. Sluoksniai buvo užauginti molekulinį pluoštelių epitaksijos metodu ant pusiau izoliuojančių GaAs (100) padėklų, padengiant juos itin plonu iki 20 nm buferiniu GaAs sluoksniu. Pagrindinis šio darbo tikslas buvo įvertinti buferinio GaAs sluoksnio poveikį skirtingą Bi kiekį talpinančio GaAsBi sluoksnio kristalinei sandarai, relaksacijai bei paviršiaus morfologijai ir optinėms savybėms. GaAsBi junginio kristali-

nės gardelės parametrai ir Bi koncentracija buvo įvertinti naudojant didelės skiriamosios gebos rentgeno spindulių difrakcijos matavimus. Relaksacijos vertės, gautos analizuojant simetrinius ir asimetrinius atvirkštinės gardelės žemėlapius, pamatuotus nuo (004) ir (115) plokštumų, atitinkamai kito nuo 0,4 iki 3,5 %. Optiniai matavimai atskleidė ženklų GaAsBi junginio draustinio energijos tarpo sumažėjimą nuo 1,34 iki 0,9 eV sluoksniams, bismuto kiekiui gardelėje didėjant nuo 0,97 iki 8,6 %.