St. Petersburg State Polytechnical University Journal. Physics and Mathematics. 2026. Vol. 19. No. 1.1
Научно-технические ведомости СПбГПУ. Физико-математические науки. 19 (1.1) 2026

Conference paper
UDC: 538.911
DOI: https://doi.org/10.18721/JPM.191.106

Heterostructures with ultrathin $In_xGa_{1-x}As/GaAs(001)$ metamorphic buffer layers and InAs/InGaAs QDs grown by molecular beam epitaxy

O.E. Lakuntsova ✉, G.V. Klimko, I.V. Sedova, A.V. Myasoedov,
A.N. Semenov, N.D. Prasolov, S.V. Sorokin

Ioffe Institute, Saint Petersburg, Russia
✉ o.e.lakuntsova@mail.ioffe.ru

Abstract. The heterostructures with ultrathin (~220 nm) $In_xGa_{1-x}As/GaAs(001)$ metamorphic buffer layers with a convex indium composition profile were grown by molecular beam epitaxy and studied using structural characterization techniques. Analysis of atomic force microscopy images revealed a relationship between the surface roughness and the growth conditions of the graded layer. The density of threading dislocations in the structures with a ultra-thin graded layer was estimated as ~10^7 cm^{-2}, which is consistent with the high average grading rate of ~90% In/μm. The reciprocal space maps of high-resolution X-ray diffraction measured for both symmetric (004) and asymmetric (224) reflections in grazing exit geometry are presented.

Keywords: Metamorphic buffer layers, convex compositional profile, molecular beam epitaxy, $In_xGa_{1-x}As$, heterostructures, reciprocal space mapping, atomic force microscopy, energy-dispersive X-ray spectroscopy, transmission electron microscopy

Funding: The work was carried out within the framework of the State Assignment No. FFUG-2024-0043.

Citation: Lakuntsova O.E., Klimko G.V., Sedova I.V., Myasoedov A.V., Semenov A.N., Prasolov N.D., Sorokin S.V., Heterostructures with ultrathin $In_xGa_{1-x}As/GaAs(001)$ metamorphic buffer layers and InAs/InGaAs QDs grown by molecular beam epitaxy, St. Petersburg State Polytechnical University Journal. Physics and Mathematics. 19 (1.1) (2026) 39–44. DOI: https://doi.org/10.18721/JPM.191.106

Конференционная статья
УДК 538.911
DOI: https://doi.org/10.18721/JPM.191.106

Гетероструктуры со сверхтонкими метаморфными буферными слоями $In_xGa_{1-x}As/GaAs(001)$ и КТ InAs/InGaAs, выращенные методом молекулярно-пучковой эпитаксии

О.Е. Лакунцова ✉, Г.В. Климко, И.В. Седова, А.В. Мясоедов,
А.Н. Семенов, Н.Д. Прасолов, С.В. Сорокин

Физико-технический институт им. А.Ф. Иоффе РАН, Санкт-Петербург, Россия
✉ o.e.lakuntsova@mail.ioffe.ru

Аннотация. Гетероструктуры со сверхтонкими (~220 нм) метаморфными буферными слоями $In_xGa_{1-x}As/GaAs(001)$ с корневым профилем изменения состава по индию выращены методом молекулярно-пучковой эпитаксии и исследованы с использованием методов структурной характеризации. Из анализа изображений атомно-силовой микроскопии установлена взаимосвязь между шероховатостью поверхности и условиями роста градиентного слоя. Оценена плотность прорастающих дислокаций в структурах со сверхтонким градиентным слоем ~10^7 см$^{-2}$, что согласуется с высокой средней скоростью изменения содержания In ~90% In/мкм.

Представлены карты обратного пространства высокоразрешающей рентгеновской дифрактометрии, измеренные для симметричных (004) и асимметричных (224) отражений в геометрии скользящего отражения.

Ключевые слова: Метаморфные буферные слои, корневой профиль изменения состава, молекулярно-пучковая эпитаксия, $In_xGa_{1-x}As$, гетероструктуры, картирование обратного пространства, атомно-силовая микроскопия, энергодисперсионная рентгеновская спектроскопия, просвечивающая электронная микроскопия

Финансирование: Работа выполнена в рамках Государственного задания № FFUG-2024-0043.

Ссылка при цитировании: Лакунцова О.Е., Климко Г.В., Седова И.В., Мясоедов А.В., Семенов А.Н., Прасолов Н.Д., Сорокин С.В. Гетероструктуры со сверхтонкими метаморфными буферными слоями $In_xGa_{1-x}As$/GaAs(001) и КТ InAs/InGaAs, выращенные методом молекулярно-пучковой эпитаксии // Научно-технические ведомости СПбГПУ. Физико-математические науки. 2026. Т. 19. № 1.1. С. 39–44. DOI: https://doi.org/10.18721/JPM.191.106

Introduction

One of the key requirements in growing heterostructures for device applications is a small lattice mismatch between the structure layers and the substrate to provide the conditions of pseudomorphic growth, since strain relaxation with the formation of misfit dislocations (MDs) also leads to the appearance of numerous threading dislocations (TDs), which can significantly degrade the characteristics of semiconductor devices. If the growth of pseudomorphic structures is not possible, an approach based on metamorphic buffer layers (MBLs) with graded composition profiles is widely used. In this case, MBL provide a smooth transition from the substrate lattice constant to the specified lattice constant. One of the possible ways for implementing a single-photon source emitting in the telecom O-band or C-band (λ = 1.3 and 1.55 μm, respectively) is also associated with the use of $In_xGa_{1-x}As$/GaAs(001) MBL followed by the formation of InAs quantum dots (QDs) in an InGaAs matrix [1 – 3]. The advantage of this approach is the ability to use $Al_{0.9}Ga_{0.1}As$/GaAs distributed Bragg reflectors, which potentially allows the fabrication of micropillars using photolithography and ion etching.

Reducing the thickness of the MBL is extremely important for the fabrication of microcavity structures with a small mode volume, as it leads to an increase in the Purcell factor and, consequently, to an increase in the rate of spontaneous radiative recombination from QDs. The key challenges are the selection of a suitable MBL design, as well as finding the optimal growth conditions that ensure both a sufficiently smooth surface morphology and low TDs density in the active region of the structure.

In this work, we study the structural properties of heterostructures with InAs/InGaAs QDs grown on top of ultrathin $In_xGa_{1-x}As$/GaAs(001) MBL with a square-root (“convex”) indium composition profile. Transmission electron microscopy (TEM), energy-dispersive X-ray spectroscopy (EDS), atomic force microscopy (AFM), X-ray diffraction both in 2θ-ω- scanning mode and reciprocal space mapping (RSM) mode were used as characterization techniques.

Materials and Methods

The heterostructures with ultrathin $In_xGa_{1-x}As$/GaAs(001) MBL were grown by molecular beam epitaxy (MBE) on semi-insulating GaAs(001) epi-ready substrates and contain $In_xGa_{1-x}As$ MBL layer, a QD layer and an inverse layer. Standard Ga and In effusion cells, as well as an As valve cracker cell were used as molecular beam sources. The growth of all heterostructures began with the deposition of a homoepitaxial GaAs buffer layer (d_{GaAs} ~ 0.2 μm) at a temperature of T_S ~ 590–600°C. The thickness of the $In_xGa_{1-x}As$ MBL with a convex composition profile was as low as d_{MBL} ~ 220 nm with initial In step of x_{min} = 0.18 and maximum In content at the end

Издатель: Санкт-Петербургский политехнический университет Петра Великого.

of graded layer x_{max} = 0.38. In this case the average In composition grading rate is as high as ~90% In/µm. The variable parameters during MBE of the graded layer were both the substrate temperature and the V/III flux ratio: the substrate temperature varied from ~380 to 470°C, while the J_V/J_{III} flux ratio varied correspondingly in the range of ~2–6.5. InAs/InGaAs QDs were deposited directly on top of the graded layer using the Stranski-Krastanov growth mode followed by the deposition of a uniform composition layer with a thickness ~200 nm at a temperature of T_S ~ 420°C [4]. The indium content in this so-called "inverse" layer (x_{inv}) is lower than x_{max}, since this layer reduces the residual strain accumulated in the upper part of the graded layer. The thickness of the inverse layer is d_{inv} ~ 200 nm, and the indium content in this layer is $x_{inv} \approx 0.28$. The parameters of the heterostructures under study, as well as the MBE growth conditions of the graded layer are listed in Table.

Table

Parameters of the studied heterostructures

Type of structure	d_{MBL}, µm	d_{inv}, µm	x_{min}	x_{max}	x_{inv}	J_V/J_{III}	$T_{S(MBL)}$, °C	$T_{S(inv)}$, °C
#1	0.22	0.2	0.18	0.38	~0.28	2	380	420
#2						4	420	
#3						6.5	470	

Notations: d_{MBL} is the thickness of graded layer, d_{inv} is the thickness of inverse layer, x_{min} and x_{max} are the minimum and maximum In content in the $In_xGa_{1-x}As$ MBL with square-root profile, x_{inv} is In content in the inverse layer, J_V/J_{III} is V/III flux ratio during MBE growth of the graded layer, $T_{S(MBL)}$ and $T_{S(inv)}$ is the substrate temperature during MBE growth of the graded and inverse layer, respectively.

TEM measurements were performed using a JEOL-2100F electron microscope at an accelerating voltage of 200 kV. The specimen was prepared using a standard technique, including mechanical grinding and polishing to a thickness of ~10 µm and subsequent Ar^+ ion milling. A cross section was prepared to study the heterostructure in the vicinity of zone axis ⟨110⟩. Microanalysis of the composition of heterostructures with MBL was carried out by EDS technique using a Bruker XFlash 6TI30 solid-state energy-dispersive X-ray detector. A DRON-8 (Bourevestnik, Russia) X-ray diffractometer was used for high-resolution X-ray diffraction measurements. The surface morphology of the metamorphic heterostructures was explored using an AFM Dimension 3100 (Veeco) microscope.

Results and Discussion

Fig. 1, *a* shows a bright-field TEM image of the structure #2. The cross-section in the image corresponds to the {110} crystallographic plane. The image demonstrates that the dense array of MDs is shifted towards the GaAs substrate presumably due to efficient strain relaxation at the initial growth stages of $In_xGa_{1-x}As$ MBL with a large initial indium step (x_{min} = 0.18) and a high grading rate (~90% In/µm) of the graded layer with convex compositional profile.

The sheet of InAs/InGaAs QDs is clearly visible due to the strain contrast. The TDs density in heterostructure #2 can be estimated at a level of $\rho_{TD} \sim 10^7$ cm^{-2}. The In composition profile in structure #2 measured using EDS technique is close to the technologically specified profile (see Fig. 1, *b*). The step in the thickness between points of the profile is as low as ~ 6 nm. To improve the accuracy of the analysis, the specimen was mounted so that its surface, (001) plane, was perpendicular to the first (longitudinal) axis of the TEM double-tilt specimen holder. The holder was tilted at an angle of approximately 15° towards the detector, and a second tilt was used to achieve an orientation at which the (002) and (00-2) reflections were observed with equal intensity in the electron diffraction pattern. This configuration allows for an increase in the level of X-ray signal reaching the detector while still providing sharp boundaries between the layers during measurement. The experimentally measured MBL profile exhibits extended tails near the interfaces with GaAs and inverse layer, which are presumably caused by local overlapping of the regions during measurements.

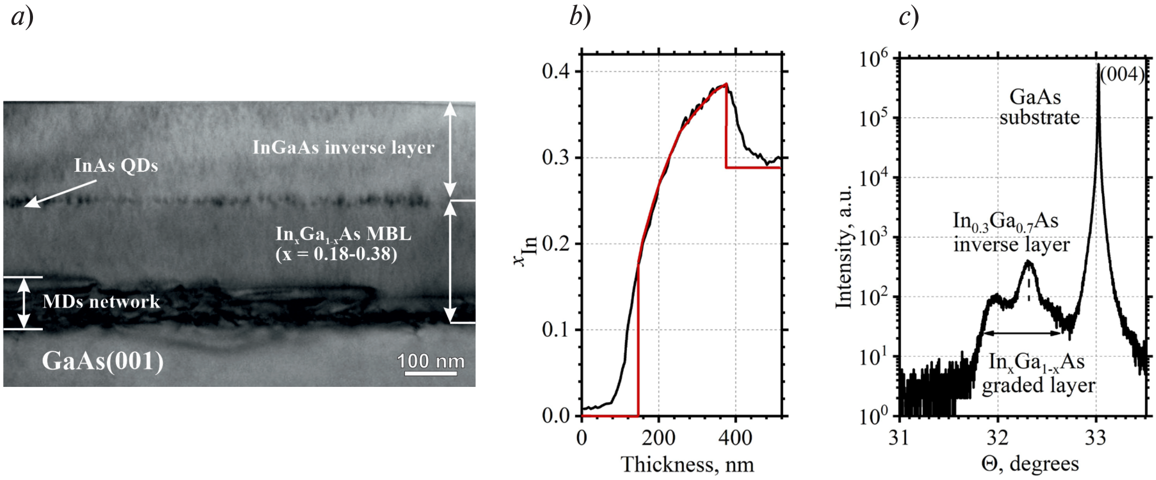

Fig. 1. Bright-field cross-sectional TEM image of the heterostructure #2 obtained in a two-beam diffraction contrast mode with strong excitation of reflection **g** = 2−20 (*a*). In composition profile measured using the EDS technique (black curve) and the technologically specified one (red curve) in structure #2 (*b*). 2θ-ω X-ray diffraction curve around GaAs (004) symmetric reflection (*c*)

Fig. 1, *c* shows the diffraction curve measured around the GaAs (004) reflection for the same structure. The narrow peak near θ ≈ 33.03° corresponds to the (004) reflection of GaAs, while the broad peak at smaller angles originates from the $In_xGa_{1-x}As$ MBL. The asymmetric shape of this peak is a direct indication of a non-linear composition profile of the graded layer [5]. The intense peak at θ ≈ 32.3° corresponds to the inverse layer.

The surface morphology and roughness of the samples were characterized by AFM. Surface roughness is one of the main criteria for the optimization of MBL because it has a significant impact on InAs QDs growth. The AFM topographical images for all the studied structures with a surface area of 100×100 μm are shown in Fig. 2. It can be seen that all structures are characterized by a “cross-hatch” morphology with surface corrugations along the ⟨110⟩ directions. This morphology is a sign of a two-dimensional growth mode and is usually associated with the formation of a network of MDs, since the average period of surface undulations corresponds to the separation of MDs projected into the interface [6]. A.M. Andrews et al. proposed a model according to which the cross-hatch is associated with the formation of an array of MDs and, accordingly, with the appearance of steps on the growth surface due to the gliding of TDs [7]. The asymmetric character of the surface undulations reflects the asymmetric distribution of MDs and is caused by the anisotropic surface migration of In adatoms in two mutually perpendicular directions [110] and [1−10]. The root mean square (RMS) surface roughness exhibits a rise from 2.89 nm to 4.23 nm with increasing substrate temperature, which agrees well with previous works showing that the surface roughness associated with cross-hatch may be reduced by low-temperature growth [8]. In segregation is important even at a growth temperature of T_S = 380 °C. To reduce the effect of In segregation on the surface, the V/III flux ratio should be increased with increasing T_S.

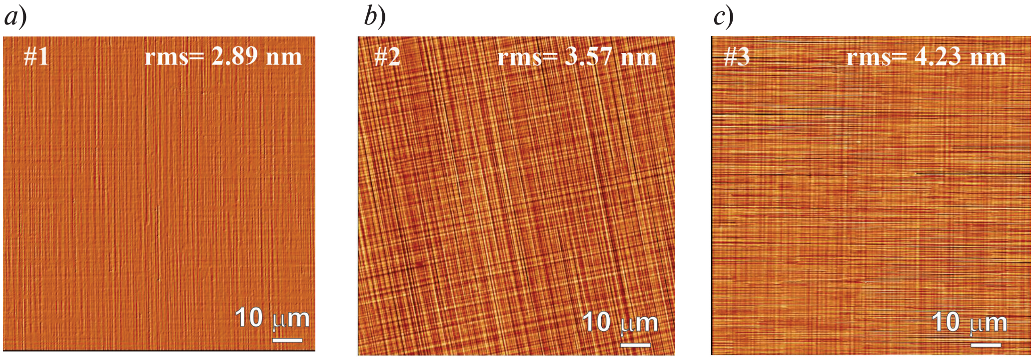

Fig. 2. AFM topographical images for structures #1 (*a*), #2 (*b*) and #3 (*c*).
The dimensions of the surface area are 100×100 μm

RSMs are commonly used to estimate the state of strain and crystallographic tilt in heterostructures with MBLs. Fig. 3 demonstrates the X-ray diffraction reciprocal space maps measured for both symmetric (004) and asymmetric (224) reflections in grazing exit geometry for the structure #2. The symmetric (004) RSMs were measured for two orthogonal azimuth angles perpendicular to $\langle 110 \rangle$ directions designated here as $\Phi = 0^\circ$ and $\Phi = 90^\circ$.

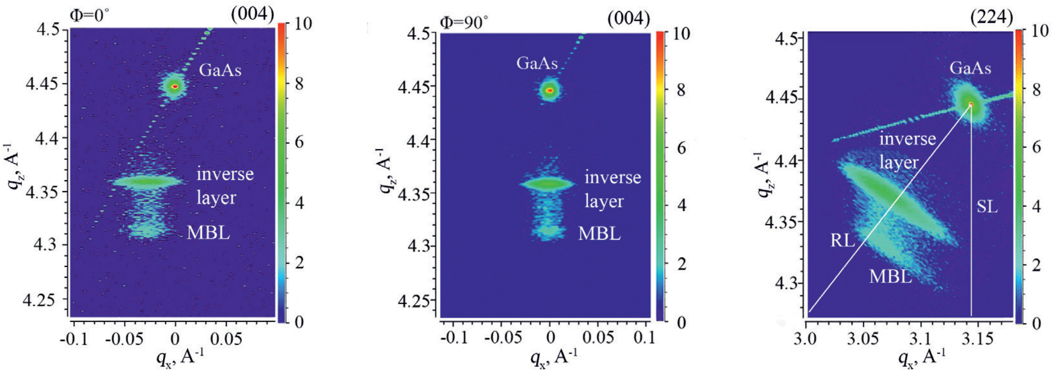

Fig. 3. The reciprocal space maps for both symmetric (004) (*a*, *b*) and asymmetric (224) reflections (*c*) measured in grazing exit geometry for the structure #2

RSMs demonstrate three clearly resolved peaks. The peak with the highest qz coordinate corresponds to the GaAs substrate, and the second most intense peak corresponds to the inverse InGaAs layer. The graded layer in Fig. 3, *a* and Fig. 3, *b* appears as a less intense band extending along the q_z axis. The peak with the lowest q_z coordinate is associated with the upper part of the graded layer due to the lower grading rate in the upper part of the MBL with a convex composition profile. The shift of the peaks from inverse and MBL layers along the q_x axis in symmetrical RSMs reflects the crystallographic tilt of these layers with respect to the GaAs substrate. The tilt arises due to an imbalance of MDs with positive and negative tilt components because of an imbalance in the dislocation populations on the various slip systems [9]. The broadening of the peaks in the direction perpendicular to the scattering vector (i.e., perpendicular to the vertical line) is associated with the mosaicity of the crystal.

The asymmetric (224) RSM is shown in Fig. 3, *c*. The RL denotes the relaxation line, which shows the positions of fully relaxed $In_xGa_{1-x}As$ alloys with different lattice constants in reciprocal space. The SL line shows a set of elastically strained alloys with in-plane lattice constants equal to the lattice constant of GaAs. The center of the peak corresponding to the MBL is close to the RL line, indicating the lattice relaxation around 90–95%. The q_x coordinate of the MBL and inverse layers are the same, indicating that the in-plane lattice constants of these layers are equal. In other words, the inverse layer is coherently grown on the relaxed MBL layer.

Conclusions

To summarize, heterostructures with ultrathin $In_xGa_{1-x}As/GaAs(001)$ MBLs with a convex composition profile were grown by MBE and studied using structural characterization techniques. AFM images of all studied structures reveal a cross-hatch morphology, confirming the two-dimensional growth mode during MBE. The RMS surface roughness increases with increasing substrate temperature, indicating that low-temperature MBL growth is preferable for the subsequent deposition of InAs/InGaAs QDs to create single photon emitters in the telecom O-band or C-band. RSM maps show that strain relaxation in ultrathin $In_xGa_{1-x}As/GaAs(001)$ MBL layers is partially achieved by layer tilting. The inverse layer is well matched to the upper part of the MBL.

Acknowledgments

TEM and AFM studies were carried out using the equipment of the Federal Center for Collective Use "Materials Science and Diagnostics in Advanced Technologies".

REFERENCES

1. **Sorokin S.V., et al.,** High-resolution X-ray diffractometry and topography of metamorphic buffers for III–V quantum well heterostructures, JETP Letters. 121 (1) (2025) 35–40.

2. **Scaparra B., et al.,** Compositionally graded InAlGaAs buffers for mid-infrared photonic devices, Materials for Quantum Technology. 3 (2023) 035004.

3. **Sittig R. et al.,** Strain engineering of optical properties in metamorphic nanophotonic structures, Nanophotonics. 11 (6) (2022) 1109–1116.

4. **Sorokin S.V., et al.,** Structural and transport characteristics of metamorphic InAlAs/InGaAs quantum wells, JETP Letters. 120 (9) (2024) 668–674.

5. **Bowen D.K., Tanner B.K.,** High Resolution X-Ray Diffractometry and Topography, 1st edition, CRC Press, London. (1998).

6. **Capotondi F., et al.,** Strain induced effects on the transport properties of metamorphic InAlAs/InGaAs quantum wells, Thin Solid Films. 484 (1–2) (2005) 400–407.

7. **Andrews A.M., et al.,** Modeling crosshatch surface morphology in growing mismatched layers. Part II: Periodic boundary conditions and dislocation groups, Journal of Applied Physics. 95 (11) (2004) 6032–6047.

8. **Choy H.K.H., Fonstad C.G.Jr.,** Effects of substrate temperature on the growth of InGaAs compositionally graded buffers and on quantum well structures grown above them, Journal of Vacuum Science & Technology B. 23 (5) (2005) 2109–2113.

9. **Kumar R., Biswas D.,** Strain relaxation and dislocation phenomena in metamorphic semiconductor buffers, Crystal Research and Technology. 51 (2016) 723–731.

THE AUTHORS

LAKUNTSOVA Olga E.
o.e.lakuntsova@mail.ioffe.ru
ORCID: 0009-0003-4202-9514

KLIMKO Grigorii V.
Klimko@beam.ioffe.ru
ORCID: 0000-0001-8893-7751

SEDOVA Irina V.
irina@beam.ioffe.ru
ORCID: 0000-0002-9540-0933

MYASOEDOV Alexander V.
a.v.myasoedov@mail.ioffe.ru
ORCID: 0000-0003-2706-7240

SEMENOV Alexey N.
semenov@beam.ioffe.ru
ORCID: 0000-0002-0719-0236

PRASOLOV Nikita D.
nikpras@mail.ioffe.ru
ORCID: 0000-0002-7519-9208

SOROKIN Sergey V.
sorokin@beam.ioffe.ru
ORCID: 0000-0003-0320-2233

Received 15.12.2025. Approved after reviewing 09.02.2026. Accepted 20.02.2026.