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Analysis of (Al)GaAs/Si buffer structures using photoluminescence measurements

© S.O. Slipchenko, V.V. Shamakhov, D.N. Nikolaev, E.V. Fomin, M.I. Kondratov, N.A. Pikhtin

Ioffe Institute, St. Petersburg, Russia
E-mail: serghpl@mail.ioffe.ru

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AlGaAs photoluminescent structures were grown on a Si substrate by metal-organic chemical vapor deposition. It was shown that the incorporation of bulk (Al)GaAs layers and AlGaAs/GaAs superlattices into the GaAs buffer layer degrades the root-mean-square surface roughness and photoluminescence intensity compared to a GaAs buffer without such inserts. An assessment of the residual strains in the structure was also performed based on photoluminescence data. It was shown that the use of AlGaAs inserts in the GaAs buffer layer increases the residual strains in the structure.

Keywords: MOCVD, buffer layers, silicon substrate, photoluminescence, residual strain.

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The technology of the heterogeneous epitaxial growth of semiconductor heterostructures is critical from the practical point of view for micro- and optoelectronics. In particular, the approaches are quite well-developed for the growth of AlGaN transistor structures on Si substrates. The relevance of development of the technology for the heterogeneous epitaxy of heterostructures in the solid solution system Al−Ga−In−As depends on the demand for the sources of laser radiation in the infrared area of the spectrum, which are integrated with the „silicon-on-insulator“ platform in a monolithic manner. However, the development of such sources of laser radiation is associated with some problems. The first problem is related to the difference in the polarity of the materials A^3B^5 and Si, causing the appearance of the antiphase boundaries. This problem is solved successfully using misoriented Si substrates [1]. The second problem is related to the substantial difference in the periods of crystalline lattices and thermal expansion coefficients (TEC) of materials A^3B^5 and Si. As a result the grown epitaxial layers A^3B^5 have multiple defects of various types (threading dislocations, packaging defects) and are also characterized by higher surface roughness. One of the approaches to solving this problem is based on using dislocation filters [2].

The quality of epitaxial structures created for the optoelectronic instruments depends on both the threading dislocation density (TDD) and the root mean square roughness (RMSR) of the surface. In this case the photoluminescent (PL) properties of the layers may be seen as the integral characteristic of the structure accounting for TDD and MSR. In some papers the authors use the analysis of PL-properties of buffer layers [3,4]. However, such approach in the analysis of the bulk layers is not effective due to diffusion erosion of the concentration profile of the photogenerated charge carriers in a thick bulk layer, which causes reduction in intensity of optical radiation. This paper analyzes the optical characteristics of the buffer layers grown on the Si substrate with the approach based on using a simple PL-structure, which is included as an additional part of the overall structure of the (Al)GaAs/Si buffer structure.

This paper continues the cycle of the studies dedicated to the development of the technology of heterogeneous epitaxy of heterostructures based on the system of solid solutions Al−Ga−In−As on Si substrates. In [5] we demonstrated the possibility to develop simple buffer structures based on GaAs, grown on the Si substrate using the method of metalorganic vapor phase epitaxy. The proposed paper is aimed at analysis of the impact of additional elements in the buffer structure design as inserts from bulk layers of AlGaAs or superlattices AlGaAs/GaAs at the main characteristics: surface morphology and PL spectrum as the integral parameter of optical characteristics of epitaxial layers grown on the selected buffer structure.

The experimental heterostructures were grown by the method of metalorganic vapor phase epitaxy in a unit with a vertical turbodisc reactor. The growth was implemented on Si (001) substrate with misorientation 4° in direction [110]. The reagents of the third group elements were trimethylgallium and trimethylalunimum, and of the fifth group elements — arsine. Hydrogen was used as the carrier gas. Three types of heterostructures were grown for the studies on the Si substrate, and one reference heterostructure was grown on the GaAs (001) substrate. The first type of the heterostructure included a buffer GaAs layer with the thickness of $2\,\mu$m. The growth was carried out as the temperature increased from 400 to 650 °C. Further a PL part was grown on the GaAs buffer layer, which included wide-band claddings from $Al_{0.2}Ga_{0.8}As$ with thickness of $0.5\,\mu$m each and a narrow-bandgap GaAs layer with thickness of $0.4\,\mu$m, placed between the wide-band plates. Using

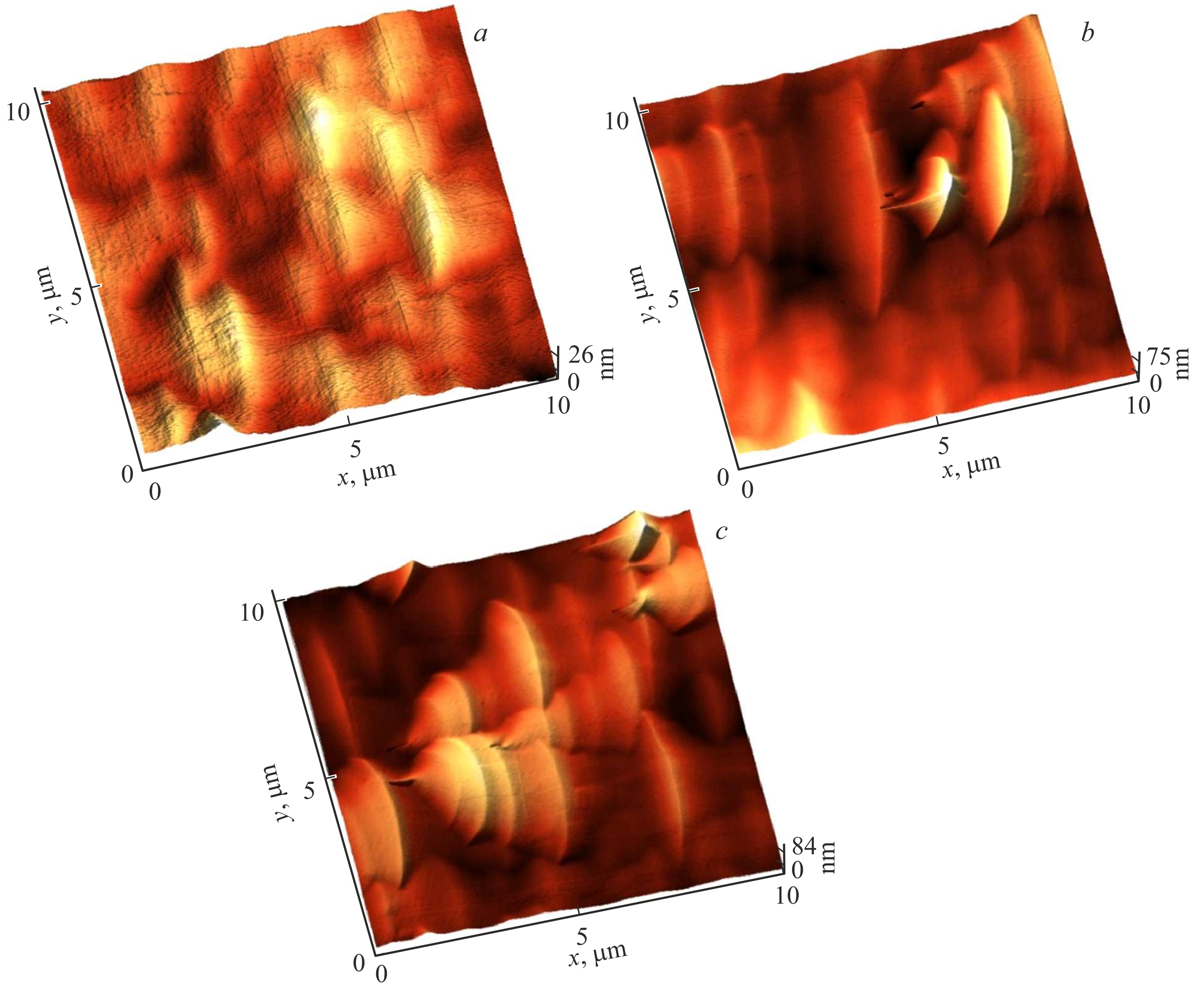

Figure 1. AFM-images of the surface of heterostructures grown on Si substrate: *a* — of the first type, *b* — of the second type, *c* — of the third type. Area of image scanning $10 \times 10\,\mu\text{m}^2$.

wide-band plates makes it possible to limit the diffusion of the photogenerated charge carriers only in the narrow-bandgap layer, therefore increases the efficiency of carrier collection, and, accordingly, increases the concentration of carriers and intensity of radiative recombination. The thickness of the narrow-bandgap GaAs layer in the PL-part of the structure was selected based on the fact that it should provide for the good localization of the charge carriers, but no effects of dimensional quantization must be observed in the layer to simplify further assessment of the residual thermal stresses. Fig. 1, *a* shows the image of the first type heterostructure surface made by the method of atomic force microscopy (AFM) in the surface area $10 \times 10\,\mu\text{m}^2$. The measured value of the MSR was 3.35 nm. Fig. 2 presents PL spectra for all studied heterostructures measured at the room temperature. For all samples the level of optical pumping was identical and amounted to 25 mW. For the structure of the first type the maximum of the PL spectrum corresponds to the wavelength 879 nm (curve *1* in Fig. 2). When the heterostructure of the second type was developed, the buffer design was amended: with the preservation of the total thickness of the buffer $2\,\mu\text{m}$, four superlattices AlGaAs/GaAs of five periods each were included therein. The used buffer design differs substantially from the classical dislocation filters that are stressed superlattices. In this case AlGaAs was used on purpose, having low mismatch of the lattice with GaAs, in order to assess the contribution of the aluminum-containing layers. Further the PL part was grown on the buffer structure, the design of which was identical to that used in the heterostructure of the first type. Fig. 1, *b* shows the AFM image of the second-type heterostructure surface made in the surface area $10 \times 10\,\mu\text{m}^2$. The measured value of MSR was 10.3 nm, which is noticeably higher than the value obtained for the heterostructure of the first type. The PL spectrum of the second type heterostructure is shown in Fig. 2 (curve *2*). The maximum of the PL spectrum is displaced to the long-wavelength area relative to the first type heterostructure and falls upon the wavelength of 881 nm. Besides, the PL intensity of the second type

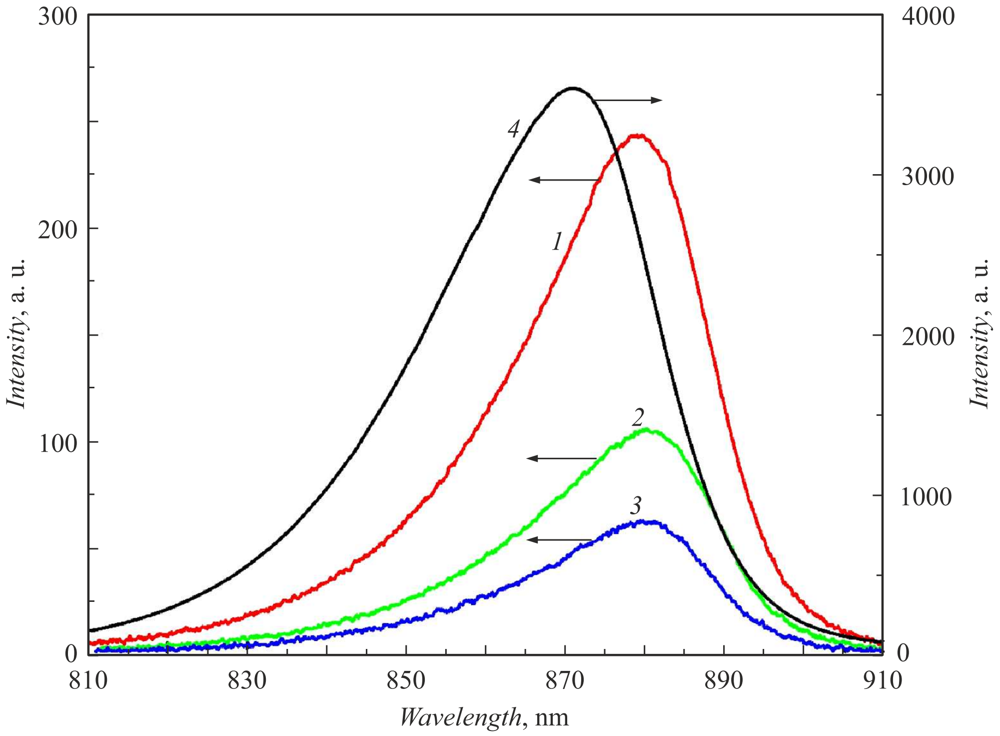

Figure 2. PL spectra measured at room temperature for heterostructures of the first (*1*), second (*2*) and third (*3*) types grown on the Si substrate, and also a reference heterostructure (*4*) grown on the GaAs substrate.

heterostructure is 2.5 times lower compared to the PL intensity of the first type heterostructure. In the third type heterostructure the superlattices were replaced with the bulk AlGaAs layers, and the total thickness of the buffer and the design of the PL-part remained unchanged. Fig. 1, *c* shows the AFM-image of the third type heterostructure surface made in the surface area $10 \times 10\,\mu\text{m}^2$. The measured value of the MSR was 12.8 nm, which is higher than the values obtained for the heterostructures of the first and second types. The PL spectrum of the third type heterostructure is shown in Fig. 2 (curve *3*). You can see that the maxima of PL spectra for heterostructures of the second and third types have coincided (881 nm). However, the PL intensity of the third type heterostructure has become even lower: 5 times relative to the first-type heterostructure and 2 times relative to the second type heterostructure. The obtained results demonstrate that the modification of the design of the buffer layer due to the inclusion of aluminum-containing layers causes noticeable improvement in the roughness of the surface and reduction of the PL intensity. Based on the obtained data, one may conclude that the increased roughness of the surface deteriorates the PL properties of heterostructures. The possible cause for the decrease in the PL intensity was related to the fact that the increase in the surface roughness results in the fact that the surface irregularities may increase the quantity of the light scattering centers. Besides, the significant roughness of the surface may be the source of appearance of the defects being the centers of nonradiative recombination. Such MSR effect on PL intensity was observed in [6]. Besides, data on PL intensity decrease may indicate TDD growth. This thesis is confirmed by the studies conducted in [4,7], where it is shown that the PL spectrum intensity is directly related to the TDD in the structure. Therefore, the reduction in the PL intensity may be related to two factors: TDD and MSR increase.

To analyze the PL properties, a reference heterostructure was also made, which was grown on the GaAs (001) substrate and included only the PL part identical in design of the PL part of heterostructures grown on the Si substrate. Fig. 2 (curve *4*) provides the PL spectrum of the reference heterostructure. From Fig. 2 you can see that the PL spectra of the first, second and third type heterostructures are displaced to a long-wavelength area relative to the PL spectrum of the reference heterostructure (maximum of the PL spectrum of the reference heterostructure falls on the wavelength of 871 nm). This indicates that the heterostructures grown on the Si substrates have residual stresses. Since the wavelength of heterostructures grown on the Si substrate is displaced to the long-wavelength area relative to such for the unstressed reference heterostructure, one may conclude that these heterostructures experience tensile strain in the parallel plane of the heterostructure interface (ε_x). The tensile strain occurs in cooling of the heterostructure after the epitaxy due to significant difference of the TEC of the GaAs layer and the Si substrate [8]. Such behavior of the PL spectra was observed in papers [3,4]. In [3] in the PL spectrum at room temperature the strong peak is observed from the transition between the electrons and heavy holes, and also a long-wavelength arm that practically merges with the main peak. The long-wavelength arm is related to the transitions between electrons and light holes as a result of degeneracy removal for the holes in the valence band due to residual stresses. Besides, if the temperature of the PL spectra measurement decreases, the intensities of transitions are redistributed, and the peaks are separated as a result of higher stresses. In [4] in the PL spectra at room temperature no long-wavelength arm is observed, as in our case. The stronger intensity of the peak related to the transition between the electrons and heavy holes with the temperature increase is caused by thermal activation of holes from the subband of light holes into the subband of heavy holes. This may result in the fact that the arm from the transition between the electrons and light holes may not be seen at room temperature. This is related to the fact that residual stresses in the structure are low, and as the degeneracy of the holes in the subband of light and heavy holes is removed, are energetically spaced by a small value. It should also be noted that the PL intensity of the best heterostructure grown on the Si substrate is 14 times lower than in the case of the reference heterostructure.

Based on the PL spectra, the residual strain was analyzed ε_x in the heterostructures of the first, second and third types. In the calculations we proceeded from the assumption that the observed maximum of the PL spectrum is related to the transition between the conduction band and the subband of heavy holes. The calculations were carried out within the framework of the model-solid theory [9,10].

The strain along the ε_z growth axis is related to the strain in the parallel plane of the ε_x heterostructure interface:

$$\varepsilon_z = -2\frac{C_{12}}{C_{11}}\varepsilon_x, \tag{1}$$

where C_{ij} — material elasticity constants.

Transition energy between the conduction band and the subband of the heavy holes (E_{e-hh})

$$E_{e-hh} = E_0 - \Delta E_{hy,v} + \Delta E_{hy,c} - \Delta E_{hh}, \tag{2}$$

where E_0 — width of the band gap of the unstressed GaAs or the maximum energy of the PL spectrum for the reference heterostructure (1.424 eV); $\Delta E_{hy,v}$, $\Delta E_{hy,c}$ — shift of edges of the valence band and the conduction band related to the hydrostatic component of the strain; ΔE_{hh} — displacement of the subband of heavy holes related to the shift component of deformation.

Selecting ε_x, we obtain the energy values corresponding to the maxima of the PL spectra for the samples of heterostructures of the first, second and third types (Fig. 2). For the calculations, the formulae and constants were used from paper [10]. The following values ε_x were obtained from the calculations: for the heterostructures of the first type (879 nm) — $2.3 \cdot 10^{-3}$, second/third type (881 nm) — $3 \cdot 10^{-3}$.

The conducted studies have shown that the use of the PL part in the heterostructures grown on the Si substrate makes it possible to obtain the integral characteristic of the optical quality and conduct the benchmarking relying on the reference structure made on the GaAs substrate. The obtained results correlate with the MSR estimate of the surface obtained in AFM-measuments. In particular, use of aluminumcontaining layers in the buffer design causes higher MSR and lower PL intensity. Besides, the position of the PL spectrum maximum makes it possible to estimate the residual mechanical strains in the structure, which arise from the TEC difference in the Si substrate and (Al)GaAs layers. For the developed heterostructures the residual strains ε_x are in the range of $(2.3-3) \cdot 10^{-3}$, and they somewhat increase due to the inclusion of the aluminum-containing layers into the buffer design.

Conflict of interest

The authors declare that they have no conflict of interest.

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