08

Modeling and Experimental Study of AlGaAs/GaAs Structures for Infrared Detector Implementation

© A.S. Dashkov,[1,2] S.A. Khakhulin,[1] N.A. Kostromin,[1,2] D.A. Barykin,[1] O.S. Komkov,[1] E.V. Pirogov,[2] M.S. Sobolev,[2] L.I. Goray,[1,2,3,4] A.D. Bouravleuv[1,3,5]

[1] Saint Petersburg Electrotechnical University „LETI"
197022 St. Petersburg, Russia
[2] Alferov Federal State Budgetary Institution of Higher Education and Science Saint Petersburg National Research Academic University of the Russian Academy of Sciences,
194021 St. Petersburg, Russia
[3] Institute for Analytical Instrumentation of the Russian Academy of Sciences,
198095 St. Petersburg, Russia
[4] Space Research Institute, Russian Academy of Sciences,
117997 Moscow, Russia
[5] Ioffe Institute,
194021 St. Petersburg, Russia
e-mail: dashkov.alexander.om@gmail.com

Received October 27, 2025
Revised December 13, 2025
Accepted December 15, 2025

A theoretical and experimental study of AlGaAs/GaAs multiple quantum well structures intended for mid-infrared photodetectors operating at room temperature has been carried out. Based on theoretical estimates, the primary requirements for the composition, layer thicknesses, and doping levels of the investigated structures were formulated. The electronic band structure, experimentally reconstructed using photoreflectance, was employed to refine the computational model implemented using the finite element method. This made it possible to accurately reproduce the band diagram and energy levels, as well as to determine the parameters required for absorption spectrum calculations. Based on these parameters, absorption spectra were calculated for different doping concentrations, demonstrating an enhancement of the absorption peak intensity with increasing doping level.

Keywords: infrared radiation detectors, AlGaAs/GaAs structures, quantum-confined heterostructures, quantum wells, intersubband transitions, photoreflectance, band diagram.

DOI: 10.61011/TP.2026.04.63273.297-25

Introduction

Modern mid-infrared (IR) detectors ($3-8\,\mu$m) play a key role in various fields, including spectroscopy, safety systems, medical diagnostics and space research [1]. One of the most promising fields of designing the mid-infrared photodetectors is to use quantum-confined AlGaAs/GaAs structures, because it is possible to precisely control an energy spectrum by selecting a thickness, composition and degree of layer doping, and they have higher temperature stability and radiation resistance as compared to HgCdTe-based detectors [1] and are compatible with industrial technologies of heterostructure growth [2,3].

Physical principles of operation of the mid-infrared detectors are based on intersubband transitions, thereby necessitating detailed theoretical modeling and experimental study of an electronic structure and kinetic processes under real operating conditions [3–5]. The present study implements a complex approach to calculation and analysis of detector characteristics, which includes numerical modeling using various theoretical models and experimental verification on grown samples of the structures under study.

Relevance of the study is necessitated by designing the approach to creating structures of the mid-infrared detectors, which provide high efficiency and stable operation in a wide range of the temperatures. Numerical optimization of a design and comparison of calculated data with experimental results made it possible to confirm adequacy of the used models and applicability of the presented comprehensive method for designing various instruments based on quantum-confined heterostructures. The obtained results may serve as a basis for designing the new-generation infrared detectors with improved characteristics for a range of practical applications.

1. Methods of theoretical studies and computational modeling

The electronic structure of the AlGaAs/GaAs quantum wells was calculated using several approaches of numerical modeling: a shooting method within an effective-mass

approximation, a finite element method and based on a solution of a transcendental equation method. The first two cases took into account nonparabolicity of a band structure and influence of an external electric field. Correctness of application of the said methods was validated on calculation of quantum-cascade structures, single quantum wells and super-multiperiod superlattices (SL) [6–8].

Computational algorithms were implemented in languages Python 3.10 and C++ using libraries SciPy [9] and NumPy [10] for solving systems of equations and eigenproblems. Special attention was paid to provision of high accuracy of the calculations. A discretization step and calculation parameters were selected so as to provide numerical stability and minimize approximation errors. In order to estimate stability of the solution when using the shooting method, standard numerical criteria of convergence were applied: control of a maximum residual of boundary conditions and checking stability of the solution when varying the discretization step and the initial conditions. In both the cases, an allowable level of the residual did not exceed 10^{-6}. These criteria make it possible to reliably trace convergence and exclude non-physical eigenstates. For the solution obtained by the finite element method, stability was also controlled via the maximum value of the residual when varying the discretization step; for a final grid, it did not exceed 10^{-6}.

These criteria of accuracy corresponded to requirements that are set when calculating the quantum-cascade structures [6–8]. In case of no convergence at the specified conditions, the solution was considered unsolved, thereby excluding use of unreliable data in further analysis.

2. Experimental studies

Electronic and optical properties of the AlGaAs/GaAs quantum wells were experimentally characterized by using methods of photoreflectance (PR) and photoluminescence (PL) spectroscopy. Photoreflectance is a non-contact method of modulation optical spectroscopy. In this method two beams of radiation are directed at the sample: a spectrometer one, which varies in a wide range of energies and a laser one with photon energy that exceeds a band gap of the structures under study. A laser interrupted at a specified frequency was used to modulate the near surface electric field. This, in turn, makes it possible to identify, against the background of all reflected radiation, those spectral features associated with the resonant absorption of light in semiconductors [11]. A principle of operation of the method is described in detail in the study [7]. This study used a high-stable laser with the wavelength of 405 nm as a source of laser radiation. The same laser was used as a structure excitation source when measuring the photoluminescence spectra.

3. Experimental samples

The studied structures with multiple quantum wells (MQW) were grown by molecular-beam epitaxy on GaAs (100) substrates with *n*-type conductivity. A buffer layer was a GaAs layer of the 200 nm thickness, which was doped with a *n*-type dopant to the carrier concentration of $1 \cdot 10^{18}\,\mathrm{cm}^{-3}$. An active region included 50 periods, wherein each of them consisted of the GaAs quantum well of the 4 nm thickness and the $Al_{0.284}Ga_{0.716}As$ barrier of the 50 nm thickness. Layers of the GaAs quantum wells were additionally doped with the *n*-type dopant to the carrier concentration of $1 \cdot 10^{18}\,\mathrm{cm}^{-3}$. Layer parameters were controlled *in situ* using reflection high-energy electron diffraction, while values of the thicknesses were verified *ex situ* by data of high-resolution X-ray diffraction [12].

4. Results and discussion

4.1. Selection and optimization of parameters of the MQW structure

The active region of the IR radiation detector was designed stage by stage. A target material system was selected to be a $Al_xGa_{1-x}As$/GaAs heteropair, since it makes it possible to grow almost unstressed heterojunction, thereby creating high-quality multi-layer heterostructures that are required for producing high-efficiency light-emitting and absorbing devices. An initial basis was designed as described in the literature [4]. The structure is subsequently updated using methods of numerical modeling, thereby making it possible to refine a geometry of and to optimize parameters of the active region in order to improve theoretical efficiency of operation of a final detector, particularly, an absorption coefficient in this case.

At the stage of modeling and optimization of the design, three different computational methods were used for the calculations: the modified shooting method [6,13], the finite element method [14] and the approximate numerical solution of the transcendental equation [15]. Practically significant and reproducible results could be obtained only in the last case. Limited applicability of the first two approached can be explained by a number of factors. In particular, the modified shooting method, which is often used when calculating quantum-cascade lasers, detectors [16] as well as superlattice and super-multiperiod superlattice structures [7,8], demonstrated no convergence in the problem under study. A key specific feature of the design under study was presence of thick barriers (as compared to the well thickness), which, as the authors believe, mostly affected accuracy of the calculations in this method. As previously noted [17], presence of the thick layers, especially near a starting point of the calculation, results in enhancing of an exponentially increasing component of the solution, which, in turn, degrades accuracy and can result in divergence of the final results. It is a consequence from

the formula (1) for calculating the wave function $\psi_c(z)$ at a specified value of energy E and a step Δz [17]:

$$\psi_c(z+\Delta z) = \Big(\big[(2(\Delta z)^2)/\hbar^2\big(eV_c(z)-E\big) + 1/\big(m^*(z+\Delta z 2, E)\big) + 1/\big(m^*(z-\Delta z/2, E)\big)\big]\psi_c(z) - 1/\big(m^*(z-\Delta z/2, E)\big)\psi_c(z-\Delta z)\Big)m^*(z+\Delta z/2, E), \quad (1)$$

where Δz is a step of a computational grid, V_c is a profile of a conduction band potential, m^* is an effective mass of the electrons, e is the electron charge, z is a coordinate along a structure growth axis.

It seems that when calculating by the finite element method the main problem is related to insufficient accuracy of discretization: the initial grid turned out to be coarse, while its refinement resulted in an increase of computational complexity and made the calculations almost unsuitable for purposes of primary designing of such structures. At the same time, the approach based on the approximate solution of the transcendental equation made it possible to obtain a primary estimate of the structure parameters. Its efficiency is explained by a number of reasons: the method includes a considerably smaller number of the input parameters and by its nature it is the closest tot the analytical one, since it does not require construction of a complete energy diagram of the detector structure, being limited to just calculation of the key energy characteristics and a ratio of effective carrier masses [15]. Besides, the calculations by this method can be performed on a common PC and require slight consumption of computational time.

Originally, the structure was designed with taking into account a specified wavelength of radiation in an assumption that bound-to-continuum transitions are implemented [4]. But during computational modeling and analysis of the published data [1,18], we have found that a diagram of transitions between a bound state and another bound or quasi-bound (near a well edge) state has some significant advantages. In this regard, further calculations included exactly a configuration with the bound and quasi-bound level, whose benefits are described in a section of discussion of numerical modeling results of the absorption spectrum.

The calculation (when $T = 300\,\mathrm{K}$) resulted in determining a target value of a molar fraction of aluminum, which was 0.284, as well as a position of a discrete quantum level that provides the transition from the bound state into the quasi-bound states and the continuum states with transition energy of 0.145 eV (8.5 μm). The obtained theoretical results were verified by experimental study of an energy band diagram of the considered structure by the methods of photoreflectance and photoluminescence.

4.2. Experimental analysis of the energy spectrum

Fig. 1 shows the spectra of photoreflectance (above) and photoluminescence (below) of the GaAs/$Al_{0.284}Ga_{0.716}As$ MQW with the 4 nm width and the barrier thickness of 50 nm.

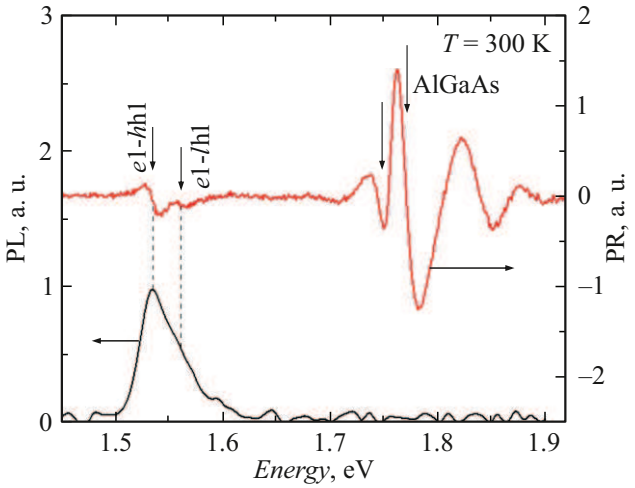

Figure 1. Spectra of photoreflectance (above) and photoluminescence (below) of the sample of the MQW GaAs/$Al_{0.284}Ga_{0.716}As$ (4 nm/50 nm).

The photoreflectance spectrum exhibits intense oscillations in a high-energy region, which are related to a signal from the AlGaAs barrier layer. A spectrum line observed at 1.78 eV corresponds to the band gap (E_g) of the $Al_{0.284}Ga_{0.716}As$ barrier layers ($E_g = 1.78$ eV [19]), which completely agrees with the technologically specified characteristics. The low-energy region in the range 1.5–1.6 eV exhibits two signals that are designated in the figure as $e1-hh1$ and $e1-lh1$. The spectrum line at energy of 1.535 eV corresponds to an interband transition $e1-hh1$ between the first electron level ($e1$) and the first heavy-hole level ($hh1$). At energy of 1.562 eV, there is a transition $e1-lh1$ between the first electron level and the first light-hole level. The obtained data correlate with measurements of the photoluminescence spectra, which also exhibit the described transitions. At energy of 1.75 eV, the photoreflectance spectrum exhibits a specific feature, which can be interpreted as an optical transition between the second heavy-hole level $hh2$ and the second electron level $e2$ that is above an electron barrier potential and related to unbound states [20]. The experimental data are in full agreement with the band structure of the quantum wells considered (Fig. 2), which is calculated by means of the $k\,p$-method within the eight-band Kane model [7]. Based on the performed analysis, we have calculated the energy of an intersubband transitions between the levels $e1$ and $e2$, which determines the wavelength of absorption of the structure under study; the obtained value was 0.149 meV.

4.3. Results of computational modeling

Since the absorption coefficient is one of the key characteristics in creating the photodetectors, additional calculations were performed for its quantitative estimation.

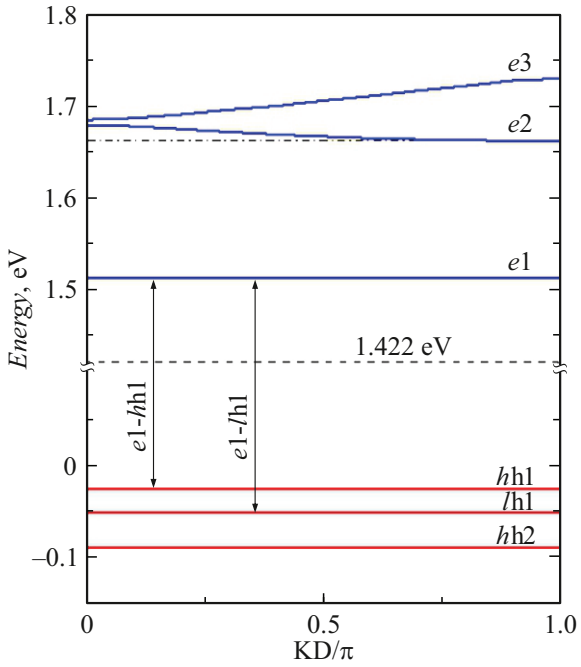

Figure 2. Band structure of the MQW $GaAs/Al_{0.284}Ga_{0.716}As$ (4 nm/50 nm).

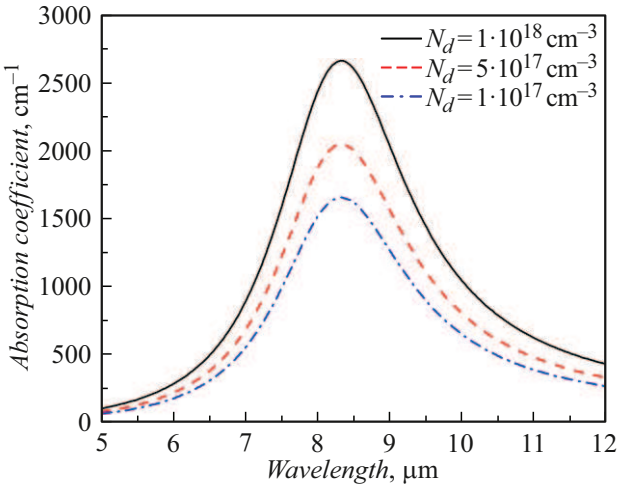

Figure 3. Dependence of the estimated absorption coefficient for the GaAs/AlGaAs MQW structure (4 nm/50 nm) for the different doping degrees at the room temperature.

Based on the experimentally determined electronic structure (conduction band discontinuity, the position of the ground electron energy level), we have refined the model used in the finite element method, thereby making it possible to reproduce the structure energy band diagram using a denser computational grid (5000 nodes per period). In the refined model, the Fermi golden rule was used to calculate probability of transitions between the ground E_1 state and the exited E_2 (quasi-localized and near the barrier edge) state, and the absorption coefficient was estimated based thereon [21,22]:

$$\alpha = \frac{e^2 kT}{2\varepsilon_0 cn\hbar} f_{12} \ln\left[\frac{1+\exp\left((E_F - E_1)/kT\right)}{1+\exp\left((E_F - E_2)/kT\right)}\right] \times \frac{\Gamma/\pi}{(E_2 - E_1 - \hbar\omega)^2 + \Gamma^2}, \quad (2)$$

where n is an average refractive index of the MQW structure, f_{12} is a oscillator strength of the transition under study, E_F is a position of the Fermi level, ω is an angular frequency of incident radiation, $\Gamma = 20$ meV is a full width at half maximum.

As noted previously, the formed band structure makes it possible to implement the transitions between the bound state and the quasi-bound state near the well edge, thereby providing a number of important advantages. First of all, these diagrams are characterized by a narrower absorption spectrum and considerably higher values of peak coefficients, which exceeds by several times the absorption for transitions of different types [18]. It provides higher spectral resolution and sensitivity of the detector, which is critical for devices designed to operate within a narrow wavelength range.

Fig. 3 shows the spectral dependences of the absorption coefficient, which are calculated by means of the numerical model for the various concentrations of the dopants. As expected, with the increase of the doping level there is an increase of intensity of the absorption peak, thereby indicating that it is necessary to use high concentrations of the dopant. The position of the spectrum maximum (8.31 μm) with satisfactory accuracy coincides with the claimed value, while peak value well agrees with the experimental data — discrepancy is $\sim (5-10)\,\%$ for the similar structures [1,18,21,22]. In addition to the numerical analysis, for the diagram under study an analytical estimate can be also obtained in an approximation of the infinite quantum well. For the structure under study, this estimate is about 6000 cm^{-1}, which corresponds to an upper limit value of peak absorption and supports efficiency of the selected configuration.

Conclusion

The study has numerically modeled and experimentally investigated the AlGaAs/GaAs MQW structures designed for mid-infrared photodetectors. The main focus was on modeling and experimental investigation of the electron energy spectrum as well as efficiency of the intersubband transitions that form the absorption spectrum in the structures under study.

The obtained results demonstrated that the approximate model based on the solution of the transcendental equation is an effective tool for primary theoretical description and analysis of the structures under study. Application of this approach makes it possible to specify justified requirements for the layer parameters and to provide satisfactory

agreement of the calculated data with the experimental results. The photoreflectance method confirmed reliability of the obtained calculations and demonstrated high efficiency when determining the electron energy spectrum, thereby making it a promising tool of monitoring the parameters of these heterostructures at the stages of designing and optimizing the infrared detectors. The described studies also included calculation of the spectral dependences of the absorption coefficient using the finite element method based on the data that were refined during the previous theoretical and experimental steps of the study.

The performed study confirmed that the selected parameters of the AlGaAs/GaAs-structures provided formation of the required electronic configuration, while the obtained values of the absorption coefficient satisfactorily agreed with data from the other studies and provided a potential for implementing the infrared detectors designed to operate at the room temperature. It is planned that further studies will comprise additional calculations and experiments, which are aimed at improving sensitivity of the device and reduction of dark current and noise characteristics, thereby enabling effective operation of the photodetector under the operating conditions.

Funding

The studies are supported by the Ministry of Science and Education of the Russian Federation (No. 075-00003-25-04, FSEE-2025-0011).

Conflict of interest

The authors declare that they have no conflict of interest.

References

[1] A. Rogalski. Infrared Phys. Technol., **43** (3), 187 (2002). DOI: 10.1016/S1350-4495(02)00140-8
[2] M.A.O. Hamed. *PhD thesis in Technical Sciences* (Manchester, The University of Manchester, 2006)
[3] A. Rogalski. *Infrared Detectors* (CRC Press, Boca Raton, 2000)
[4] A.M. Filachev, I.I. Taubkin, M.A. Trishenkov. *Tverdotel'naya fotoelektronika: Fotorezistory i fotopriemnye ustroistva* (Fizmatkniga, M., 2012) (in Russian).
[5] V.V. Kopytov, G.V. Akinshina. Nauka. Innov. tekhnol., (in Russian). **43**, 134 (2005).
[6] C. Jirauschek. IEEE J. Quant. Electron., **45** (9), 1059 (2009). DOI: 10.1109/JQE.2009.2020998
[7] A.S. Dashkov, S.A. Khakhulin, D.A. Shapran, G.F. Glinskii, N.A. Kostromin, A.L. Vasiliev, S.N. Yakunin, O.S. Komkov, E.V. Pirogov, M.S. Sobolev, L.I. Goray, A.D. Bouravleuv. J. Semicond., **45** (2), 022901 (2024). DOI: 10.1088/1674-4926/45/2/022701
[8] A.S. Dashkov, L.G. Gerchikov, L.I. Gorai, N.A. Kostromin, A.D. Buravlev. FTP, **57** (5), 321 (2023) (in Russian). DOI: 10.21883/FTP.2023.05.56197.17k
[9] Electronic source. SciPy. *Fundamental algorithms for scientific computing in Python.* Available at: https://scipy.org/ (data of access: 24.10.2025).
[10] Electronic source. NumPy. *The fundamental package for scientific computing with Python.* Available at: https://numpy.org/ (date of access: 24.10.2025).
[11] O.S. Komkov. FTT, **63** (8), 991 (2021). (in Russian). DOI: 10.21883/FTT.2021.08.51146.032
[12] L.I. Goray, E.V. Pirogov, M.S. Sobolev, A.S. Dashkov, M.M. Borisov, S.N. Yakunin, A.L. Vasiliev, P.A. Yunin, A.D. Bouravleuv. Mater. Sci. Semicond. Process., **169** (2024), 107875 (2024). DOI: 10.1016/j.mssp.2023.107875
[13] B. Jonsson, S.T. Eng. IEEE J. Quant. Electron., **26** (11), 2025 (1990). DOI: 10.1109/3.62122
[14] L.R. Ram-Mohan. *Finite element and boundary element applications in quantum mechanics* (Oxford University Press, Oxford, 2002)
[15] L.K. Martinson, E.V. Smirnov. *Kvantovaya fizika*: uchebnoe posobie dlya vuzov (Izd-vo MGTU im. N.E. Baumana, M., 2021) (in Russian).
[16] C. Jirauschek, T. Kubis. Appl. Phys. Rev., **1** (1), 011307 (2014). DOI: 10.1063/1.4863665
[17] P. Harrison, A. Valavanis. *Quantium wells, wires and dots: theoreticall and computation physics of semiconductor nanostructure* (Josh Wiley & Sons Inc., West Sussex, 2016)
[18] B.F. Levine. J. Appl. Phys., **74** (8), R1 (1993). DOI: 10.1063/1.354252
[19] H.C. Casey Jr., M.B. Panish. *Heterostructure Lasers, Part A: Fundamental Principles* (Academic, NY., 1978), Ch. 4, 5.
[20] R. Kudrawiec, J. Andrzejewski, J. Misiewicz, D. Gollub, A. Forchel. Phys. Status Solidi (A), **202** (7), 1255 (2005). DOI: 10.1002/pssa.200460911
[21] M. Helm. *The basic physics of intersubband transitions.* Chapter In *Semiconductors and semimetals,* **62**, 1 (Elsevier, Linz, 1999)
[22] S.D. Gunapala, B.F. Levine, L. Pfeiffer, K. West. J. Appl. Phys., **69** (9), 6517 (1991). DOI: 10.1063/1.348861

Translated by M.Shevelev