Interpretation of photoluminescence spectra of metamorphic InAlAs/GaAs heterostructures

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Abstract. The results of analyzing the photoluminescence spectra of metamorphic In_{0.75}Al_{0.25}As/In_{0.95}Al_{0.05}As/GaAs heterostructures grown by molecular-beam epitaxy method are presented. In the spectra of low-temperature photoluminescence, three emission peaks have been detected, which correspond to carrier recombination in different areas of the structure. These include a part of the In_{0.75}Al_{0.25}As “virtual substrate” grown at high temperature, and the area of a triangular potential well formed by the metamorphic buffer layer and the “virtual substrate”. Photoluminescence related to defects in the high-temperature part of the “virtual substrate” was also measured.

1. Introduction and samples

InAs and its alloys are some of the most demanded materials for creating microwave transistors, as well as devices for mid-wavelength infrared optoelectronics. The growth of the epitaxial layers of these materials on a GaAs substrate is carried out using a metamorphic technology [1]. GaAs substrates, compared with another substrates of the III-V group, have a number of advantages such as higher reliability, low cost and large available plate sizes (100-150 mm) [2].

The purpose of this study is to analyze the obtained photoluminescence spectra of the In_{0.75}Al_{0.25}As/In_{0.95}Al_{0.05}As/GaAs metamorphic heterostructures and evaluate the effect of low-dimensional effects on the samples under study.

The samples were grown by molecular beam epitaxy (MBE) method in the Ioffe Institute (Russian Academy of Sciences). In table. 1, the sequence of layers of the structures under study can be seen. Due to the large mismatch of the lattice constants of the GaAs substrate and the subsequent In_{0.75}Al_{0.25}As layer, called the “virtual substrate”, it is impossible to grow the epitaxial layer directly, since the relaxation of strain will lead to the large number of defects in the active layer of the future device. Therefore, metamorphic buffer layer (MBL) In_{0.05}Al_{0.95}As was used to grow such structures. This layer matches the substrate with the subsequent layer by gradually changing the lattice parameter. Metamorphic technology allows to obtain a “virtual substrate” with the required lattice parameter, which serves as a basis on which the active layers are grown [3]. In fig. 1 the band structure of one of the samples is shown, as provided by a calculation taking the strain into account [4].

Table 1. Structure of the studied samples

| Sequence of layers                     | Sample #1 | Sample #2 | Sample #3 |
|----------------------------------------|-----------|-----------|-----------|
| High-temperature part of the “virtual substrate” In_{0.75}Al_{0.25}As | 140       | -         | 1030      |
| InAs                                   | 1         | -         | 1         |
| Low-temperature part of the “virtual substrate” In_{0.75}Al_{0.25}As | 20        | 100       | 20        |
| Metamorphic buffer layer In_{0.95}Al_{0.05}As | 1200      |           |           |
| Buffer layer GaAs                      | 200       |           |           |
| Semi-insulating GaAs (001) substrate   | 3*10^5    |           |           |
2. Experiment and results
The samples were examined by the low-temperature (from 10K to 80K) photoluminescence method using an experimental setup based on the VERTEX 80 Fourier transform infrared spectrometer (FTIR). This method is chosen because it is highly sensitive and non-destructive. It does not require special preparation of the samples for the measurements. In fig. 2 a typical PL spectrum of the sample #1 is shown.

![Figure 1. Band diagram of the sample #1 indicating the transition energies of the In0.75Al0.25As/In0.05.0.8Al0.95.0.2As/GaAs heterostructure.](image1)

Three peaks of radiation characteristic for most of the samples, corresponding to charge carrier recombination in different areas of the structure, were observed.

2.1. Interpretation of the peak with the energy of 1.055 eV
It was assumed that this peak corresponds to the charge carrier recombination in the area of a triangular potential well formed by the upper part of the metamorphic buffer layer and the “virtual substrate” (see Fig.1). The transition energy is close to the calculated value of 1.044 eV. The shift towards higher energies as compared to the calculated value can be associated with the quantization of the charge carriers in the triangular potential well. The well width (L=160 nm) is comparable to the de Broglie wavelength in the corresponding material at T = 10 K. On an inset of Fig. 1, the first quantization level is shown. One upper level also exists, but it is situated close to the continuum. An unusual feature of this heterostructure is that, unlike the conventional single heterojunction and metal-oxide-semiconductor (MOS) structures, quantum wells are present for both electrons and holes. Therefore, the observed increase in the energy of the PL peak above the calculated value might be explained by low-dimensional effects. In addition, under the influence of unaccounted residual compressive strain [5], the band gap of the upper part of the MBL also increases.

In fig. 3 typical PL spectra of the structure under study depending on the pumping laser power is shown. This behavior of the peaks’ intensity is typical for all the samples studied. It can be seen that the width at half-maximum of the 1.055 eV peak under consideration weakly depends on power: 17.4 meV at P=17 mW and 22 meV at P=380 mW, and the position of the peak does not change.

The peak intensity increases almost linearly in log scale with increasing pump power (Fig. 4), which is typical for direct interband transitions in quantum wells. Similar behavior was also observed in a number of other papers [6], [7].

In fig. 5, it can be seen that as the temperature increases, the spectrum is expected to shift to lower energies. The peak with an energy of 1.055 eV is absent at a temperature above 30 K. This is due to the fact that the charge carriers accumulated in the quantum well receive sufficient kinetic energy to overcome the potential barrier and leave it.

A comparison was made for the samples with different maximum composition x_max of the metamorphic buffer layer [3]: 0.77 for a sample #4, 0.79 for #5, 0.81 for #6 and 0.83 for #7. In fig. 6 the PL spectra of these samples are shown. In this series of samples, an active region was grown on the “virtual substrate” [8].
As it can be seen in Fig. 6, the peak under consideration is the most intense in each of the PL spectra of these samples. The shift of the peak with the decrease in the inverse step towards higher energies is explained by an increase in the band gap of the solid solution of the final MBL composition. The decrease in the intensity of this peak with that in the maximum composition $x_{\text{max}}$ can be explained by reduction of the quantum well depth.

### 2.2. Interpretation of the 1.144 eV peak

The samples shown in Fig. 7 differ from each other by the absence (sample #2) of the high-temperature part of the “virtual substrate” and its presence (sample #1).

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The PL spectrum shows that for the sample #2 the peak is not observed. Thus, it can be assumed that the peak with an energy of 1.044 eV corresponds to carrier recombination in the high-temperature part of the “virtual substrate”. In fig. 8 the PL spectra of the samples with different thickness of this layer are shown: 1030 nm for the sample #3 and 140 nm for the sample #1. As it can be seen, the peak of the sample with a thicker layer was 4.5 times more intense in amplitude than that of the sample with a thinner layer. The assumption that this peak corresponds to the high-temperature part of the “virtual substrate” is also confirmed by the calculation of transition energy. This value was 1.129 eV. The shift of the peak position of the PL spectrum towards higher energy is explained by the effect of residual compressive strain in the “virtual substrate”. In the PL spectrum, a shift of the peak position to lower energies can be seen. It can be explained by a smaller effect of residual compressive strain on the thicker layer and, accordingly, a smaller increase in the band gap of the “virtual substrate” than in the sample #1.

This conclusion corresponds to previous studies by other authors. For example, in [9], it is seen in the PL spectra that for the sample in which an additional layer of the “virtual substrate” at a higher temperature was grown, another photoluminescence peak appears. In [10], [11], where identical InAlAs/GaAs structures were studied, the presence of a similar peak of the “virtual substrate” is mentioned.

2.3. Interpretation of the 0.998 eV peak
The power dependence of the 0.998 eV peak is shown in Fig. 9. It can be seen that this peak behaves sublinearly and at a sufficiently high power goes into saturation. The temperature dependence of the peak width at half-maximum (Fig. 10) has also been considered.

![Figure 9](attachment:figure9.png)

**Figure 9.** Dependence of the 0.998 eV peak intensity on the pump power for the sample #1.

![Figure 10](attachment:figure10.png)

**Figure 10.** Dependence of the 0.998 eV peak width at half-maximum on the temperature for the sample #1.

This dependence is typical for optical transitions through defect levels. In [7], it is concluded that the estimated peak corresponds to the PL caused by the presence of defects in the area of the metamorphic buffer layer. However, Fig. 7 shows that there is no peak with an energy of 0.998 eV for the sample #2 (for which the high-temperature part of the “virtual substrate” has not been grown). This allows us to suggest that this PL is related to the presence of a defect in the high-temperature part of the “virtual substrate”.

3. Conclusion
Thus, we analyzed the photoluminescence spectra of the structures under study, which showed three typical PL peaks for all samples. The possible regions of the heterostructure in which carrier recombination occurs were determined. The observed shift in the experimental energy values in comparison to the calculated ones was explained by the effect of mechanical compressive strain, as well as low-dimensional effects in the structures.

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