REPORT DOCUMENTATION PAGE

Form Approved OMB No. 0704-0188

1. REPORT DATE *(DD-MM-YYYY)* 19-07-2006	2. REPORT TYPE Final Report	3. DATES COVERED *(From – To)* 01-Jul-02 - 13-Mar-07

4. TITLE AND SUBTITLE

Towards Resonant-State THz Laser Based on Strained p-Ge and SiGe QW Structures

5a. CONTRACT NUMBER
ISTC Registration No: 2206

5b. GRANT NUMBER

5c. PROGRAM ELEMENT NUMBER

6. AUTHOR(S)

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5d. PROJECT NUMBER

5d. TASK NUMBER

5e. WORK UNIT NUMBER

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8. PERFORMING ORGANIZATION REPORT NUMBER

N/A

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)

EOARD
PSC 821 BOX 14
FPO AE 09421-0014

10. SPONSOR/MONITOR'S ACRONYM(S)

11. SPONSOR/MONITOR'S REPORT NUMBER(S)
ISTC 02-7003

12. DISTRIBUTION/AVAILABILITY STATEMENT

Approved for public release; distribution is unlimited.

13. SUPPLEMENTARY NOTES

14. ABSTRACT

The main focus of the project is to investigate the possibilities for population inversion between two-dimensional (2D) acceptor states and THz lasing in strained selectively doped SiGe quantum well (QW) structures, as well as the microscopic mechanism of a population inversion in resonant-state p-Ge laser (RSL) and conditions for continuous-wave (cw) operation of RSL and its parameters (the radiation spectrum, the range of frequency tuning, the output power, and the interval of working temperature) in this regime. For this purpose it is proposed:
1. to study the formation of resonant acceptor states; to determine energy spectrum of 2D shallow acceptor states in QWs (as a function of electric field, QW width, doping level, alloy composition, and impurity center position), and 3D resonant acceptor states in p-Ge under stress (as a function of strain); 2. to study radiative transitions between resonant and localized shallow acceptor states split by size quantization and strain in 2D and by stress in 3D; to investigate the possibilities for population inversion between split-off and ground states;
3. to study effect of electric field heating of holes on transport phenomena and THz luminescence; 4. to calculate carrier life times of resonant states, the probability of coherent capture and re-emission processes by resonant states as well as elastic resonant scattering in doped strained 2D structures and in strained bulk p-Ge; to calculate the probabilities of optical transitions between 2D resonant and local states of impurities; 5. to calculate hot-carrier distribution function taking into account resonant-state scattering and to develop theoretical models of population inversion.

15. SUBJECT TERMS
EOARD, Physics, Solid State Physics

16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT UL	18, NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON DONALD J SMITH
a. REPORT UNCLAS	**b. ABSTRACT** UNCLAS	**c. THIS PAGE** UNCLAS		57	**19b. TELEPHONE NUMBER** *(Include area code)* +44 (0)20 7514 4953

Standard Form 298 (Rev. 8/98)
Prescribed by ANSI Std. Z39-18

ISTC 2206p

Final
Project Technical Report
of ISTC 2206p

Towards Resonant-State THz Laser Based on Strained p-Ge and SiGe QW Structures

(From 1 July 2002 to 30 June 2006 for 48 months)

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July 2006

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ISTC 2206p

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(From 1 July 2002 to 30 June 2006 for 48 months)

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1. Abstract.

The main objectives of the project are to investigate the possibilities for population inversion between two-dimensional (2D) acceptor states and THz lasing in strained selectively doped SiGe quantum well (QW) structures; and to realize widely tunable cw lasing in stressed bulk p-Ge.

The stimulated THz emission from boron-doped single-QW Si/SiGe/n-Si structures with optical cavity was realized. The THz emission spectra were obtained. The emission lines are attributed to optical transitions between the resonant and excited localized acceptor states in the QW. The conditions for THz emission excitation were determined.

Stimulated emission of THz radiation was observed in p-Ge under uniaxial stress. The resonator formed by well-parallel sample planes due to total internal reflection was necessary to obtain the stimulated emission. The continuous-wave operation of the p-Ge RSL was demonstrated. The lasing begins at voltages of impurity breakdown. The minimum values of bias voltage and current for lasing were 1V (2V/cm) and 3mA, respectively.

Spectra of photoconductivity (caused by photo-thermo excitation of impurities) and absorption of uniaxially stressed p-Ge were measured. The spectra contain several lines corresponding to different optical transitions between the ground and several excited acceptor states. Pressure dependence of the spectral positions of the lines was determined. The resonant state formation induced by strain in p-Ge was observed directly for the first time.

New theoretical methods of non-variational calculations of the resonant state characteristics have been developed: (i) the method of configuration interaction (PTI) and (ii) direct calculations of the energy spectrum and wave functions of shallow acceptors by means of plane-wave expansion of the acceptor envelope function. Computer programs have been developed for calculation of the acceptor energy spectra, including the resonant states, as well as the resonant capture probability and resonant elastic scattering of holes in stressed p-Ge and strained $Si/Si_{1-x}Ge_x/Si$ QWs. The distribution functions of heavy and light holes and the population of the resonant and localized acceptor states, as well as the optical gain have been found.

Keywords: THz lasing, quantum-well structures, strained semiconductors, resonant acceptor states, absorption, transport.

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ISTC 2206p

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List of contents

1. Introduction (Brief description of the work plan: objectives, expected results, technical approach)

Objectives

The main objectives of the project are to investigate the possibilities for population inversion between two-dimensional (2D) acceptor states and THz lasing in strained selectively doped SiGe quantum well (QW) structures; and to realize widely tunable cw lasing in stressed bulk p-Ge.

For this purpose it was supposed:

1. To resolve the microscopic mechanism of a population inversion in p-Ge resonant-state laser (RSL);

2. To find the conditions for continuous-wave (cw) operation of RSL; to determine the spectrum of stimulated THz emission, the range of frequency tuning, the output power of emitted radiation, and the interval of working temperature;

3. To develop a design and technology of MBE growths of selectively doped SiGe/Si and Ge/GeSi QW structures and of fabrication of QW laser structures;

4. To perform structure characterization by means of different techniques such as X-ray diffraction, atom-force microscopy, transmission electron microscopy, Auger analysis, as well as electrophysical (Hall effect, magnetoconductivity, CV methods) and optical (photoluminescence, Raman scattering) methods;

5. To study the resonant acceptor states in SiGe QWs: to determine their energy spectrum and carrier lifetime as a function of electric field, QW width, doping level, alloy composition, and impurity center position; to find out optical transitions between the resonant and localized states of shallow acceptors in doped 2D structures, to develop non-variational methods of calculations and perform computer simulations;

6. To analyze the possibilities and the conditions for intra-impurity population inversion in SiGe QWs: spontaneous THz luminescence and absorption measurements, transport measurements at low and high electric fields, computer simulation of distribution function of hot carriers at capture-emission carrier exchange between the resonant states and the continuum;

7. To realize and investigate stimulated THz emission from SiGe QW structures; to determine the spectrum of stimulated THz emission, the output power of emitted radiation, and the interval of working temperature.

Expected Results

As a result of the proposed research it was supposed:

1.1. To find the energy spectra, capture and impact ionization rates, optical transition probabilities of 3D shallow acceptor states split by strain;

1.2. To calculate the carrier capture and re-emission probabilities for resonant states, as well as the probabilities of optical transitions between different impurity levels, continuum states and between impurity and the continuum states; to find the distribution function and population of the resonant states; to develop a microscopic model of intra-center inversion for RSL;

2.1. To determine the spectrum of stimulated THz emission, the range of frequency tuning, the output power of emitted radiation, and the interval of working temperature;

2.2. To clear up the role of impurity breakdown, dislocation density, crystallographic direction and resonator quality on a excitation and characteristics of cw operation;

3.1. To grow by MBE SiGe/Si and Ge/GeSi QW structures with different acceptor doping level, profile and alloy composition;

3.2. To develop the design of the SiGe laser structures, including the potential and doping profile and a resonator (it can be the same structure with well-parallel planes or with metallic mirrors);

4. To determine characteristics of MBE grown structures by means of standard methods indicated in p. 4 of previous section;

5.1. To determine the energy spectrum and carrier lifetime of 2D shallow acceptors in SiGe QW as a function of electric field, QW width, doping level, alloy composition, and impurity center position;

5.2. To calculate the probabilities of optical transitions between different 2D impurity levels, continuum states and between impurity and continuum states;

6.1. To clear up the effect of lateral and transverse electric field on the population of 2D resonant states; to find the hot-carrier distribution function from luminescence and absorption spectra;

6.2. To calculate the distribution function of hot carriers taking into account the capture-emission carrier exchange between the resonant states and the continuum, and the resonant state population;

7. To realize stimulated THz emission from SiGe QW structures; to determine the spectrum of stimulated THz emission, the output power of emitted radiation, and the interval of working temperature.

Technical Approach and Methodology

To achieve the project objectives, the following technological, experimental and theoretical methods were employed.

Selectively doped SiGe structures (*task 3*) have been grown at IPM by MBE machines ("Balzers" UMS 500P and "Katun") with solid sources and MBE utilities with sublimation (Si) and gaseous (Ge) sources. The photolitography facilities at IPM, and the equipment for contact deposition at IPM, IRE and PTI have been used to prepare the laser structures.

Structure characterization (*task 4*) have been performed at IPM by means of X-ray diffraction analysis, atom-force microscopy, transmission electron microscopy, and Auger analysis. Hall effect and CV measurements as well as photoluminescence and absorption measurements have been used for the characterization of p-Ge and SiGe/Si structures. Transport and magnetotransport studies of Ga-doped p-Ge and B-doped SiGe/Si QW structures under weak and strong electric fields in the temperature range from 4.2 to 300 K have been performed.

THz radiation spectra (*tasks 2, 5 to 7*) have been studied by means of "Hitachi" grating spectrometer at IRE and FTIR spectrometers at IPM and PTI.

New theoretical non-variational methods have been developed and used for calculation of energy spectrum and lifetime of resonant acceptor states in uniaxially strained semiconductors and two-dimensional structures (*tasks 1, 5 to 7*). PTI theoretical group has developed the method of configuration interaction and IPM group has evolved a direct method of plane-wave expansion of wave functions in a crystal of finite area. They have developed programs for computer simulation based on these theories. For calculation of hot-carrier distribution function with taking into account the resonant states, the Monte Carlo method and direct numerical solution of kinetic equation have been used.

2. Methods, Experiments, Theory

Growth and characterization of SiGe quantum-well structures.

1. The technology of molecular-beam epitaxy of p-SiGe/Si structures for THz lasers was developed at IPM. Test SiGe/Si structures were fabricated by two methods: 1) by sublimation of Si and Ge deposition from a gas source, and 2) electron-beam evaporation of Si and Ge using solid sources. The structures grown by first technique contained 5, 7 and 20 quantum wells with the following parameters: $d_{SiGe} = 350A$, $x = 0.173$, $d_{Si} = 1390A$. The structures were grown on a Si:P(100) substrate ($\rho_{300K} = 10\Omega*cm$). Boron δ-doped layers were placed in the middle of each quantum well. The sheet B concentration determined by the SIMS method was $2*10^{12}cm^{-2}$.

Structures grown by second technique contained a silicon buffer layer, single SiGe quantum well, undoped Si spacer, a B-doped layer and undoped Si layer. The impurity concentration in the doped layer was ~ $2x10^{17}cm^{-3}$. The QW parameters were preliminarily verified by the X-ray diffraction analysis. Both uniformly and selectively doped Ge_xSi_{1-x}/Si(001) structures with single GeSi quantum well have been grown. The selective doping has been done by evaporation of Si doped with boron to 10^{19} cm^{-3}. The structures differed by the SiGe alloy composition and the carrier concentration. According to the SIMS data, the maximum boron concentration in doped layers was $8 \cdot 10^{17}$ cm^{-3}. A change of the hole concentration in the QW was achieved by using one-side (only above the GeSi layer) or symmetric (above and under the GeSi layer) doping.

The following Si/SiGe/Si structures were used:

Multiple-layer (5, 8 and 20 periods) $Si_{1-x}Ge_x$/Si structures with boron doped $Si_{1-x}Ge_x$ quantum wells have been intended for the impurity photoconductivity studies.

The $Si/Si_{1-x}Ge_x$/Si structures with one and three SiGe quantum wells MBE-grown pseudomorphically on n-type Si substrates were used for THz emission, photoluminescence and photoconductivity measurements. The Ge content x in SiGe alloy has varied from 0.07 to 0.48. The structures with three SiGe quantum wells grown on a compensated n-Si substrate were also used.

The relaxed compositionally graded $Si_{1-x}Ge_x$/Si(001) buffer layer with low threading dislocations density have been grown by chemical vapour deposition method. The roughness of surface of the grown structures has been reduced by the chemical and mechanical polishing down to values compared with the roughness of Si(001) substrates. It is shown that the fabricated $Si_{1-x}Ge_x$/Si(001) buffer layers with low threading dislocations density and smooth surface can be used as "artificial substrates" for growth of Ge/Si heterostructures by molecular beam epitaxy.

Boron doped $Si/Si_{0.85}Ge_{0.15}$/Si structures with different thicknesses of undoped Si cap layer varied from 30 to 120 nm were grown at IPM in order to investigate the effect of surface states on THz emission. Single-QW SiGe structures were grown at 550^0C on slightly doped n-type Si(001) substrate by molecular-beam epitaxy using solid sources. Ge and Si were evaporated using electron beam gun. Boron was evaporated from high-temperature effusion sell with self-supporting tungsten filament. SiGe QW of 20 nm thickness was δ-doped in the middle with boron with concentration of $6 \cdot 10^{11}$ cm^{-2}. Two δ-doped B layers were positioned within the buffer and cap layers at the distance of 30 nm from the QW interfaces. According to the capacity-voltage measurements, the residual impurity concentration in undoped layers was less than $5 \ 10^{15}$ cm^{-3}.

Single-QW and triple-QW Si/SiGe/Si structures selectively doped with boron have been MBE grown on Silicon-On-Insulator (SOI) substrate in order to exclude a carrier injection from the substrate into SiGe QW. Structure parameters verified by means of CV measurements.

The technology of MBE growth of strained multiplayer SiGe structures on strain-relaxed $Si_{1-x}Ge_x$/Si(001) buffer layers for THz sources was settled at IPM, Nizhny Novgorod. This technology allows us to grow the structures with more than 100 SiGe layers. The dislocation

density in the buffer layers was $< 3*10^5$ cm^{-2}. The surface roughness measured by means of AFM gave it to be < 0.5 nm that is comparable with the roughness of initial Si(001) substrate. It means that there are practically no misfit dislocations. The X-ray diffraction studies have shown that SiGe/Si superlattice grown on the relaxed buffer is unstrained in total.

2. Sample characterization has been made by means of transport, magnetotransport, CV and SIMS measurements, as well as by X-ray diffractometry and Q-DLTS method. SIMS data show, in particular, the boron related maxima in the center of QW and in barrier layers. Estimated values of boron concentration are consistent with those determined from growth conditions.

All grown structures have been characterized with Hall effect measurements. The measurements have shown the presence of a two-dimensional hole gas in all studied structures.

The hole mobility determined by low-temperature (T=4.2 K) Hall effect strongly depends on the alloy composition and the doping level in QWs (Fig. 1). While increasing the hole concentration from $1.5 \cdot 10^{11}$ to $3.0 \cdot 10^{11}$ cm^{-2}, the hole mobility decreases from $5.1 \cdot 10^3$ down to $4.7 \cdot 10^3$ cm^2/(V·s). The relatively small hole mobility in GeSi QW is connected with the alloy scattering.
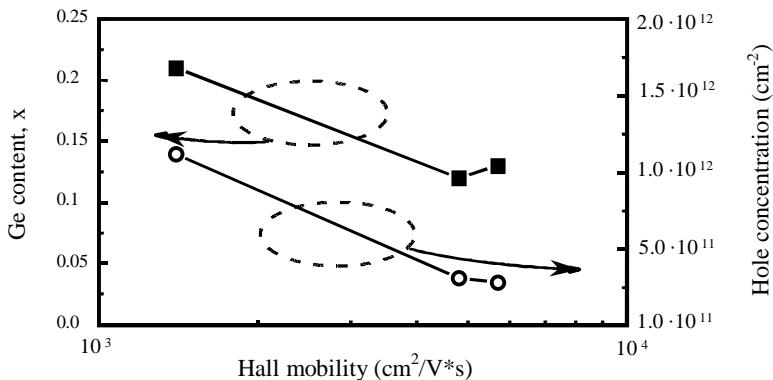

Fig. 1. The dependence of hole mobility on the composition and the doping level in GeSi quantum well.

The hole mobility decreases with an increase of the Ge content in the GeSi layer. The highest hole mobility has been observed for the structures with a small Ge content in a QW and with a small ($<5 \cdot 10^{11}$ cm^{-2}) carrier concentration. The Hall measurements data for three structures are given in Table 1. Temperature dependences of hole concentration give the activation energy in the range of 24 to 39 meV, which is less than the ionization energy of boron impurity (45 meV) in bulk Si.

Table 1.

Sample #	QW width, Å	Ge content	Mobility, cm^2/V×s	Hole concentration, cm^{-2}
419	250	0.12	5.1×10^3	1.5×10^{11}
447	250	0.13	4.7×10^3	3.0×10^{11}
482	200	0.21	1.4×10^3	1.0×10^{12}

3. Depth distributions of impurities and Ge in p-type Si/Si$_{1-x}$Ge$_x$/Si structures were investigated by means of SIMS and CV measurements to clear up the origin of surface charge. The triple-QW structures of different Ge contents in SiGe alloy were studied (x = 0.15, 0.2 and 0.25). SiGe QWs and Si barriers were δ-doped with boron of the concentration of $6*10^{11}$ cm^{-3}. The charge at the Si/SiO$_2$ boundary is associated with surface segregation of Ge and, partially, B impurities at epitaxial growth. The structure scheme and Ge depth distributions are shown in Figs. 2 and 3.
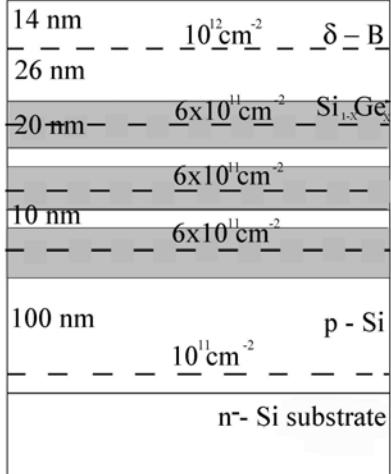
Fig. 2. Scheme of triple-QW SiGe structure.
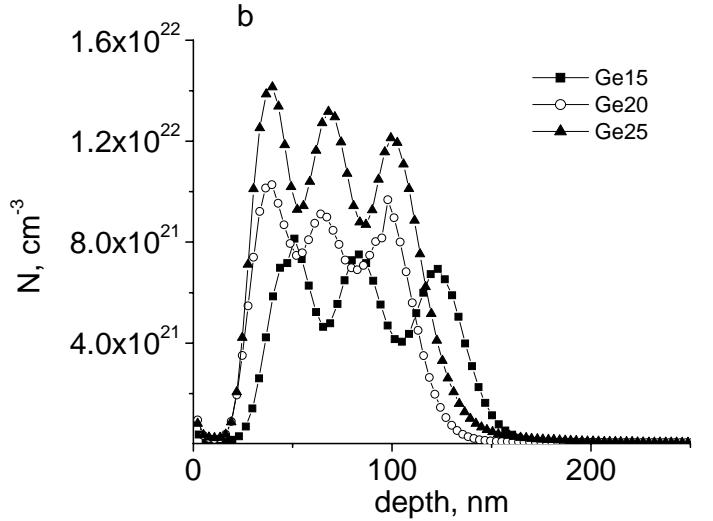
Fig. 3. Ge depth distributions in Si/SiGe/Si structures of different Ge content in SiGe alloy.
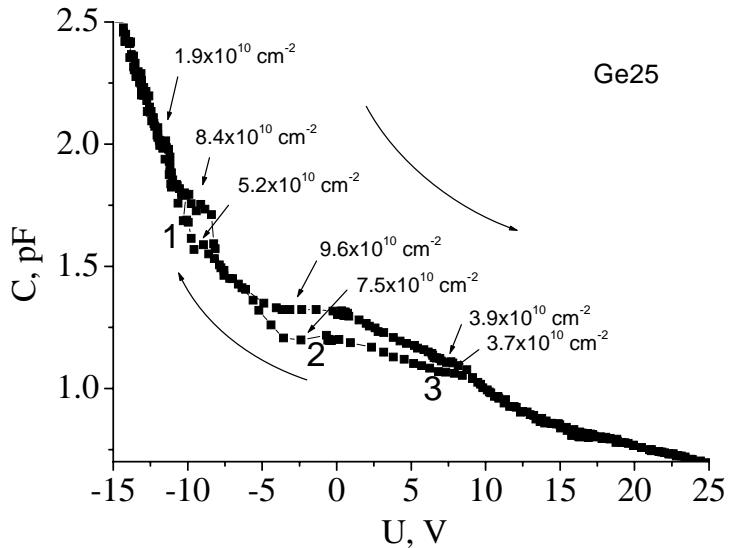

Fig. 4. CV characteristic for structure Ge25. The numbers 1, 2, 3 indicate the QW-related plateaus. The values of p_w for QW and δ-B layer are shown.

4. Samples with three boron δ-doped SiGe layers with Ge content of 0.15 – 0.25 were MBE-grown on n-type Si(100) substrate. The Schottky diodes were created for CV measurements by means of mercury probe. The high-frequency (1 MHz) CV measurements were used for characterization of the heterostructures. CV characteristic for one of the structure is presented in Fig. 4. The plateaus of nearly constant capacitances C*, which correspond to recharging of QWs (1 to 3) and δ-boron layer in the cap layer are clearly seen. The hysteresis is revealed in CV characteristic; arrows show the directions of changing applied voltage. The estimated hole concentrations p_w in the QWs or δ-B-doped layer are given in Fig. 4, too. The values of p_w in QWs and δ-B layer, N_B^{CV}, for the structures with 0.15, 0.2 and 0.25 Ge content are presented in Table 4. The shift of CV characteristics towards the negative voltages is caused by a large positive charge at the surface traps. This charge at the Si/SiO$_2$ interface was estimated and

presented in Table 2. One can see that increase in Ge content in the SiGe QW leads to increase in positive charge at the Si/SiO_2 interface. The large positive charge observed at the surface of p-Si/SiGe/Si heterostructures was shown to result from the surface segregation of Ge during the epitaxial growth. The charge on the hetero-interface of strained Si/SiGe/Si structures is shown to determine the carrier distribution in the structures. In particular, the hole population of QWs is low in comparison with boron concentration observed by SIMS, as was demonstrated by the estimation of hole concentration in SiGe QWs from CV characteristics. It was found that population of quantum wells strongly increased after exposure of the SiGe/Si structures under voltage. Annealing in hydrogen ambient at 430 C caused strong passivation of boron in the QWs and in δ-doped barriers and does not lead to a decrease in the large positive charge at surface states.

Table 2. Parameters of structures and the sheet boron concentrations obtained by different methods.

Structure	$Si_{1-X}Ge_X$, x:	N_B^0, cm^{-2}	N_B^{SIMS}, cm^{-2}	N_h^{CV}, cm^{-2}
Ge15	15	$2.8x10^{12}$	$6.3x10^{11}$	$(1.3-1.6)x10^{11}$
Ge20	20	$2.8x10^{12}$	$7.5x10^{11}$	$(1.3-1.9)x10^{11}$
Ge25	25	$2.8x10^{12}$	$1.24x10^{12}$	$(1.9-2.4)x10^{11}$

5. Recharging of electrically active defects in MBE-grown SiGe/Si heterostructures with both one and three SiGe quantum wells under applied voltage was studied. The electrically active centers and population of quantum wells were characterized as a function of Ge content. The structures with both one and three SiGe layers used in this study were MBE-grown on n-type FZ-Si(100) substrates at the temperature of 400^oC. The Ge content in SiGe alloy was varied from 0.07 to 0.48. The SiGe QWs were δ-doped with boron in the QW middle. Two B δ-layers were positioned within the buffer and cap layers. The background concentration of holes in MBE-grown layers did not exceed $3x10^{15}cm^{-3}$.

CV measurements, current–voltage (IV) measurements and charge deep level transient spectroscopy (Q-DLTS) were used for characterization of the structures.
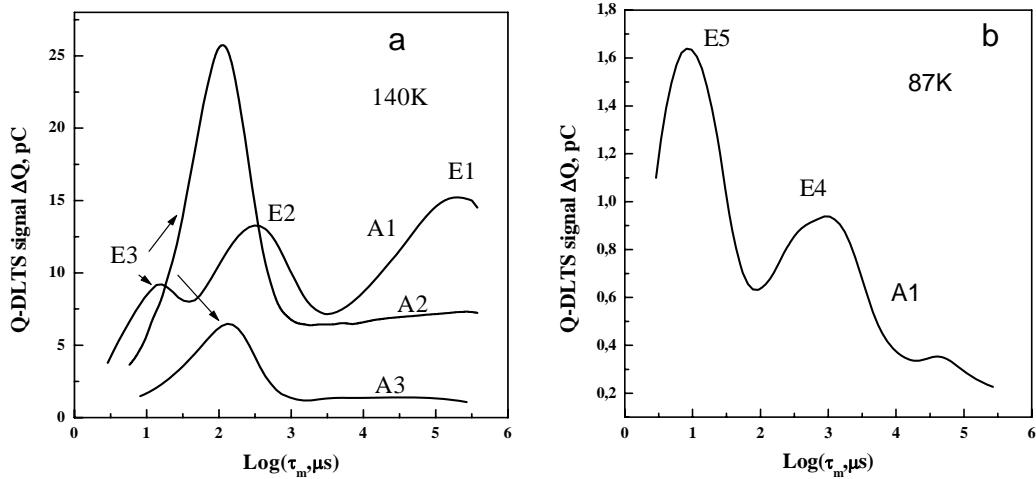

Fig. 5. DLTS spectra for structures A1, A2, A3 at different T. a: $\Delta U = 0.1$ V, b: $\Delta U = 0.5$ V. τ_m is the rate window.

Q-DLTS spectra for the single-QW structures A1, A2, A3 (with 0.07, 0.1 and 0.15 Ge content, respectively) are presented in Fig. 5 a, b. The system ASEC-03 employed in the present work for measurements of Q-DLTS spectra keeps the sample temperature fixed and scans the rate window $\tau_m = (t_2 - t_1)/ln(t_2/t_1)$, where t_1 and t_2 are the time moments of recording the Q-DLTS signal $\Delta Q =$

Q(t_2) – Q(t_1). The parameters of deep levels observed are given in Table 1. In the structure A1 with lower Ge content, five deep levels were found. Only one of them (E3) was observed in the structure A3.

6. In order to optimize the design of SiGe/Si heterojunction for laser application, stability of electronic parameters under applied voltage (electric field effect) and deep-level centers in selectively doped MBE-grown SiGe/Si structures with low background concentration were studied as a function of Ge content. Hysteresis loops in C-V and I-V characteristics were observed and analyzed. An increase in Ge content is found to lead to a reduction of the hysteresis in C-V characteristics, to emergence of the hysteresis in I-V characteristics, and to appearance of electric field "memory" effects in SiGe/Si structures. SiGe/Si structures with low background concentration and low selective doping are found to be very sensitive to the presence of interface states. Deep QW interface states lead to large relaxation times of conductivity and/or capacitance of SiGe/Si structures. Relaxation time decreases with increase of Ge content in SiGe alloy. At different Ge content a correlation exists between a set of deep levels and the relaxation times.

7. The vertical transport through SiGe structures was studied. Temperature activation of holes from the QW was found to determine the current through vertical Si/SiGe/Si structures at T > 160 K. At lower temperatures (T < 130 K), the current is attributed to a thermally activated tunneling of holes from QW. Activation energy of this process, E_a, demonstrates tendency to discrete increase with applied voltage. Steps in E_a(U) dependence can be connected with space-quantization levels in QW.

8. The temperature dependence of conductivity σ along the SiGe layer and hole mobility in Si/Si$_{1-x}$Ge$_x$/Si QW structures was studied at IRE RAS. The SiGe QW was sandwiched between Si buffer and cap layers and was δ-doped with boron in the QW middle with the concentration of 6×10^{11}cm^{-2}. Both the buffer and cap layers were doped with one B-δ-layer. Two activation-law regions were observed in the σ(T) dependence (Fig. 6). At low T, from 4 to 20 K, activation energy (~2 meV) was shown to be due to thermal excitation of holes from the Fermi energy to a
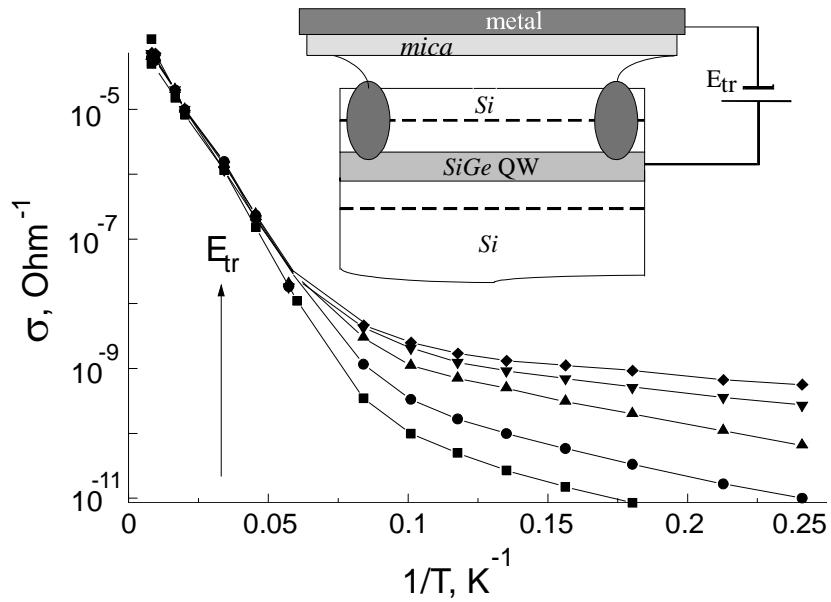

Fig. 6. Lateral conductivity of SiGe QW in transverse electric field vs T.
Insert: Schematic picture of the structure.

mobility edge. The calculations of a potential profile for our structures performed at PTI taking into account pinning the Fermi energy on the surface due to surface charge show that the Fermi

level is near the first level of size quantization in QW. The surface charge creates a built-in transverse electric field (perpendicular to the SiGe layer), its value was found to be near 20 kV/cm. To prove this, we carried out field-effect measurements. The external potential applied across the QW essentially increases the lateral conductivity and decreases the activation energy. The increase of hole concentration is a result of a shift of Fermi energy due to a change of a transverse potential.

9. The negative magnetoresistance of boron-doped SiGe/Si quantum-well structures due to magnetic field suppression of quantum interference corrections to the conductivity was found in the temperature range from 2 to 20 K. The effect of a random potential caused by charged boron δ-layers in barriers on quantum corrections to the conductivity was observed by means of transverse electric field-effect measurements. The transverse electric field increases the hole concentration in QW due to a shift of Fermi energy resulting in a decrease of the activation energy and value of conductivity. The activation energy is due to thermal excitation of holes from the Fermi energy to a mobility edge. The increase of free hole concentration reduces the random potential and increases the quantum corrections. Elastic and inelastic scattering times of holes as well as the magnitude of the random potential were determined from the magnetic field dependence of the NMR. The effect of transverse electric field on the negative magnetoresistance (NMR) of SiGe QWs was studied. A saturation of NMR, observed in high magnetic fields, disappears as electric field increases. The effect is related to increasing of hole concentration in the well.

10. The GeSi structures were characterized by photoluminescence (PL) technique. Modulation doped and undoped testing Si/Si$_{0.85}$Ge$_{0.15}$/Si QW structures have been MBE grown at IPM on the n-Si(100) substrate with the donor concentration $N < 5 \times 10^{15}$ cm^{-3}. The buffer (160 nm) and cup (30 to 120 nm) were δ-doped with boron with concentration N$_\delta$ from $1*10^{11}$ cm^{-2} to $6*10^{11}$ cm^{-2} on a distance of 30 nm from each hetero-interfaces. The SiGe quantum well was doped in the middle with δ-layer of B with concentration of $6*10^{11}$ cm^{-2}. The structure surface was checked by means of atom-force

Fig. 7. PL spectra of SiGe single-QWs.

microscopy, which indicate no dislocations. Besides of the line due to charge carrier recombination in Si layers with transverse optical phonon emission (Si$_{TO}$), the lines in the PL spectra were found resulted from the radiative recombination in GeSi layers (GeSi$_{NP}$), and assisted by the transverse acoustic (TA) and transverse optical phonon emission (GeSi$_{TO}$) (Fig. 7). Spectral position of the PL lines in GeSi QW is in a good agreement with the theoretical calculations using the SiGe alloy composition and QW width obtained from X-ray analysis.

11. Impurity photoconductivity (PC) spectra of the p-type SiGe/Si QW structures were studied. Shown in Fig. 8 are the PC spectra measured with BOMEM DA3.36 Fourier-transform spectrometer for different temperatures (Fig. 8, a) and bias (Fig. 8, b). The structures were grown on Si:B substrate ($\rho_{300K} = 12$ Ω*cm). They consist of 270 nm buffer Si layer, 5 Si$_{1-x}$Ge$_x$ QWs (x = 0.24, d$_{QW}$ = 12.2 nm), separated by 34 nm Si barriers, and 100 nm Si cap layer. The structures were uniformly doped with boron ($N_A \approx 10^{15}$ cm^{-3}). The photoresponse consists of two band of different nature. The high-frequency band (330-700 cm^{-1}) corresponds to the ionization of the

boron impurity in bulk Si. The low-frequency band (210-330 cm^{-1}) seems to be resulted from the ionization of the boron acceptors in SiGe QWs. The spectral dips are clearly seen in the low-frequency band at 245, 278, 321 and 343 cm^{-1} resulted from optical transitions between ground and excited states of boron acceptor in bulk Si.
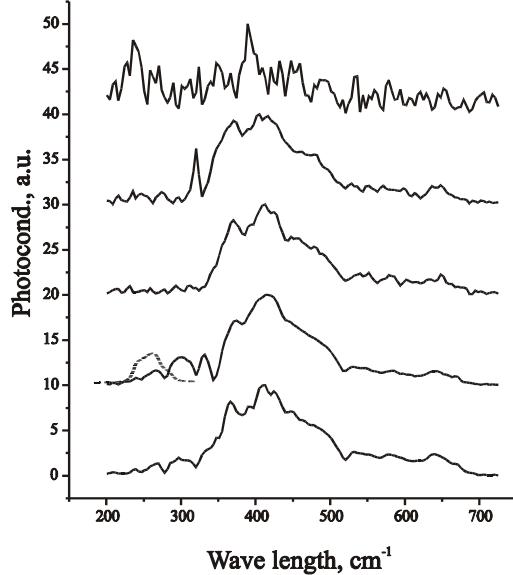

Fig. 8, a.
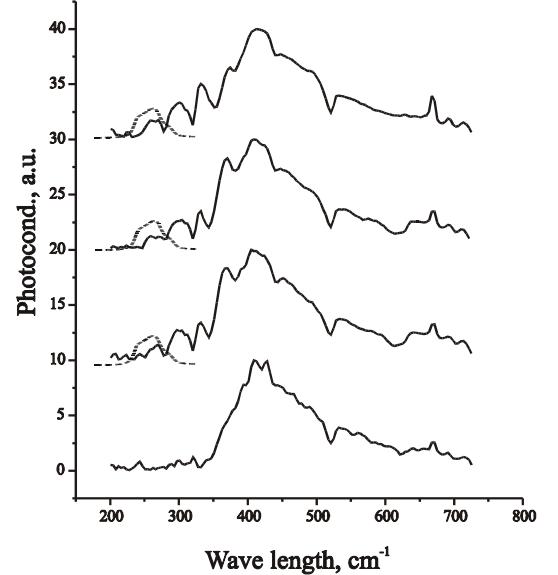
Fig. 8, b.

Fig. 8. Photoconductivity spectra of the Si$_{1-x}$Ge$_x$/Si(100) quantum well structure #349
   a: at the temperatures (upwards): 4.2, 12.6, 15, 26, 32.5 K,
   b: at bias (upwards): 8.3, 30, 50 V/cm (b) (scan speed 0.5cm/sec) and 50V/cm (scan speed 0.1cm/sec).

The dashed line corresponds to the calculated PC spectrum of the boron acceptors situated in the QW center of the sample. There is a satisfactory agreement between the experimental and calculated results. The photoconductivity maximum at 300 cm^{-1} is shifted in comparison with calculated one (260 cm^{-1}). This can be due to a built-in electric field caused by pinning the Fermi energy on the surface of the structure. In several structures, a new photoconductivity band attributed to the photoionization of boron acceptors in SiGe QWs was discovered (Fig. 9). The structure consists of a single 14.5 nm Si$_{1-x}$Ge$_x$ quantum well with x=0.23 grown on a 300nm buffer Si layer and covered by the 84nm Si cap layer. The new band is at lower frequencies if compared with boron photoionization band in bulk Si.
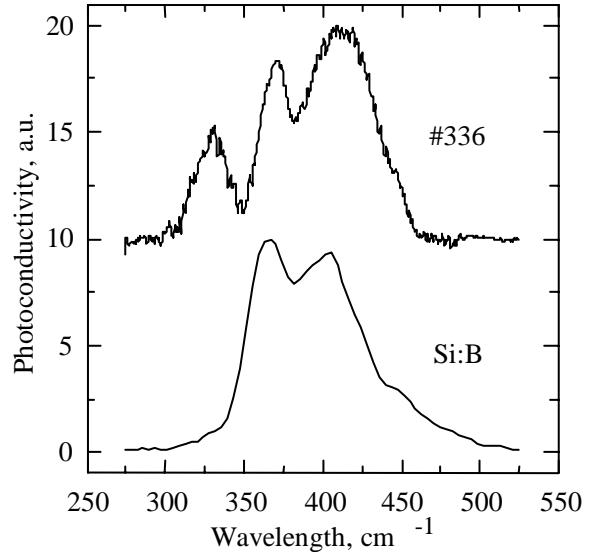

Fig. 9. PC spectra of structure #336 and bulk Si:B sample.

12. THz photoconductivity of *p*-Si/SiGe quantum well (QW) structures as a function of QW parameters: the thickness (10nm÷25nm) and the Ge concentration (10÷30%) has been studied.

The measured photoconductivity spectra of QW structures are shown in Fig. 10, the photoconductivity spectrum of bulk Si:B (x=0) being presented for comparison. A low-frequency band (210 ÷ 330 cm^{-1}) is connected with boron ionization in the SiGe QW. According to a theory, the ionization energy of an acceptor in SiGe alloy is lower than for bulk Si and has a minimum for the acceptors located in the center of a QW. The low-frequency band of photoconductivity in the structures is in a good agreement with the calculated value of the boron ionization energy in the center of the QW. The photoconductivity in the range of 330 ÷ 700 cm^{-1} is related to boron ionization in bulk Si (buffer layer and substrate).

In addition to the impurity bands in the photoconductivity spectra of QW structures, a wide high-frequency band was found, the band position being depended on Ge content in QW. We connect the discovered high-frequency photoconductivity band with hole transitions from QW into long-living states in Si barriers. The hole capture into barrier states dominates over their return into QW, the large lifetime being probably resulted from tunneling processes. Thus, the photoexcitation leads to decrease of hole density in QW, i.e. to the negative photoconductivity.


Fig. 10. Photoconductivity spectra of SiGe/Si heterostructures and bulk Si:B (x=0) for different Ge content x in SiGe alloy. QW widths are10 nm; 20 nm and 25 nm for x = 0.3, 0.21 and 0.12, respectively. T = 4.2K.

Theory

1. A new approach to calculate parameters of resonant states was proposed by the theoretical group at PTI RAS. It makes possible, in particular, to determine the probabilities of the resonant scattering and capture at resonant states. The approach is based on the method of configuration interaction, which has been first introduced by Fano for an analysis of field ionization of a helium atom. Following Fano, two different Hamiltonian have been used for the initial approximation for localized and continuum states, respectively. On the other hand, wave functions have been constructed, following Dirac, in the same way as in the general theory of scattering. The method was applied to resonant states induced by (i) acceptors in Ge under uniaxial stress and (ii) defects in the barrier of AlGaAs/GaAs quantum-well structures.

2. The theoretical approach for calculation of the energies and wave functions of localized, resonant and the continuum states of shallow acceptors in the uniaxially compressed Ge, taking into account the split-off hole subband and anisotropy effects, was developed by the theoretical group at IPM RAS. The acceptor envelope function was expanded in the basis of free hole envelope functions (which are eigenstates of the Hamiltonian in the absence of the Coulomb potential). This method allowed us to calculate the photoconductivity spectra of strained Ge without using the Born approximation and describe satisfactorily the observed photoconductivity bands in uniaxially compressed p-Ge.

The results obtained by different approaches developed by PTI and IPM groups are in good agreement.

3. Detailed analysis and specific calculations have been made for resonant acceptor states induced by shallow acceptors in uniaxially deformed germanium under a pressure applied along [001] and [111] axes. The energy position of the lowest resonant state as well as the life time in the resonant state, the probabilities of elastic scattering and capture at the resonant state have been calculated as a function of pressure applied. It has been shown that elastic resonant scattering in uniaxially deformed p-Ge is strongly anisotropic. Similar strong anisotropy is also characteristic for probabilities of capture at the resonant states. This specific angular dependence considerably influences on the dependence of resonant-state population on the electric field and temperature.

4. The influence of central-cell corrections (the chemical shift) on the spectrum of the acceptor states in uniaxially strained Ge was studied theoretically. A model spherical potential is applied combined with the acceptor Coulomb potential.

5. The developed computer program allowed us to find the populations of localized as well as resonant acceptor states depending on electric field strength and pressure. Non-equilibrium population of acceptor states was calculated by the solution of a system of rate equations in the frames of two-level model including impact and thermal ionization, cascade and Auger capture processes. The balance equations have been solved numerically. The intra-center population inversion was shown to exist in a wide range of electric fields and external strain.

6. Comprehensive theoretical study of operation of the strained hot-hole p-Ge Resonant State Laser (RSL) was performed. The distribution functions of heavy and light holes have been found by means of the solution of the Boltzmann kinetic equation, taking into account interactions with acoustic and optical phonons, as well as resonant and non-resonant ionized impurity scattering. The obtained distribution function has been used for calculation of generation-recombination coefficients as functions of electric field and stress.

7. The direct method of plane-wave expansion of wave functions developed at IPM was used, in the envelope function approximation, for calculation of the acceptor energy spectrum in strained QW structures. The acceptor Hamiltonian used was a 4*4 matrix operator including the Luttinger Hamiltonian, the deformation term, the QW confinement potential due to the valence band discontinuity and the Coulomb potential. Resonant states of shallow acceptors in Si/SiGe QW heterostructures have been studied theoretically. The acceptor wave function has been expanded in the terms of hole wave functions in the absence of impurity Coulomb potential. This expansion includes terms related to the different subbands of size quantization. The resonant states arise when impurity levels pertained with higher subbands fall into the energy continuum of the lowest subband.

8. The theoretical study of resonant acceptor state in 2D system has been performed by using the configuration interaction approximation developed by the theoretical group at PTI RAS. The energies and wave functions of acceptors in some of the SiGe/Si structures have been found using developed computer programs. The computer codes allow us to calculate eigenenergies and lifetimes of the ground and excited resonant acceptor states in $Si/Si_{1-x}Ge_x/Si$ QW structures as a function of Ge content x in SiGe alloy.

9. The Monte-Carlo program for calculation of 2D and 3D hot-carrier distribution function was developed for study of non-equilibrium hole kinetics in strained p-Ge and SiGe quantum-well structures. The simulation takes into account acoustic and optical phonon scattering as well as complex structure of the valence band. Distribution function calculated by this technique is used

to improve calculation of the impact ionization coefficients for acceptor impurities in these materials. The calculated coefficients are used to analyze possibility to achieve intra-center population inversion for deep acceptors, such as copper, in p-Ge.

10. The technique, which allows us to solve Schroedinger equation with Luttinger Hamiltonian for complex valence band structure, is established. The method enables the analytical representation of the wave function of the impurity states for both Coulomb and short-range types of impurity potentials.

3. Results

Study of impurity optical transitions in Ge and Si.

1. In a framework of the investigation of possibility to get THz emission due to impurity breakdown in Si:B, the dependence of THz spectra of Si:B structure with Ti/Au contacts on the current through the structure have been studied. Populations of three lower excited states of boron versus current and temperature have been found from experimental data analysis. Fig. 11 shows typical experimental spectrum. The FTIR scan was taken with a pumping current of 1.5 A at 4 K at a spectral resolution of 4 cm^{-1}. Shown in Fig. 12 is the dependence of impurity states population on the current through the structure at 10K extracted from experimental data. Boron concentration is $5*10^{15}$ cm^{-3}, compensation is 1 %.
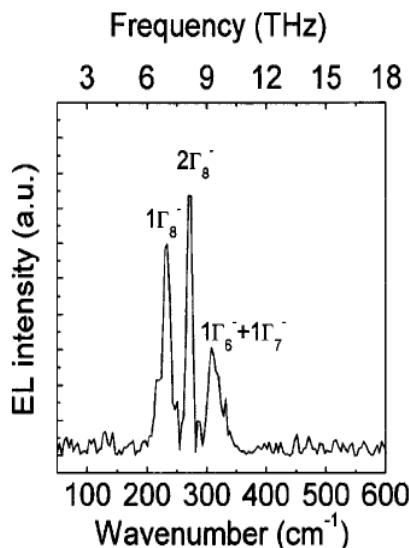

Fig. 11. Emission spectrum of a boron-doped silicon device. The peaks correspond to the impurity intracenter transitions of the $1\Gamma^{8-}$ state, $2\Gamma^{8-}$ states, and the mixed state of $1\Gamma^6$ and $1\Gamma^7$ to the ground state $1\Gamma^{8+}$.
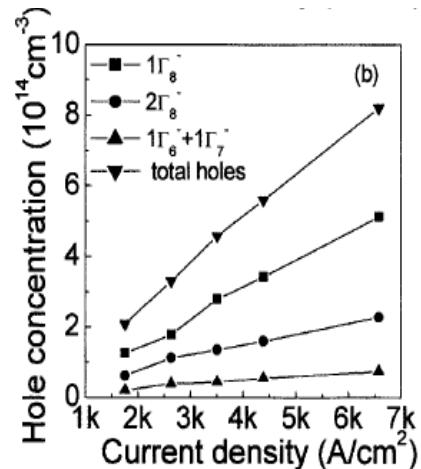
Fig. 12. The dependence of excited states population versus current density through 385 µm sample at 10 K, extracted from THz luminescence spectra.

2. The mechanism of boron impurity breakdown in silicon has been analyzed. Two-level model has been used for impurity states. The breakdown of impurity levels and acoustic phonon assisted cascade capture of free carriers into localized states have been taken into account. The value of threshold electric field calculated appeared to be much less than experimentally obtained. Distribution function analysis has shown that intra-band phonon scattering does not suppress free carriers heating; even at 100 V/cm one can find carriers with kinetic energy of the order of impurity binding energy, which results in a breakdown. To fix this issue, transitions from the valence band to impurity states assisted by the optical phonon emission have been taken into account. Analytical expressions have been obtained for the probability of this process as

well as for corresponding capture coefficient. Calculated dependence of capture coefficient on electric field is shown in Fig. 13. The results obtained will be used for calculation of impurity states populations in electric field.

3. The dynamic model for study of hole transport in Si based THz devices has been developed. The model describes temporal evolution of current and electric field, as well as impurity population and concentration in the valence band across the device. It includes injection of holes through metal-semiconductor contacts, drift and diffusion of holes inside the semiconductor part of the devices, impact ionization as well as cascade

Fig. 13. Amplitude of capture coefficient (optical phonon assisted, into acceptor ground state) vs. electric field.

capture of carriers with acceptor states. The program for solving a system of rate equations for localized acceptor and valence band states populations has been developed. The results are shown in Figs. 14 and 15. Numerical modeling of impurity breakdown in a structure with Shottky barriers has been performed and good agreement with experimental IV-characteristic has been obtained.

4. The THz emitters based on intra-center transitions have been used to investigate B and Ga acceptor states in Si. The first direct observation of $1\Gamma_7^+$ acceptor state has been presented in electroluminescence spectra. The state of such symmetry is impossible to observe in absorption experiments.

5. Intracenter optical transitions between hydrogenic levels in doped silicon, germanium, and gallium arsenide provide a simple and attractive approach to THz emitters. Recent measurements [P.-C. Lv, et al., Appl. Phys. Lett, **85**, (2004)] have shown that the energies of lines of the same origin in absorption and emission spectra differ by several meV. Besides of this, the emission

Fig. 14. Occupations of ground and excited levels vs applied voltage for 385 μm Si:B sample at T=4.5K.

Fig. 15. I-V curves of the 385 μm B:Si sample at T=4.5K.

spectra show line splitting. The origin of these effects is supposed to be due to electron-phonon interactions, which causes Jahn-Teller effect. The Jahn-Teller effect on shallow acceptor levels (splitting due to interaction with phonons) as well as polaron effect have been theoretically investigated. The shift of the ground acceptor state due to interaction with acoustic phonons has been calculated in 2nd order of the perturbation theory for Ga, P, and B impurities in Si. The results of calculations with central cell correction taken into account are in good agreement with experimental results (Fig. 16). The results are presented in Table 3. The nonlinear theory of polaron effects in shallow acceptors under elastic strain (acoustic phonon interaction) was also developed, using the approach developed by G. Bir [G. A. Bir, Sov. Phys. JETP **51**, 556 (1966)], where the splitting of four-fold degenerated ground acceptor state (Γ_8^+ symmetry) is proved to be split when interacting with acoustic phonons.

Fig. 16. Emission spectra of Si:Ga at 20 K. Peaks at 49.9, 52.7, 54.4 and 56.9 meV correspond to the transitions between split levels $1\Gamma_8^-$ and $1\Gamma_8^+$. Double peak (35.1 and 32.6 meV) is related to transitions from split state $1\Gamma_8^-$ into $1\Gamma_7^+$. The inset shows the states

	Coulomb center	Ga	B
$\Delta E(\Gamma_8^+)$, *meV*	3.02	4.2	2.57

Table 3. Results of calculations of the splitting of the ground acceptor state Γ_8^+ in silicon.

The scheme of low energy levels of Coulomb acceptor in Si, calculated according R. Buczko and F.Bassani (Phys. Rev. B 45, 5838 (1992)), is shown in Fig. 17. Calculations show that the

Fig. 17. Scheme of energy levels of Coulomb acceptor. The line lengths indicates relative oscillator strengths of transitions.
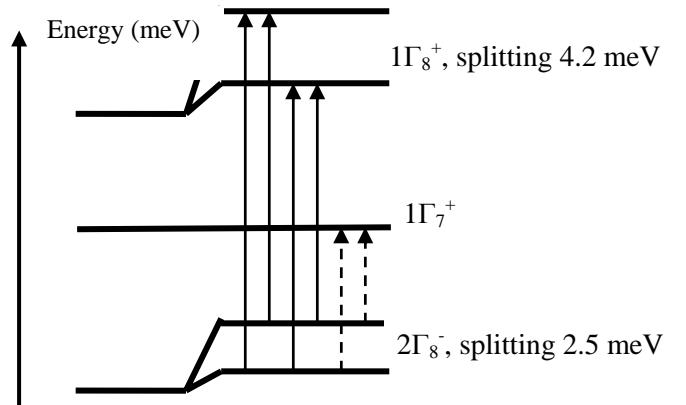
Fig. 18. Splitting of shallow acceptor levels found from the experiment.

transition of the $2\Gamma_8^-$ level to the $1\Gamma_8^+$ ground state has the largest oscillator strength. The scheme of optical transitions in the electroluminescence spectrum of Si:Ga is represented in Fig. 18 (transition energies: 56.9, 54.4, 52.7, 49.9, 35.1, 32.6 meV) The appearance of multiple lines is

caused by the polaron effect that shifts and splits the ground $1\Gamma_8^+$ state by 4.2 meV and the excited $2\Gamma_8^-$ state by 2.5 meV. The calculated value of the splitting of the ground state $1\Gamma_8^+$ for shallow Coulomb acceptor is 3.02 meV.

6. The effects of uniaxial compressive stress on the terahertz electroluminescence from P-doped silicon devices have been studied. A shift in the emission peaks of donor state transitions: $2p_0{\rightarrow}1s(E)$ and $3p_{+/-}{\rightarrow}1s(E)$ has been observed for a stress of about 0.1 GPa along the [100] direction. Optical transitions from excited states to $1s(E)$ strain-split states are shown to have pronounced polarization effect. Transitions involving the $1s(T1)$ ground state, however, showed no polarization. These results suggest that it may be possible to realize an impurity-doped silicon terahertz emitter tuned by externally applied stress.
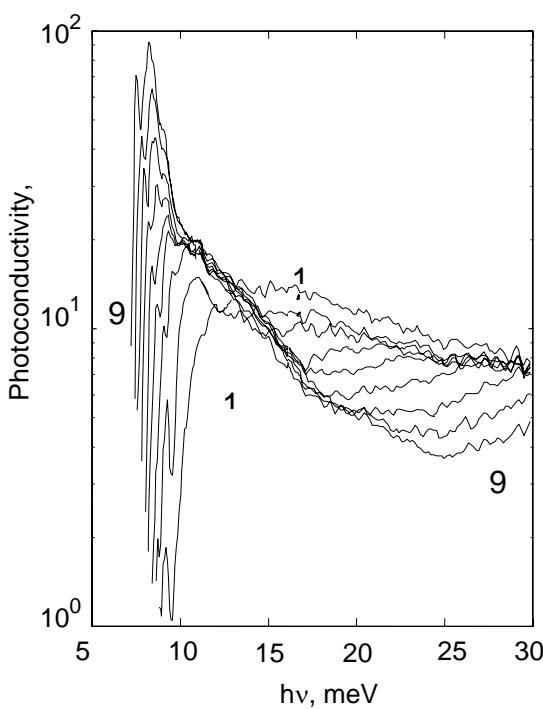

Fig.19. Photoconductivity spectra of strained p-Ge at pressures from 0 (curve 1) to 7.4 kbar (curve 9) with 0.93 kbar step.
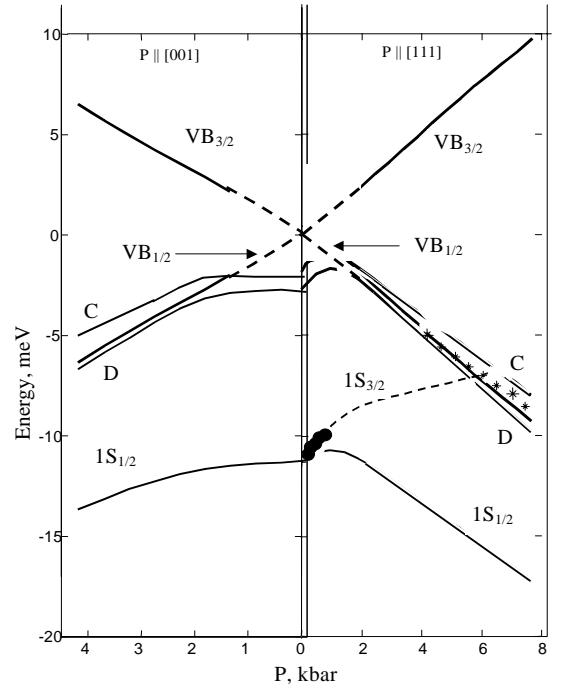
Fig. 20. Energy positions of acceptor levels C and D and valence subbands in dependence on pressure.

7. To identify optical transitions responsible for excitation of THz stimulated radiation in unaxially compressed Ga-doped p-Ge, the spectra of optical absorption and photoconductivity (PC) were investigated with FTIR spectrometer in a wide range of pressures in [111] and [001] directions. The PC spectra are shown in Fig. 19. The dependence of valence band splitting between the branches of light and heavy holes as a function of pressure was established (Fig. 20). Constants of deformation potential for valence band were determined from the dependences. Spectra of photoconductivity (caused by photo-thermo excitation of impurities) for lower energies are presented in Fig. 21. The spectra contain several lines corresponding to different optical transitions between the ground and several excited acceptor states. Pressure dependence of the line spectral positions was determined. For the first time, the resonant state formation induced by strain in p-Ge was observed directly.
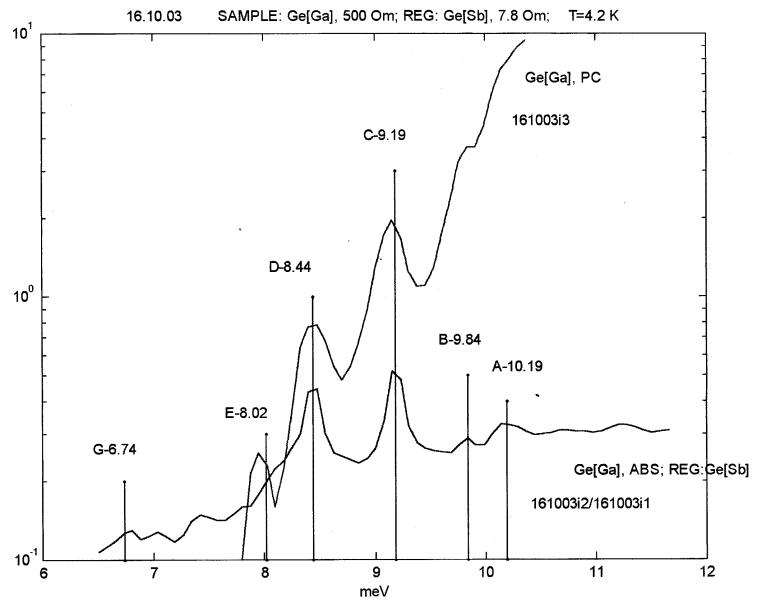
Fig. 21. Photoconductivity (upper curve) and absorption spectra of strained p-Ge. P=4 kbar, T=4.2 K.
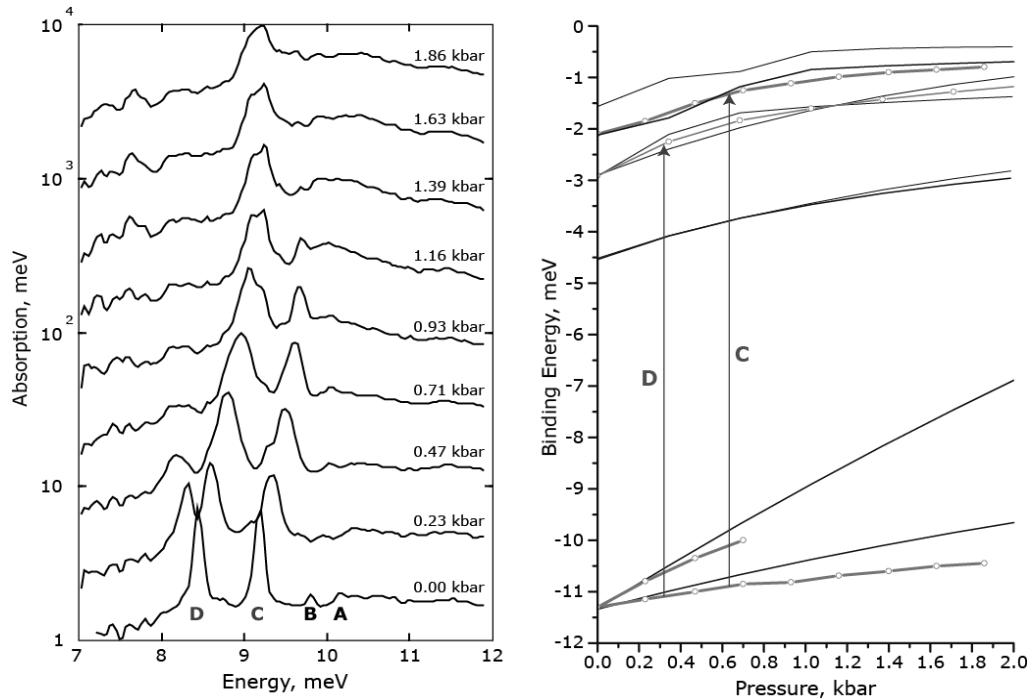
Fig. 22. Absorption spectra at different values of stress (left panel) and calculated acceptor level energies (solid lines at the right panel). Open points demonstrate the agreement of experimental and theoretical results.

8. Calculations of energy splitting of ground state of Ga acceptor impurity in uniaxially strained Ge were performed by the basis expansion technique developed by the theoretical group at IPM taking into account the central cell potential. Comparison of the calculation results with the valence-band splitting energy obtained from the experiment (p. 7) allows us to determine the precise value of the valence band deformation potential as $b = 3.58$ meV/kbar for Ge compressed in [111] crystallographic direction. The splitting of the valence band edge calculated using this deformation potential value is in perfect agreement with that extracted from photoconductivity and absorption spectra. Calculations of energy positions of excited states of Ga impurity in

uniaxially compressed p-Ge were performed, as well. The agreement between experimentally measured absorption spectra and allowed intra-center optical transitions was established (Fig. 22).

Investigation of the mechanism of lasing in bulk p-Ge. Studies of cw operation.

1. Energies and wave functions of excited and ground localized acceptor states as well as of the lowest resonant acceptor state were calculated using plane-wave expansion method with the eigenstates of the bulk-semiconductor Luttinger Hamiltonian as a basis. This approach allows one to clear up the origin of the resonant acceptor states and to show that the "ground" resonant state originates from the excited $4\Gamma_8^+$ state having binding energy of 1.3 meV in the absence of deformation rather than from the ground acceptor state (see Fig. 11).
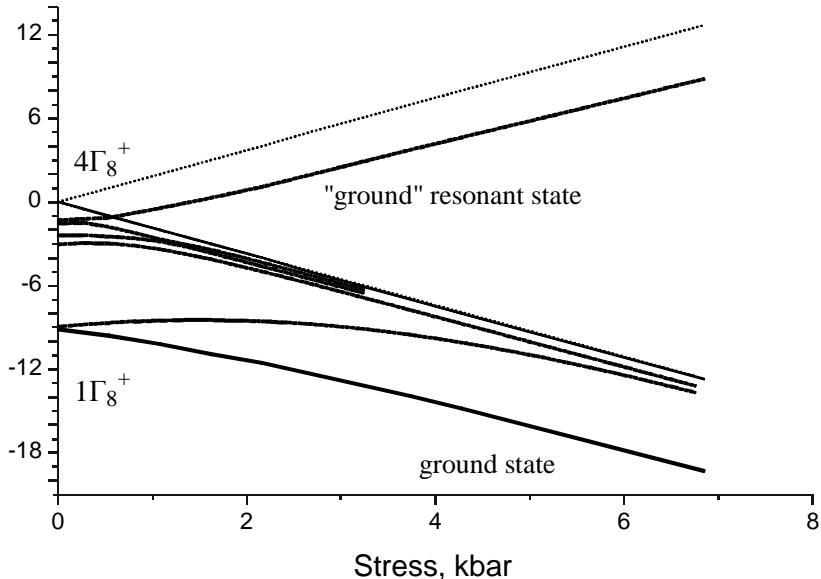

Fig. 23. Stress dependence of the $1\Gamma_8^+$ and $4\Gamma_8^+$ acceptor-state energies in strained Ge.

2. By using the developed method of solving Schroedinger equation with Luttinger Hamiltonian for complex valence band structure and the analytical representation of the wave function of the impurity states for both Coulomb and short-range types of impurity potentials, the coefficients describing the stress splitting of the ground impurity state have been calculated. We have obtained the splitting of $\Delta E=0.399\alpha P$ for Coulomb potential, where P is the applied stress and α is the valence band deformation potential. Similarly, we obtain $\Delta E=0.7466\alpha P$ for the case of short-range potential.

Table 4. Parameters of the model potential used to describe Ga acceptor in Ge.

Binding energy within effective mass approximation	Binding energy of Ga in Ge.	Amplitude of the model spherical potential for a well with the 10A radius	Amplitude of the model spherical potential of a well with 5A radius
9.65 meV	11.32 meV	45 meV	375 meV

3. The influence of central-cell corrections (the chemical shift) on the spectrum of the acceptor states in uniaxially strained Ge was studied theoretically. A model spherical potential is applied combined with the acceptor Coulomb potential. The radius and the amplitude of the model potential are chosen to fit experimentally measured binding energy of the ground acceptor state in unstrained Ge. The results of such a fitting are given in Table 4. The energy positions of the lowest resonant state as a function of applied stress are presented in Fig. 24. Thus, it is shown

that the central cell potential influences on the energies of the resonant states much stronger than on the energies of the excited localized states. The effect is as stronger as smaller is the radius of the central cell potential used to fit the binding energy. To summarize, the effect of the central cell potential on the resonant acceptor states should be taken into account when analyzing spectra of stimulated emission in uniaxially stressed p-Ge.

4. In addition to the basis expansion method used earlier, the method of configuration interaction has been adapted for studies of effect of central-cell potential on the resonant-state width and the resonant scattering and capture amplitudes. The theory was applied to the case of acceptor resonant states in strained p-Ge; results are shown in Fig. 25.
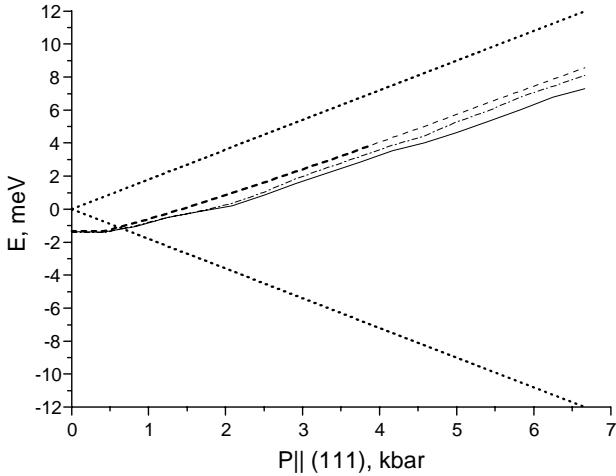

Fig. 24. The energy position of the lowest resonant state induced by Ga in strained Ge as a function of applied stress; influence of the central cell potential. Dashed line: without central cell correction; dash-dot line: central cell potential of 10 A radius; solid line: central cell potential of 5 A radius.
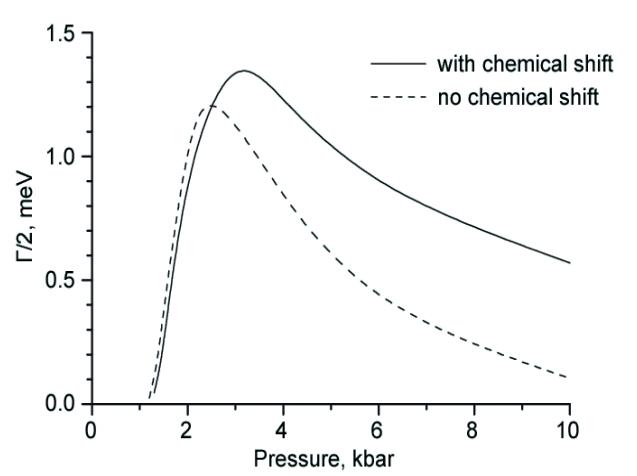
Fig. 25. Width of the acceptor resonant state under the heavy hole band in strained p-Ge with (solid line) and without (dashed line) central cell potential effect.
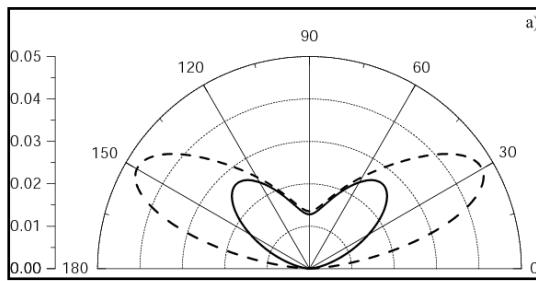
Fig. 26. a)Angular dependence of resonant scattering amplitude on the wave-vector of incident particle,
b)Angular dependence of the amplitude of capture into the resonant state on the wave-vector of incident particle.
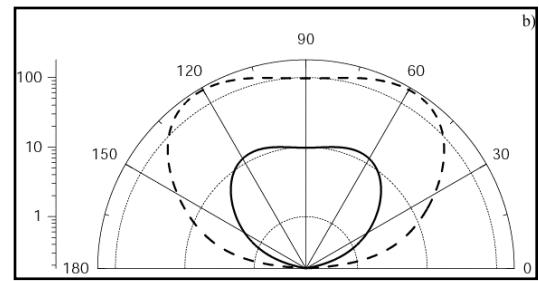
5. The angular dependences of scattering and capture of carriers on the resonant states were calculated taking into account both charged impurity and phonon scattering as well as resonant scattering. Both the scattering and capture are strongly anisotropic. The results are shown in Fig. 26. One can see that the capture into the resonant state is absent when the hole momentum component perpendicular to the z axis is zero, i.e., when the hole moves along the stress axis. In this case, hole states in the light-hole band cannot be coupled with the resonant states.

6. Hot carriers distribution function in uniaxially strained p-Ge was calculated for the case of stress and electric field applied in [100] and [111] crystallographic directions by means of
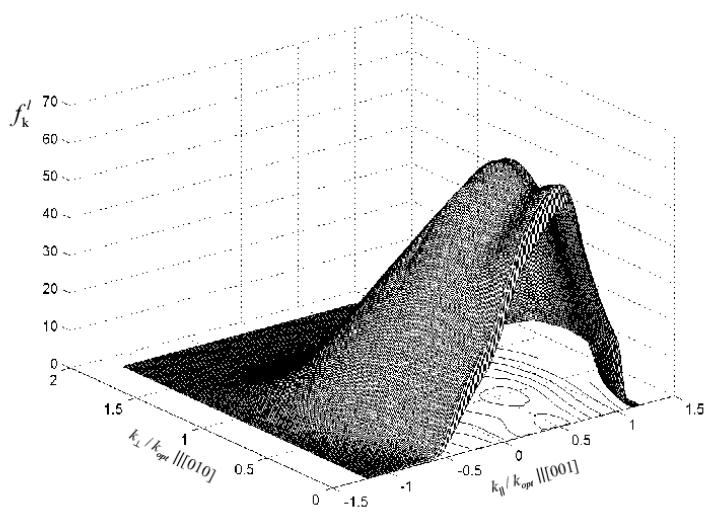
Fig. 27. Light-hole distribution function for p-Ge at P = 4 kbar and E = 10 V/cm.
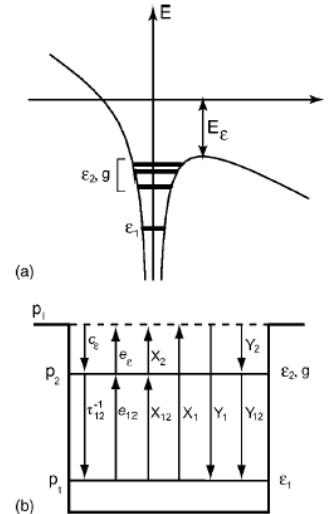
Fig. 28. (a) Coulombic center in an electric field.
(b) Scheme of "two-level" model and processes involved.
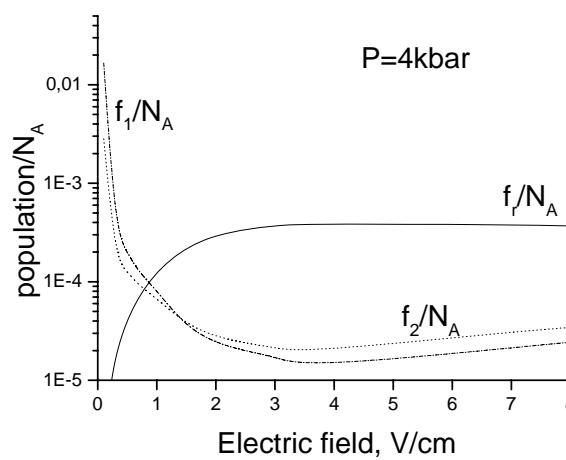
Fig. 29. Electric field dependence of acceptor-state population.
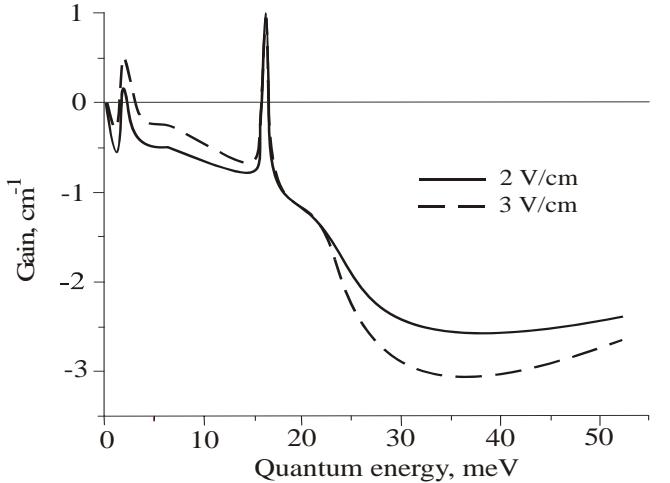
Fig. 30. Optical gain spectrum in uniaxially strained p-Ge for 4 kbar pressure along [100] direction.

Monte-Carlo program developed for study of non-equilibrium hole kinetics in strained semiconductors. The hole heating by external electric field, as well as inter- and intra-subband scattering with acoustic and optical phonons have been taken into account. The example of the light-hole distribution function for p-Ge at P = 4 kbar and E = 10 V/cm is shown in Fig. 27. The distribution function obtained has been used for calculation of generation-recombination coefficients as functions of electric field and stress. The calculated distribution function was used also to improve calculation of the impact ionization coefficients for acceptor impurities in these materials. The calculated coefficients were used to analyze possibility to achieve intra-center population inversion.

7. Kinetics of holes in strained p-Ge resonant-state laser (RSL) under an applied electric field has been studied. Non-equilibrium population of localized acceptor states was obtained as a solution of the system of rate equations within the two-level model: the ground impurity level and some effective excited level combined from all excited levels (Fig. 28). For shallow acceptors, the

energy distances between the excited states are very small, therefore one can assume that all these states have the same population as the effective level. The Pool-Frenkel effect was also taken into account, i.e., the decrease of the impurity ionization energy in the external electric field by the energy $\Delta\varepsilon=2(e^3E/\kappa)^{1/2}$ (Fig. 28, a). The degree of degeneracy was taken as the number of excited Coulombic states with ionization energies larger than $\Delta\varepsilon$ multiplied by the degeneracy factor of each level in respect to angular momentum. The model includes impact and thermal ionization, cascade and Auger capture processes.

The populations of localized as well as resonant acceptor states depending on electric field strength and pressure were found numerically using the developed computer program. The intra-center population inversion was shown to exist in a wide range of electric fields and external strain. Electric field dependences of population of the resonant and two lowest localized acceptor states for P=4 kbar are presented in Fig. 29.

8. The probabilities of optical transitions have been found and the optical gain spectrum has been calculated (Fig. 30). The calculations show that the stimulated THz emission is possible at low fields due to optical transitions between the resonant $1s$ state and the localized $2p_{\pm 1}$ states of an acceptor as well as between the continuum and $2p_{\pm 1}$ states. The calculation results explain the nature of the new line found experimentally (see Fig. 39) in the spectrum of low-voltage generation.

9. Spectra of spontaneous THz emission at impact ionization of a shallow acceptor (Ga) in Ge have been measured at PTI for the first time. The spectra were measured using the Fourier spectrometer in the 5.5 - 5.6 K temperature range. It was observed the narrow lines with

Fig. 31. Spectra of the emission and photoconductivity signals.
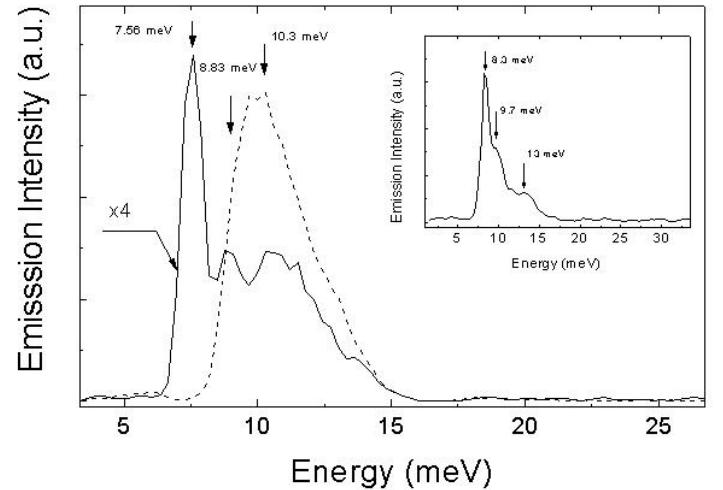
Fig. 32. The polarization resolved THz electroluminescence spectrum of stressed p-Ge(Ga). P~3.5 kbar. T=5.5 K, E=5.2 V/cm. Solid line - e⊥**P**, dotted line – e∥**P**. **P**∥[111]

maxima at ~1.99 THz (8.2 meV) and ~2.36 THz (9.7 meV) which correspond to the optical transitions of holes from excited states of the impurity to the ground state (Fig. 31). A broad emission band with the maximum at 3.15 THz (13 meV) was observed, as well. This band corresponds to the optical transitions of hot holes (an effective temperature is ~ 26 K) from the valence band to the impurity ground state. The contribution of hot hole transitions from the

valence-band states increased with electric field. At the same time, the optical transitions of holes between subbands of the valence band are also revealed in the emission spectrum.

10. Detailed studies of the spectra and polarization of the THz electroluminescence from uniaxially stressed p-Ge(Ga) ([111] direction) have been performed. The THz emission spectrum contains the luminescence lines of different polarization with respect to the stress direction (Fig. 32). The polarization degree attains ~80-90% for major THz emission lines. A depolarization of the THz emission under electric field applied was observed.

11. The reconstruction of absorption spectra of acceptor-doped Ge under uniaxial stress is studied. It is known that in unstressed material the most intensive lines correspond to the optical transitions from the ground state to the first ($2\Gamma_8^-$, D-line) and third ($3\Gamma_8^-$ and $1\Gamma_7^-$, C-line) excited p-states. The transition into the lower excited state $1\Gamma_8^-$ (G-line) is one order less because of smaller matrix element. Under uniaxial strain, on the contrary, G-line becomes more intensive at high enough stress. The oscillator strengths for these transitions are calculated with using acceptor wave functions found in axial approximation. The results are shown in Fig. 33. At the polarization perpendicular to the strain direction, the transitions with the change of total momentum by unity are only allowed. At the polarization parallel to the strain direction, the transitions are allowed only if the total momentum projection on the strain axis is conserved. It means that the transitions from the ground state into the first and second excited states for parallel polarization are impossible. The results obtained explain the ignition of G-line in the absorption spectra of p-Ge under stress.
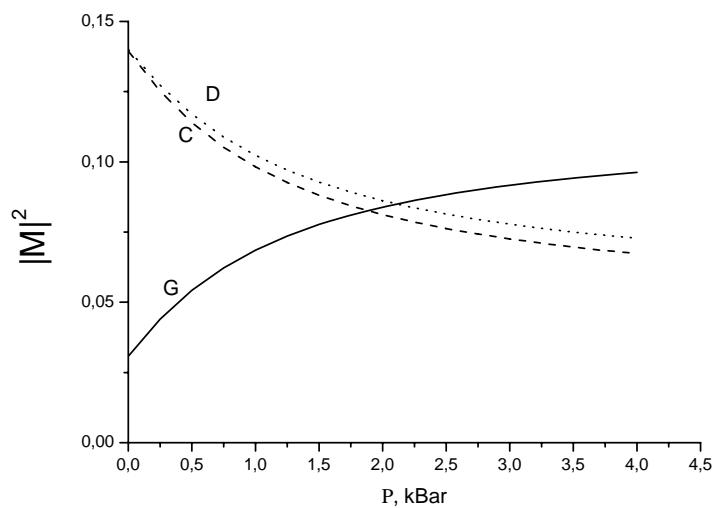
Fig. 33. Matrix elements for intra-center transitions.

12. Current-voltage characteristics of stressed p-Ge were measured. The pressure dependence of the threshold electric field for shallow impurity (Ga) breakdown due to impact ionization was obtained. The dependences turn out to be different for field directions parallel and perpendicular to the stress. This is connected with different heating carriers by field for different crystallographic directions due to different effective masses of holes. The threshold field decreases from 8 V/cm at zero pressure to ~2 V/cm at the pressure near 6 kbar and then practically saturates. The vertical part of current-voltage characteristics indicating the formation of current filament becomes less pronounced at high pressures.

13. Streaming motion of charge carriers in strained p-Ge in crossed electric and magnetic fields was studied by means of measurements of spontaneous radiation intensity. The radiation is due to optical transitions between strain-split valence subbands. An increase in intensity observed at some critical magnetic field H_c (Fig. 34, a) indicates carrier accumulation in the upper valence subband due to magnetic trap formation. The calculated dependence of H_c on valence band splitting is shown by solid lines in Fig. 34, b.
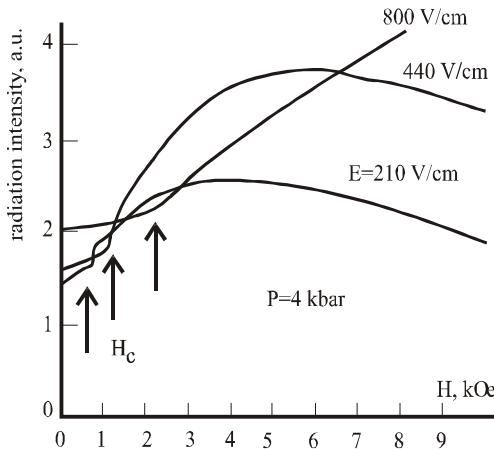
Fig. 34, a. Magnetic field dependence of spontaneous radiation intensity.
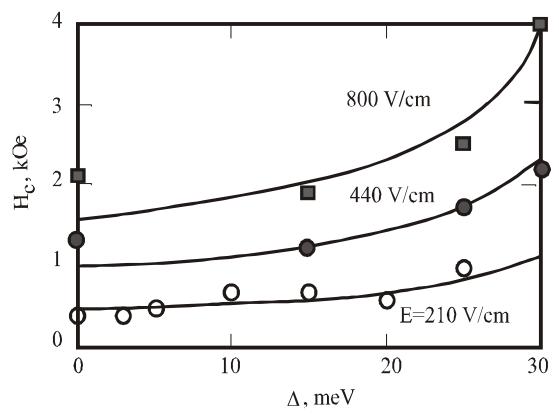
Fig. 34, b. Critical magnetic field H_c vs valence band splitting Δ. Lines show the calculated $H_c(\Delta)$ dependence.

14. The gallium-doped Ge crystals with Ga concentration of $3*10^{13}$ to 10^{14} cm^{-3} were used in the experiment at liquid helium temperature. The samples of a square cross section of 0.5 to 1 mm^2 and 6 to 10 mm long were cut in the [111] or [100] crystallographic directions. Uniaxial pressure P and electric field E were applied along the samples. Voltage pulses of 0.2 to 1 µs duration were applied to two contacts positioned on the long (lateral) plane of the sample. The distance between the contacts was from 4 to 9 mm. THz luminescence was registered by the cooled gallium-doped Ge photodetector. For the samples with planes parallel within 4`, the steep rise in radiation intensity up to 10^3 times was observed at some threshold stress P_c. The minimum P_c values were 4 kbar and 3 kbar for the [111] and [100] crystallographic directions, respectively.

The resonator formed in our case by well-parallel sample planes due to total internal reflection was necessary to obtain the stimulated emission. Indeed, the jump in emission disappeared after rough grinding of one of the long sample planes. Polishing and etching restored the resonator and the stimulated emission appeared again.

We have found that for a crystal with optical mirrors (lateral sample planes) parallel within 0.5'-4', one can observe THz emission only in the pulsed regime beginning at approximately 2.5 kV/cm. To obtain the lasing at low voltages, we used the dislocation-free Ge or material with small dislocation density; a resonance cavity of high enough quality is necessary, as well. The low-voltage operation was achieved for the plane parallelism better than 20 arcsec. Fig. 35 presents the dependence of the THz emission intensity and the current through the sample vs voltage. The lasing begins at voltages of impurity breakdown. At

Fig. 35. Signal and current vs voltage.

the impurity breakdown conditions, a current filament arises. That is why the conditions for low-voltage lasing are much more hard than for high voltages when the current density is uniform in whole sample. At low voltages, only the current filament acts as an active region. Therefore, one needs to have high-quality resonator to excite low-voltage lasing. At low voltages, due to small power dissipated in the sample, stimulated emission could be excited in a continuous-wave (cw)

regime. The minimum values of bias voltage and current for lasing were 1V (2V/cm) and 3mA, respectively.
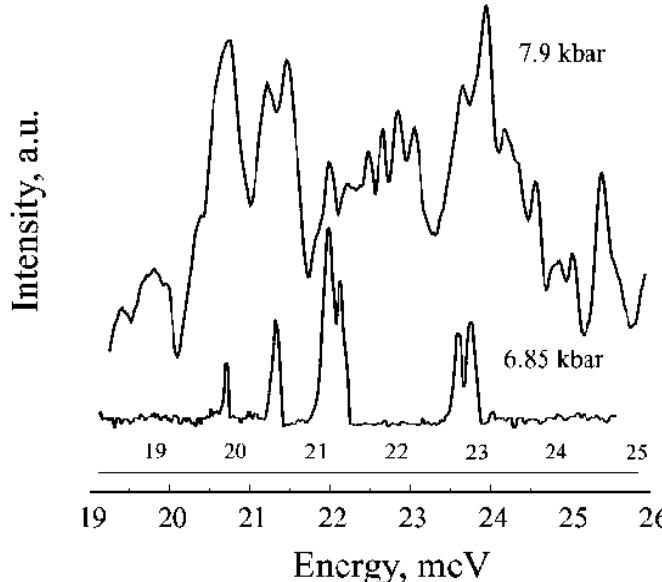
Fig. 36. THz emission spectra at 14V/cm (upper curve) and 3kV/cm pulsed (0.5μsec) electric field.
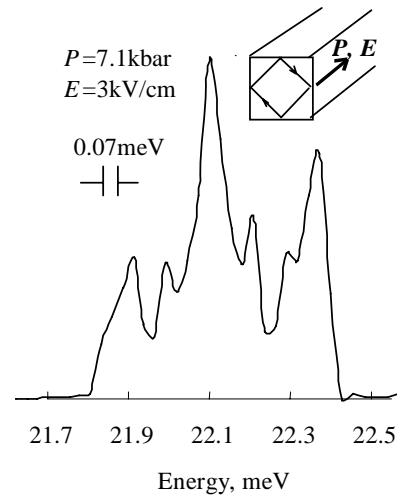
Fig. 37. Modal structure of the main peak in the spectrum of Fig. 1.

15. The spectrum of stimulated radiation from compressed p-Ge measured by the grating monochromator is presented in Fig. 36 (lower curve). The spectrum was measured at the pressure of 6.85 kbar under excitation with short (0.5 μsec) pulses of high voltage (3 kV/cm). It consists of several peaks. The peak energies increased with pressure. The energy of the most intensive peak (21.2 meV in Fig. 36) is varied from 21.2 to 42 meV by increasing pressure from 6.85 to 11 kbar at $P \parallel [111]$. The main peak measured in more details shows the structure caused by resonator modes (Fig. 37). The line spacing (≈ 0.11 meV) for the specimen with the cross section of $1*1$ mm^2 coincides with that found from the condition $N\lambda = nL$, where λ is the radiation wavelength, n is the refractive index ($n=4$ for Ge), L is the optical path length (see the inset in Fig. 37), and N is an integer.

Fig. 38. Pressure dependence of stimulated emission frequency. Open point corresponds to cw regime.

16. Uniaxial deformation removes the degeneracy of the valence band of Ge at $k=0$ and splits it into two subbands separated by the energy gap proportional to the applied pressure P. The degenerate ground state of an acceptor is also split into two states. The energy separation $\delta\varepsilon$ between the split-off state and the ground state increases with strain. At certain pressures one of the split-off states enters the valence band continuum and becomes resonant while the ground state remains in the forbidden band. The comparison of calculated energies of optical transitions from the resonant $1s$ state to the localized $1s$ and $2p_{\pm 1}$ states and the experimental stress

dependence of the energy of the main peak allows us to identify the main peak as the resonant $1s$ to $2p_{\pm 1}$ transition and the peaks at 19.9 and 20.5 meV as the transitions from resonant $1s$ to $2p_0$, $2s$, respectively. The peak of energy 23 meV is supposed to be radiative transition of hot free holes with the energy of s-resonant level to $1s$ localized state. The stimulated emission frequency tuned by stress (from 3 to 9 kbar) corresponds to the frequency range of 3 to 10 THz (Fig. 38). The open point shows the frequency in the cw regime at 4 kbar.

17. The spectrum of low-voltage THz radiation was registered by the He-cooled InSb detector tuned by magnetic field. The detector and the p-Ge sample were placed in the same cryostat at the distance of 20 cm one from another to avoid magnetic field influence on the sample. The spectrum of THz radiation from 7.9 kbar compressed p-Ge for different electric field is shown in Fig. 39. At electric fields of 7 and 10 V/cm, the THz emission is mainly due to a spontaneous radiation. The stimulated emission peaks are observed near 14 V/cm. Besides of the peaks due to intra-center optical transitions, it was observed one more peak at quite different energy: it is 15 meV at 7.9 kbar (curve 3). The comparison with the calculations shows that this peak is a result of optical transitions from the light-hole subband to the ground state of acceptors (see Fig. 30). Shown in Fig. 39,a is the part of the emission spectrum within the main line. The line structure is caused by resonator modes. The distance between the lines coincides approximately with the
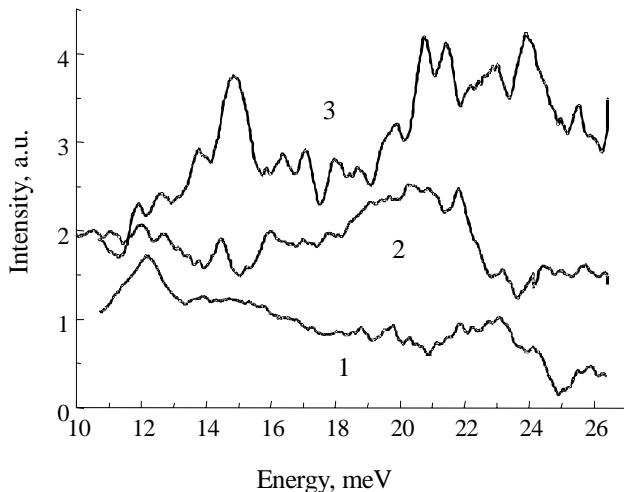
Fig. 39. Radiation spectrum for different electric fields.
E, V/cm: 1 – 7; 2 – 10; 3 – 14.
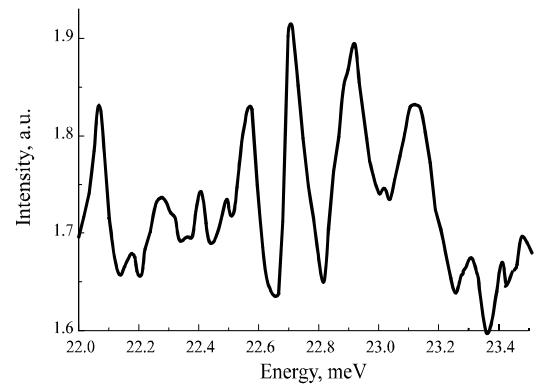
Fig. 39, a. Part of the emission spectrum
indicating the modal structure.

value found from the condition $k\lambda = nL$, where λ is the emission wavelength, n is the refractive index (n=4 for Ge), L is the optical path length, and k is an integer. The line widths allow us to estimate from below the resonator quality Q. Q is not less than 200.

The short-wave part of the spectrum of Fig. 39 is shown in Fig. 36 (upper curve). The emission spectrum contains several peaks at the energies of 20.5, 21.5, 23, 24 and 25.5 meV. These energies correspond to direct optical transitions between resonant and different localized acceptor states. The peak positions are shifted, due to higher pressure, by ~1 meV to higher energies as compared with those observed at high pulsed voltage. Note that hole motion at high fields is ballistic while at low fields it is diffusive. Nevertheless, as seen from the spectra presented in Fig. 36, the lasing in both cases is due to stimulated intracenter optical transitions.

18. It is known that Gunn effect exists in strained p-Ge at the same conditions as THz emission observed. The interaction of the stimulated THz emission and the Gunn effect in strained p-Ge was studied. Shown in Fig. 40 is the evolution of the probe voltage (a), current (b), and THz emission intensity (c) vs applied voltage for the case of static domain. We have shown that the negative differential conductivity in the uniaxially strained Ge is due to strong non-parabolicity of the valence band; that is why the Gunn effect threshold coincides with the onset of streaming motion. The redistribution of hot holes (with different effective masses) over various branches of the Ge valence band (Fig. 41, right panel) leads to the formation of electric domains, static or travelling depending on contact conditions. In this case, the electric field along the sample is very non-uniform, and there are regions of high and low fields. The high-field domain length increases with increasing applied voltage; while the values of the electric field in the domain and
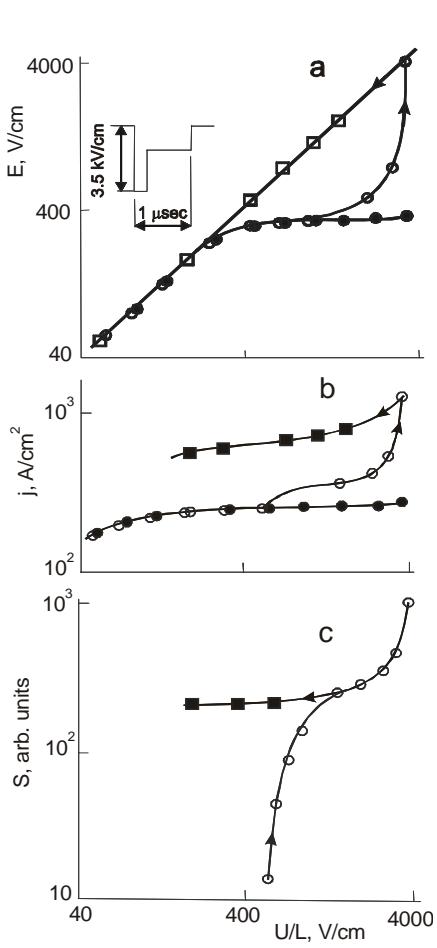
Fig. 40. Probe voltage (a), current (b) and signal S (c) vs bias.
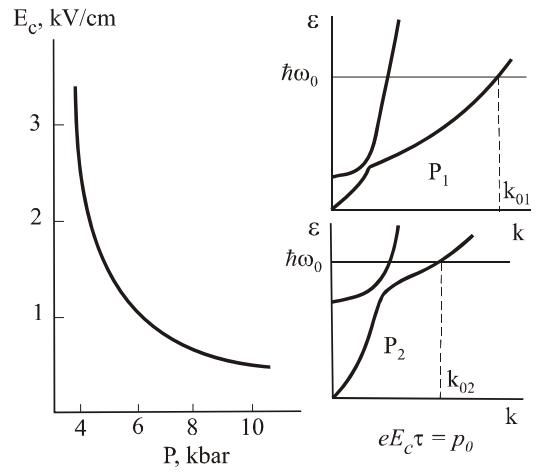
Fig. 41. Pressure dependence of Gunn-effect threshold field and valence band diagrams.
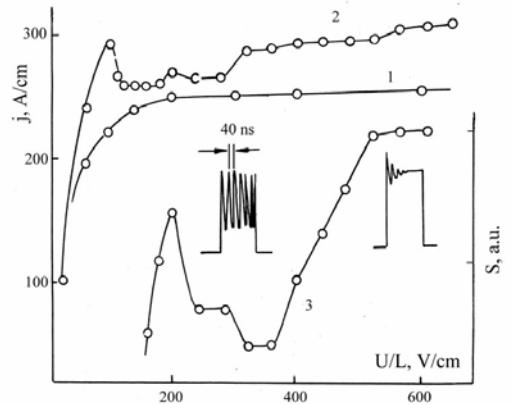
Fig. 42. Voltage dependence of mean current without (1) and with (2) Gunn oscillations and stimulated emission intensity (3).

outside it do not depend practically on the applied voltage; therefore, the current saturation region appears in the current-voltage characteristics of the sample. The stimulated emission occurs at a certain critical domain length. It was shown that the domain length increases with increasing both voltage and pressure at a fixed voltage. For this reason, the lower the applied voltage is, the higher the applied pressure must be in order that the domain length reaches this critical value. For a sufficiently high intensity of the stimulated emission, the domain disappears,

the field distribution over the sample becomes uniform, and the current jump occurs (an increase up to the value corresponding to this uniform field).

The mutual influence of stimulated THz emission and traveling Gunn domains in strained p-Ge, which can appear at the same conditions, has been studied. The evolution of these two effects is shown in Fig. 42. At a stress just below the stimulated emission threshold, current oscillations were observed, the average current being saturated (curve 1). At a stress above threshold, the average current (curve 2) and radiation intensity (curve 3) changed in a similar way, until the oscillations became damped (see the inserts), indicating the transition from a moving to a static domain. Finally, for sufficiently intense radiation, the oscillations disappeared and there was only the static domain. The next rise of the intensity destroys the static domain.

Investigations of the resonant acceptor states in doped SiGe QWs

1. The theoretical study of resonant acceptor state in 2D system has been performed by using two approaches: the configuration interaction approximation developed by the theoretical group at PTI RAS and the direct method of plane-wave expansion of wave functions in the envelope function approximation developed at IPM. In the latter, The acceptor Hamiltonian used was a 4*4 matrix operator including the Luttinger Hamiltonian, the deformation term, the QW confinement potential due to the valence band discontinuity and the Coulomb potential. The calculations were performed for Si/SiGe QW structures similar to those studied experimentally at IRE RAS and IPM RAS. The energies and wave functions of acceptors in some of the SiGe/Si structures have been found using developed computer programs. The computer codes allow us to calculate eigenenergies and lifetimes of the ground and excited resonant acceptor states in $Si/Si_{1-x}Ge_x/Si$ QW structures as a function of Ge content x in SiGe alloy.

The energy spectrum of shallow impurity in QW structures is known to be sensitive to both the well width and the impurity position in the well. As it follows from our calculations, the binding energy of an acceptor placed in QW center depends non-monotonously on QW width and reaches the minimum value at $d_{QW} = 15$ nm. In order to compare the calculation results with
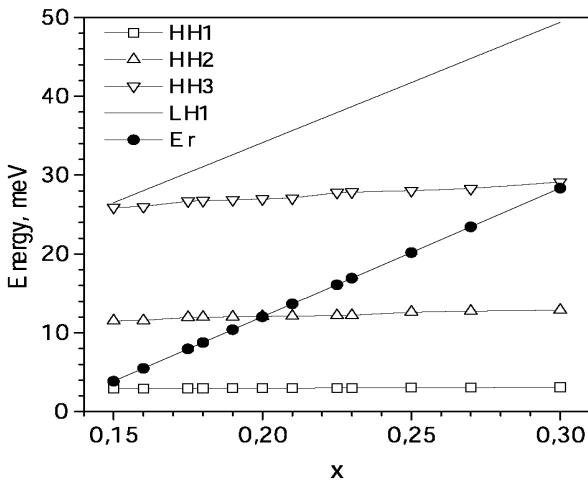
Fig. 43. Dependence of the resonant state energy on Ge content x in $Si/Si_{1-x}Ge_x/Si$ QW.
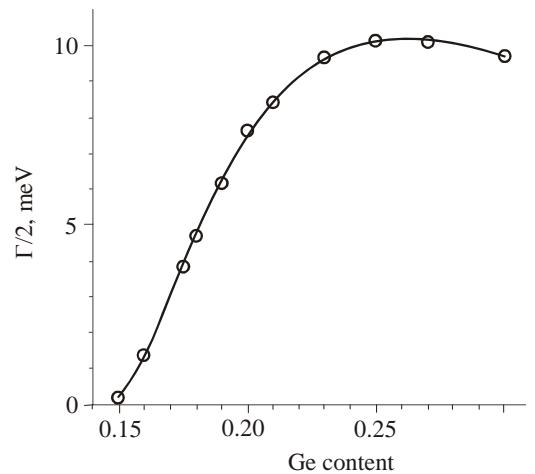
Fig. 44. The width of the boron resonant state in 20 nm SiGe quantum well as a function of x.

the available experimental data we have to take into account the chemical shift of the binding energy which is known to be significant for shallow acceptors in Si. The chemical shift for the shallow impurity in a QW structure can be estimated using additional modeling potential, which is appreciable near the impurity position. Fig. 43 presents the dependence of acceptor-state energies, as well as the position of the levels of space quantization on Ge content x for 200A

SiGe QW. Fig. 44 presents the dependence of the width of the boron resonant state split from the ground state as a function of x.

The acceptor wave function has been expanded in the terms of hole wavefunctions in the absence of impurity Coulomb potential. This expansion includes terms related to the different subbands of size quantization. The resonant states arise when impurity levels pertained with higher subbands fall into the energy continuum of the lowest subband. Eigenenergies of the "ground" and several excited acceptor resonant states pertained with the 2nd subband in Si/Ge$_{0.24}$Si$_{0.76}$ heterostructure #349 (biaxial deformation of SiGe layers $\varepsilon = 6 \times 10^{-3}$, $d_{QW} = 122$ Å) are given in the Table 5.

Table 5. Eigenenergies of several resonant acceptor states pertained to the 2nd subband of size quantization in Si/Ge$_{0.24}$Si$_{0.76}$ heterostructure #349 ($\varepsilon = 6 \times 10^{-3}$, $d_{QW} = 122$ Å). The energy separation between the 2nd and the 1st subbands is 20 meV.

	Eigenenergy calculated from the edge of the 2nd subband of size quantization/
"Ground" state ($2p_0$ – like)	-19.5 meV
$3p_0$–like state	-8.7 meV
$3d_{\pm 1}$–like state	-8.4 meV

2. THz emission spectra of GeSi/Si QW structures under high-voltage pulsed bias have been studied. The electroluminescence measurements were carried out in combination with the measurements of THz photoconnductivity (PC) spectra. The PC measurements have been performed using a broadband THz light source based on an electric-current heated tungsten filament. Shown in Fig. 45 are the spectra of electroluminescence and photoconductivity of the same QW structure. One can see that both spectra contain two maxima at the energies of 5.9 and
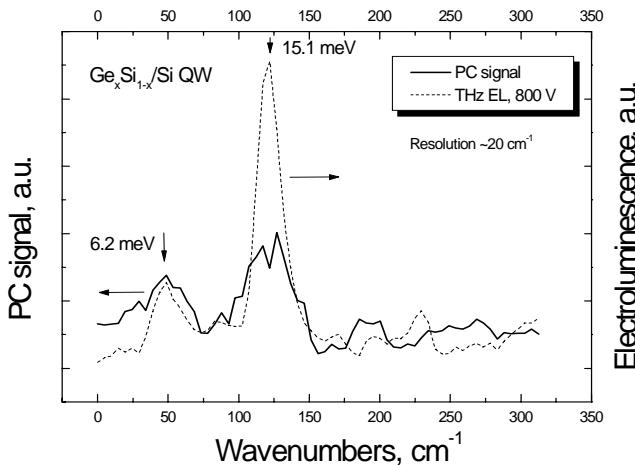
Fig. 45. Photoconductivity and luminescence spectra of Si/Si$_{0.85}$Ge$_{0.15}$/Si QW structures.
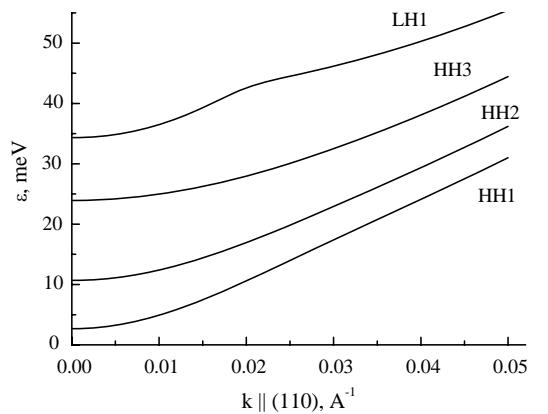
Fig. 46. Energy dispersion of valence band of Si/Si$_{0.85}$Ge$_{0.15}$/Si QW structure.

15.1 meV. To clear up the mechanism of luminescence and photoconductivity, we performed calculation of energy levels in SiGe QWs, which showed that the energy splitting of heavy and light hole bands is about 13 meV. The peak at 6 meV is attributed to optical transitions between the heavy-hole band and A$^+$ states. The peaks near 15 meV are coming from optical transitions between the light-hole band and A$^+$ states. Measurements of lateral conductivity and

magnetoconductivity in the temperature range of 1.6 to 4.2 K confirmed that A^+ centers play essential role in lateral conductivity.

3. The binding energy of A^+ center in $Si/Si_{0.85}Ge_{0.15}/Si$ QW structures ($d_{QW} = 20$ nm) was calculated for two types of impurity potential:

1.) Debye potential: $V = -\dfrac{e}{\kappa r}\exp\left(-\dfrac{r}{a}\right)$, where κ is dielectric constant, and a is the screening length, which has been treated as a fitting parameter. The results are presented in Table 6.

2.) Spherical QW of 20 nm radius. The depth of QW is a fitting parameter. The results are presented in Table 7.

Table 6. Debye impurity potential.

$E(A^+)$, meV in bulk $Si_{0.85}Ge_{0.15}$,	a, nm	$E(A^+)$, meV in $Si/Si_{0.85}Ge_{0.15}$ QW ($d_{QW} = 20$ nm)	LH-subband energy (counted from the lowest HH-band)	$E(A^+)$, meV LH-related state
-2.0	2.9	-2.7	31.65	29.6
-1.5	2.5	-2.1	31.65	29.9

Table 7. Spherical impurity potential.

$E(A^+)$, meV in bulk $Si_{0.85}Ge_{0.15}$	QW potential depth, meV	$E(A^+)$, meV in $Si/Si_{0.85}Ge_{0.15}$ QW ($d_{QW} = 20$ nm)	LH-subband energy (counted from the lowest HH-band)	$E(A^+)$, meV LH-related state,
-2.0	57	-2.9	31.65	29.5
-1.5	50	-2.4	31.65	29.9

4. Energy dispersion of hole subbands has been calculated, as well (Fig. 46). The energy gap between two lowest subbands (8 meV) is in a good agreement with the energy difference between experimental peaks. The energy of the first peak is twice higher than calculated energy of A^+ center, what might be due to impurity levels expansion into the band, which is partially populated. THz absorption spectrum have been calculated for transitions: localized state of A^+-center — free 2D holes for different incidence angles. The results are shown in Fig. 47.
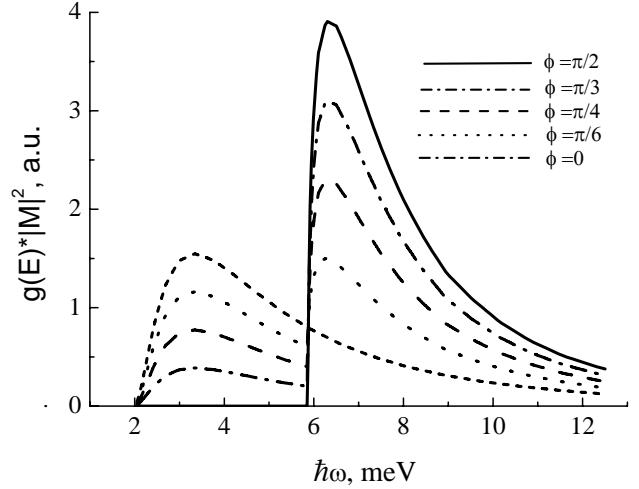
Fig. 47. Calculated THz absorption spectra for different incidence angles ϕ.

Realization and investigation of stimulated THz emission from SiGe QW structures

1. $Si_{1-x}Ge_x$/n-Si structures with optical resonator were used to obtain a stimulated THz emission. The structures have been MBE-grown pseudomorphically on n-type Si substrates. The SiGe QW was sandwiched between Si buffer and cap layers and was δ-doped with boron in the QW middle with the concentration of $6\times10^{11}cm^{-2}$ (Fig. 48, a). Both the buffer and cap layers were doped with one B-δ-layer. Two kinds of structures were used. In type-I QWs, the well was 20nm thick and Ge content x in SiGe alloy was 0.15. The thickness of cap and buffer layers was 60 and 130nm, respectively. The boron δ-layers in the barriers, with concentration from $4\times10^{11}cm^{-2}$ to $10^{12}cm^{-2}$, were positioned each at the distance $d_1=30nm$ from respective QW interfaces. The QW thickness in type-II structures was about 13.5nm. Other parameters were: $x=0.15$, 0.1, and 0.07, and $d_1=19nm$ and $d_2=62nm$. The concentration of B in the δ-layers was $6\times10^{11}cm^{-2}$. The pulsed bias of 0.2 to 4 μs duration has been used in order to avoid overheating. Bias was applied to the SiGe
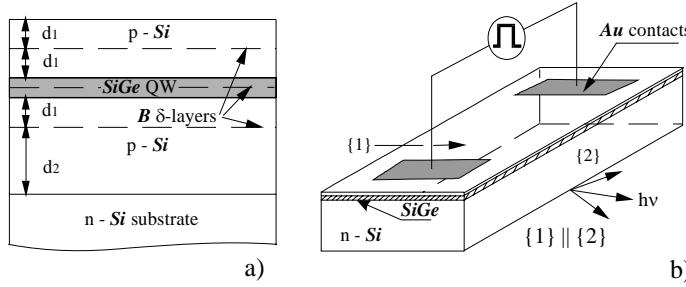
Fig. 48. Schematic view of structure (a) and laser design (b)
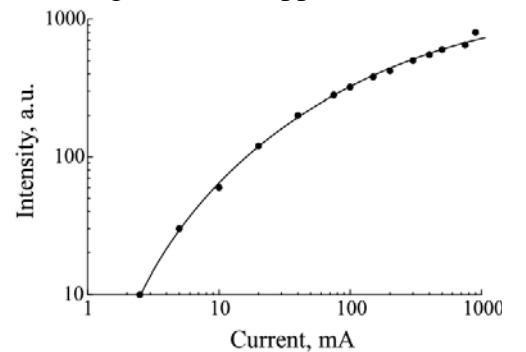
Fig. 49. THz emission intensity vs current
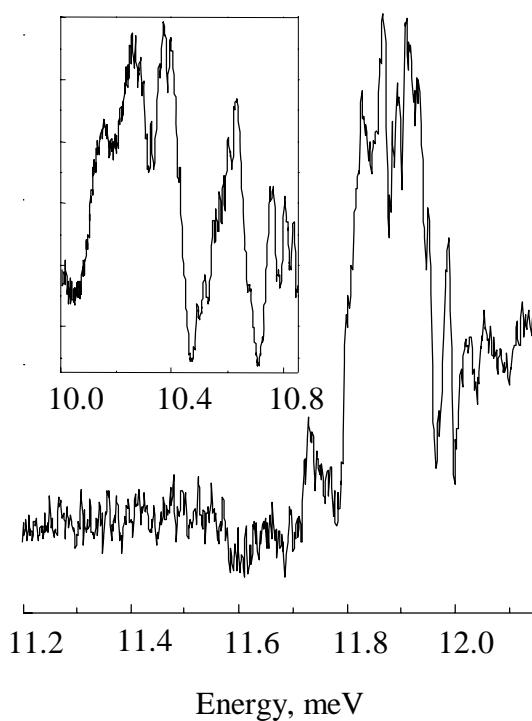
Fig. 50. Stimulated emission spectra of structures of the first type at 1000 V.
The inset shows additional lines appeared at 1500 V.
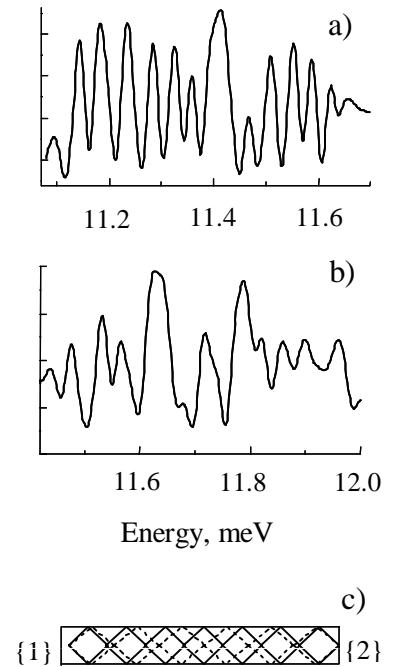
Fig. 51. Modal structure of the main emission line at 1000 (a) and 1500 V (b) and schematic of optical paths (c).

layer via thermal-diffusion made Au contacts (Fig. 48, b) with the distance of 6mm. Emission spectrum was measured by a grating monochromator and registered with a cooled Ga-doped Ge photodetector. Measurements were made at liquid He temperatures. An optical resonator was formed due to the total internal reflection between the parallel top and bottom surfaces of the sample, which were perpendicular to the growth direction, and two lateral facets ({1} and {2} in Fig. 48, b), which were parallel polished. $Si_{1-x}Ge_x$/n-Si structures with x = 0.26, 0.32, and 0.48 were also studied. The structures with three SiGe quantum wells grown on a compensated n-Si substrate were also used.

For the samples with the optical resonator, we observed that an intense THz emission arose at a threshold voltage above 100 - 300V/cm for different samples. Shown in Fig. 49 is the dependence of photodetector signal on pumping current. In the single-QW structures with the optical resonator, it was possible to observe the stimulated THz emission only for Ge content x=0.07, 0.1, and 0.15. In the structures with x=0.26, 0.32, and 0.48, the stimulated THz emission did not arise.

2. The spectra of the THz emission from SiGe/Si structures were obtained by means of the grating monochromator. Spectra of the emission were measured within the energy range from 9.8 to 15.5 meV. Shown in Fig. 50 are parts of the spectra for samples of the first type with x=0.15. The peak near the wavelength 104 μm was observed (Fig. 50) at some threshold voltage. The spectral position of the peak varied from 103 to 108 μm for different samples. At higher voltages, it was possible to observe additional maxima at larger wavelengths (see the inset in Fig. 50). The intense THz emission was also observed in structures of the second type with x = 0.15; there is a line near 100 m in the emission spectrum. The structure of the main peak due to resonator modes is shown in Fig. 51. Only one spatial mode is excited at 1000 V (Fig. 51, a). The mode spacing (~ 0.04 meV) corresponds to the optical path inside the structure for the total internal reflection. As the voltage increases, it was possible to excite several spatial modes and the picture became rather complicated. The modal structure shown in Fig. 51, b corresponds to the coexistence of at least two spatial modes. Their optical paths are presented in Fig. 51, c. The linewidths of this modal structure were determined by the spectral resolution of the monochromator (by the width of the output slit), but they allow us to estimate the value of resonator quality from below. The estimated resonator quality is Q > 300.

The modal structure of the emission indicates its stimulated nature. We attribute the observed stimulated THz emission of $Si/Si_{1-x}Ge_x$/Si QW structures to the inverted population of the boron resonant states induced by the internal strain. For $Si/Si_{0.85}Ge_{0.15}$/Si structures, the valence band splitting is ~ 31 meV. According to variational calculations, the shallow-acceptor binding energy is about 27 meV; the same value was obtained for the binding energy of the acceptor state split off from the ground state. Thus, it can be expected that internal strain in $Si/Si_{0.85}Ge_{0.15}$/Si is sufficiently high for resonant states to appear. Formation of resonant states can be facilitated by a built-in transverse electric field induced in our structures by the surface charge. The transverse potential bends QW valence bands and gives rise to resonant states even if the internal strain is not sufficiently high. The calculated energy diagram for the SiGe structure
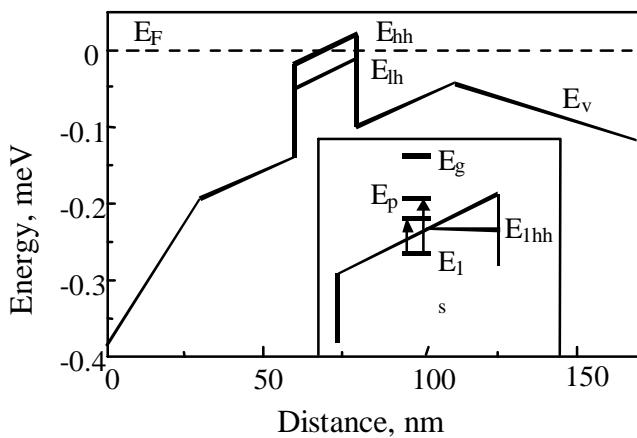
Fig. 52. The energy diagram for an SiGe/Si structure.

under study is shown in Fig. 52. The inset in Fig. 52 shows the scheme of acceptor levels and the lower size-quantization level $1hh$. We believe that the main peak of the THz emission is associated with stimulated optical transitions (shown by arrows in Fig. 52) between the resonant 1 and first excited (localized) p acceptor states. The energy of this transition is consistent with that found from calculations. It is natural to connect the additional maximums observed at lower energies with optical transitions from the same resonant state to higher excited localized states.
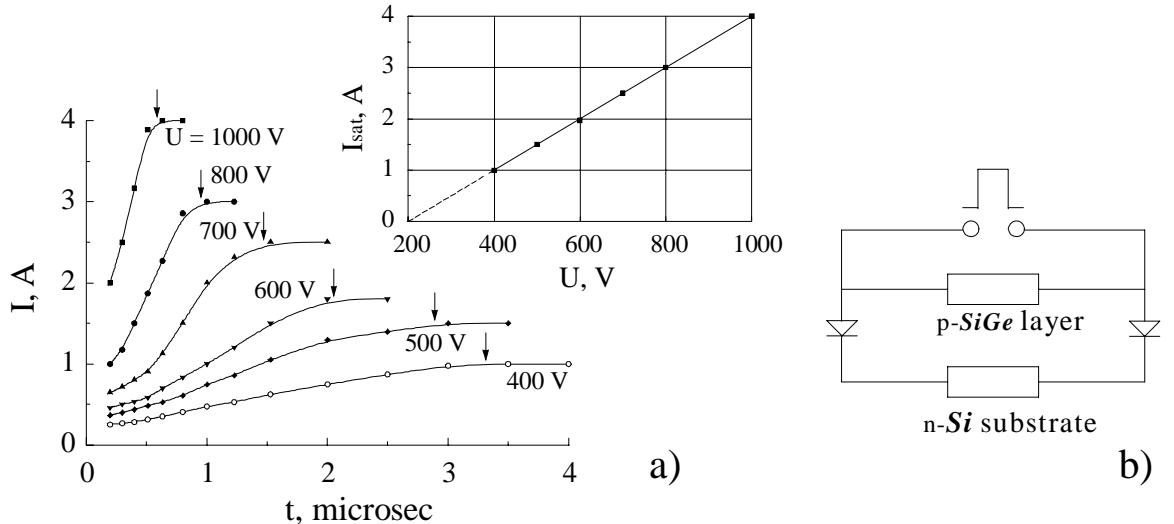
Fig. 53. (a) Time dependence of current at various voltages (the arrows show the onset of stimulated emission) and (b) the equivalent circuit of the structure. The inset shows the voltage dependence of the saturation current.

3. The stimulated THz emission was arisen in two different situations. In the first case, the onset of the emission was observed at electric fields ~100 V/cm as the current through a sample was small (not exceeding 10 mA). The duration of emission pulse did not exceed 0.3 μs. The excitation of the emission in this case depends on conditions on both the structure surface and contacts. The second case was realized at sufficiently long (up to 10 μs) voltage pulse when the Joule heating of the SiGe layer produces ionization of donors in the substrate. It should be noted that the emission intensity virtually does not depend on the current flowing through the substrate,
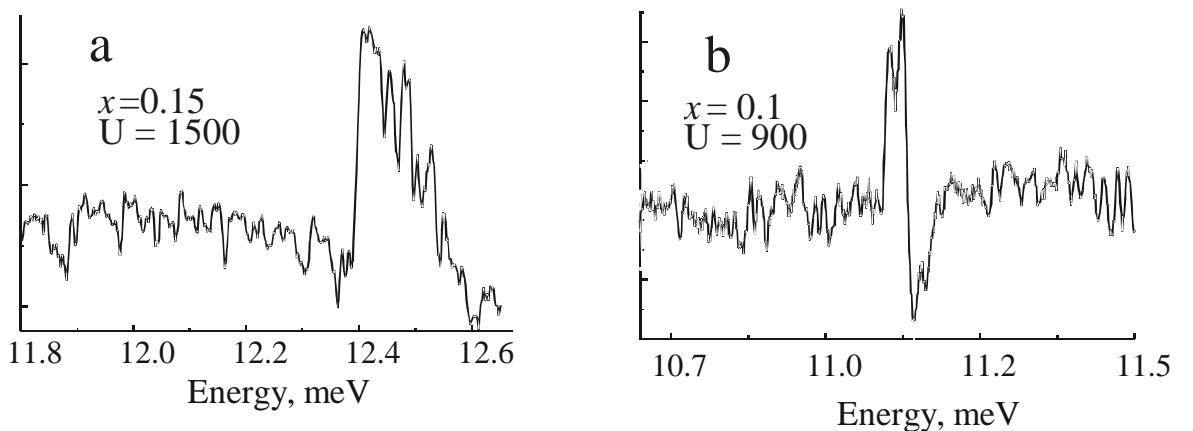
Fig. 54. THz emission spectra of single-QW SiGe/n-Si structure of 0.15 (a) and 0.1 (b) Ge

which additionally indicates that stimulated emission is due to the processes in the SiGe layer.

The dynamics of this process is shown in Fig. 53, a. It is seen that the higher the applied voltage is, the less time is required for the total depopulation of donor states in the substrate. As a rule, the intensive emission appears at the beginning of current saturation (this instant is shown by arrows in Fig. 53, a). As a result of donor ionization, the resistance of the substrate decreases strongly (to 200 Ohm for this sample). The voltage drop across one (blocking) of the p-n junctions formed between p-contacts and the n-Si substrate (Fig. 53, b) creates sufficiently high transverse voltage (200 - 300 V) between the QW and the substrate. This voltage bends valence bands in the QW and improves the conditions for the formation of resonant states. In addition, the compensation of acceptors in p-layers due to the injection of electrons from the substrate promotes the intra-center inversion, as well.

Spectra of the emission for Si/Si$_{1-x}$Ge$_x$/Si structures of $x = 0.1$ and 0.15 for the second regime are shown in Fig. 54. It is seen that the energies of lines in the emission spectra depend on the Ge content in SiGe alloy increasing with increasing x. The change in the line energy in SiGe structures of different Ge content can be attributed to different acceptor-level splitting, which should be larger for higher Ge content due to larger strain thus giving larger optical transition energy.

4. The cause and conditions for the emission excitation in the low-current regime were studied. The problem arisen consists in the following. In the case of p-Ge resonant-state laser (RSL), population inversion is realized for the resonant states of shallow acceptors induced by an external stress. Initially, the ground state of an acceptor is frozen at low temperatures and the free hole concentration is very small. Electric field depopulates the acceptor ground state due to impact ionization, while the resonant state acts as a trap for carriers due to a capture-emission exchange with the continuum and is filled to some degree. In the case of our SiGe/Si structures, impact ionization was not observed at electric fields sufficient for lasing because of larger shallow-acceptor binding energy in Si$_{1-x}$Ge$_x$ alloy in comparison with that for p-Ge. Calculations showed that this energy is about 27 meV for the structures with 0.15 Ge content. On the other hand, the Fermi level is near QW valence band edge and the free hole concentration at equilibrium conditions is of the order of the acceptor concentration in the QW. That is why the population inversion should be difficult to reach even if impact ionization could occur. Nevertheless, the stimulated emission is observed and the question emerges, what is its excitation mechanism.

The evolution of THz emission and current along the SiGe layer at the leading front of voltage pulse was studied. The time dependences of radiation intensity and current are shown in
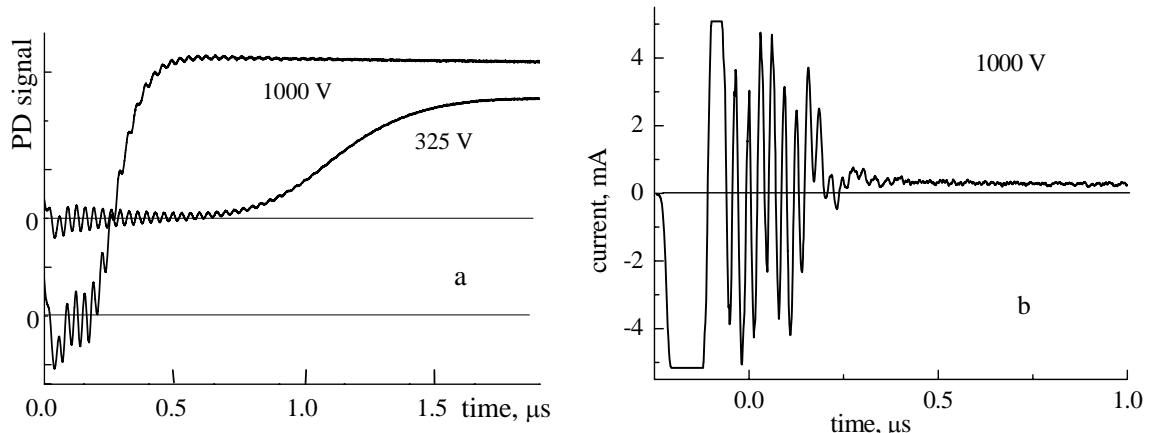
Figure 55. Time dependences of emission intensity (a) and current (b).

Figs. 55, a, b. The main features of the time dependences of the sample current and THz emission intensity are damped oscillations and a time delay in the emission excitation depending on voltage (Fig. 55). All these phenomena can be attributed to a non-stationary injection of carriers through contacts. This is confirmed by current-voltage characteristics of the samples $I \propto U^{3/2}$. The damped oscillations of current (and emission) are similar to those observed in avalanche diodes and are connected with the excitation of space-charge waves. The oscillation period does not depend on time indicating that they are due to drift waves of free carriers.

3. The essential role of the injection was confirmed by means of probe measurements. The probe contact was deposited between the current contacts. The measurements were performed for two samples with different probe electrode positions: 1 and 3 mm from one of the current electrodes. Fig. 56 shows the time dependence of probe voltage normalized to the applied voltage, U_p/U, for different U. The measurements were performed for two samples with different probe electrode positions: 1 and 3 mm from one of the current electrodes. Fig. 56 shows the probe voltage normalized to the applied voltage, U_p/U, in dependence on time for different U. The maximum in probe voltage is observed indicating a transit of the packet of injected carriers. The U_p value is in this case about 0.8 of the applied voltage. The time delay of the maximum is inversely proportional to the applied voltage. This dependence is presented in Fig. 57 for two probe positions. It is seen that the transit time of the carrier packet is shorter for closer probe contact. The delay time of the probe voltage correlates also with that of the onset of emission and the decay time of oscillations in the current and emission (Figs. 55).
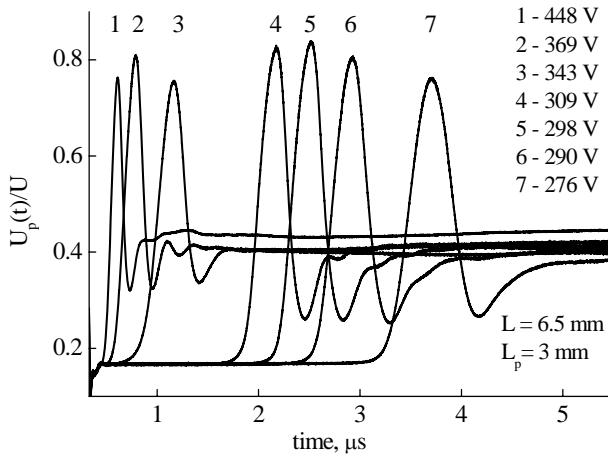
Fig. 56. Time dependence of probe voltage.
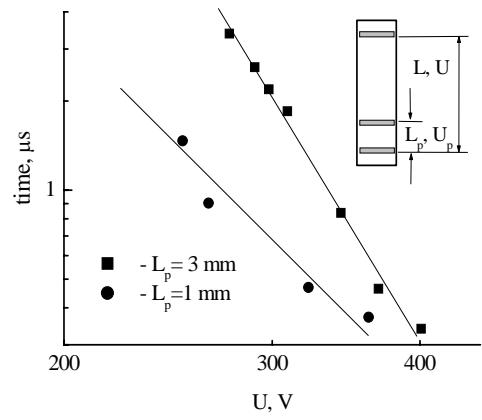
Fig. 57. Dependence of delay time of probe voltage peak on applied voltage.

The drift direction of the voltage peak indicates that it corresponds to the packet of electrons, i.e. it takes place the electron injection into the n-Si substrate. This allows us to suggest the mechanism of population inversion consisted of two steps: non-stationary electron injection through contacts into n-Si substrate and, in turn, electron injection from the substrate into SiGe layer resulting in a depopulation ("compensation") of acceptor states in SiGe QW. Then, the situation becomes similar to that in strained p-Ge. The injection stops when contact screening is restored. That is why the low-current THz emission is excited in this case only during a short time of the existence of injection. In the case of ionization of donors in the substrate, the high electron concentration in the substrate provides the injection into p-SiGe layer in total area between current contacts and the stimulated THz emission can exist during long time not depending on the contact screening.

Conclusion

The data obtained during the Project performance shows that the stimulated THz emission in strained p-Ge and SiGe/Si structures doped with shallow acceptors is the result of the population inversion of resonant acceptor states. In p-Ge, broadband frequency tuning by strain was realized and the possibility of cw operation was demonstrated. It was shown that the use of the SiGe/Si structures is promising for developing THz resonant-state lasers.

References

List of published papers and reports with abstracts.

1. M.S. Kagan, I.N. Yassievich. *Resonant states and THz lasing in SiGe quantum well structures delta-doped with boron*. Physica E, 2002, V. 13, PP. 916-919.

An intense terahertz emission of stimulated character from boron delta-doped SiGe/Si quantum well structures has been observed. The stimulated emission arises under strong electric fields (300–1500 V/cm) applied parallel to interfaces. The mechanism of population inversion is based on the formation of resonant acceptor states in strained SiGe layer.

2. V.Ya.Aleshkin, V.I.Gavrilenko, D.V.Kozlov. *Shallow acceptors in Si/SiGe quantum well heterostructures*. Phys. Stat. Sol. (c), 2003, V. 235, PP. 687-689.

The non-variational approach for calculation of energy spectra of shallow-acceptor resonant states in Si/SiGe QW heterostructures, taking into account the anisotropy effects has been developed. The method is based on the expansion of the acceptor wavefunction in the basis of the free hole wavefunctions in the QW. These functions are eigenfunctions of the Hamiltonian in the absence of the Coulomb potential and refer to different subbands of size quantization. The resonant state was revealed among all the states in the energy continuum of the certain subband (e.g. 1st) by the high fraction of an upper (e.g. 2nd) subband wavefunctions in the wavefunction expansion of the particular state.

3. V.Ya.Aleshkin, A.V.Gavrilenko, V.I.Gavrilenko, D.V.Kozlov, A.T.Dalkjan, V.N.Tulupenko. *On the impurity photoconductivity of uniaxially stressed p-Ge*. Phys. Stat. Sol. (c), 2003, V. 235, PP. 680-682.

Far infrared photoconductivity of stressed p-Ge in the high frequency spectral range corresponding to transitions from the acceptor ground state to the split-off subband has been observed for the first time. The theoretical approach for calculation of the energies and wave function of localized, resonant and the continuum states of shallow acceptors in the uniaxially compressed Ge was developed. The acceptor envelope function was expanded in the basis of free hole envelope functions (which are eigenstates of the Hamiltonian not containing the Coulomb potential). This method allowed to calculate the photoconductivity spectra of strained Ge without using the Born approximation and describe satisfactorily the observed photoconductivity bands in uniaxially compressed p-Ge.

4. A.Blom, M.A.Odnoblyudov, I.N.Yassievich, K.A.Chao. *Resonant states in doped quantum wells*. Phys. Stat. Sol. 2003, V. 235 (1), PP. 85-88.

Resonant states can play an important role on the electronic transport, noise and optical properties of heterostructure devices. A non-variational method have been used to study the resonant states formed by shallow donors inside and outside quantum wells. The method allows us to evaluate the position and the width (lifetime) of the resonant states, as well as matrix elements for optical transition probabilities. A quantitative difference is found between the width found and that resulting from the resolvent operator approach, which can be connected with

neglecting an intraband scattering in the latter method. We also show how the impurity states, localized and resonant, evolve in dependence of the donor position from infinity into the quantum well.

5. V.Ya.Aleshkin, A.V.Antonov, V.I.Gavrilenko, D.V.Kozlov, Z.F.Krasil'nik, D.N.Lobanov, A.V.Novikov. *Impurity photoconductivity in SiGe/Si:B quantum well heterostructures.* Proc. "Nanophotonics" Workshop, Nizhny Novgorod, Russia, 2003, V. 2, PP. 227-230 (in Russian)

Impurity photoconductivity spectra of the p-type SiGe/Si QW heterostructures have been studied. A new photoconductivity band observed at lower frequencies if compared with boron photoionization band in bulk Si has been discovered. The carried out spectral measurements at different temperatures and different bias voltages have shown that the discovered low-frequency photoconductivity band is definitely of different origin than the photoconductivity resulted from the photoionization of boron acceptors in bulk Si and is attributed to the photoionization of boron acceptors in GeSi QWs.

6. S.V. Svetlov, V.Yu. Chalkov, V.G. Shengurov, V.I. Gavrilenko, M.N. Drozdov, Yu.N. Drozdov, Z.F.Krasil'nik. *Growth of multilayer Si/Si$_{1-x}$Ge$_x$ structures with δ–doped layers by sublimational MBE of Si in german environment.* Proc. "Nanophotonics" Workshop, Nizhny Novgorod, Russia, 2003. V. 2, PP. 277-279 (in Russian)

The growth conditions of multilayer structures containing thin (20-35 nm) layers of SiGe solid solution selectively doped with B or Ga by sublimational MBE of Si in german environment have been investigated. The widths of growing Si and SiGe layers are shown by means of X-ray analysis and SIMS to be repeated with high accuracy, the impurity concentration in δ-doped layers (10^{18} cm^{-3}) being corresponding to the impurity atoms transfer from the highly doped source to the growing layer. The formation of sharp profiles of germanium and impurity concentrations at low growth temperature (500°C) is promoted by the hydrogen atoms on the growing surface arising at the german dissociation.

7. I.N. Yassievich. *Donor states in modulation-doped Si/SiGe heterostructures.* Proc. "Nanophotonics" Workshop, Nizhny Novgorod, Russia, 2003, V. 1, PP. 55-59 (in Russian)

Non-variational method for calculation of resonant as well as localized donor states parameters has been developed. It can be also used for evaluation of wavefunctions of the donor states and calculation of optical absorption spectrum for Si/Si$_x$Ge$_{1-x}$.

8. I.V. Altukhov, E.G. Chirkova, V.P. Sinis, M.S. Kagan, R.T. Troeger, S.K. Ray, J. Kolodzey. *Effect of Potential and Doping Profiles on Excitation of Stimulated THz Emission of SiGe/Si Quantum Well Structures.* Proc. "Nanophotonics" Workshop, Nizhny Novgorod, Russia, 2003, V. 1, PP. 71-73 (in Russian)

The stimulated THz emission is shown to be excited in Si/Si$_{1-x}$Ge$_x$/Si quantum-well structures with Ge content in SiGe alloy x=0.07, 0.1, and 0.15. In the structures with x=0.26, 0.32, and 0.48, the stimulated THz emission did not arise. The energy of lines observed in the emission spectra depends on the Ge content in SiGe alloy increasing with increasing x. Two different regimes for excitation of the emission in the same sample are observed.

9. A.A. Prokofiev, M.A. Odnoblyudov, I.N. Yassievich. *Resonant states in modulation doped SiGe heterostructures as a source of THz lasing.* In: "Towards the first silicon laser", edited by L. Pavesi, S. Gaponenko, L. Dal Negro, Kluwer Academic Publishers, Dordrecht, The Netherlands (2003).

Detailed theoretical study of acceptor resonant states in boron doped $Si/Si_{1-x}Ge_x/Si$ structures, as well as results of computer simulation of possible structures for multiquantum-well resonant-state lasers is presented.

10. A. Blom, M.A. Odnoblyudov, I.N. Yassievich, and K.A. Chao. *Donor states in modulation-doped Si/SiGe heterostructures.* Phys. Rev. B68, 2003, 165338.

An universal non-variational approach for calculating the properties of shallow donors inside or outside heterostructure quantum wells is presented. The method allows us to obtain not only the binding energies of all localized states of any symmetry, but also the position and width of the resonant states which may appear when a localized state becomes degenerate with the continuous quantum well subbands. The approach is used for calculation of optical absorption spectra, which are strongly non-isotropic due to the selection rules. The calculations were done for Si/Si_xGe_{1-x}.

11. V.Ya. Aleshkin, A.V. Antonov, V.I. Gavrilenko, D.V. Kozlov, Z.F. Krasil'nik, D.N. Lobanov, A.V. Novikov. *Impurity photoconductivity in SiGe/Si:B multi-quantum-well heterostructures.* Proc.11th Int. Symp. "Nanostructures: Physics and Technology", St.Petersburg, Russia, 2003, PP. 131-132

The impurity photoconductivity spectra in strained SiGe/Si:B quantum well structures have been studied experimentally at $T \geq 4.2$ K. In addition to the photoconductivity band resulted from the photoionization of boron acceptors in the bulk Si the new low-frequency band has been found. The photoconductivity dependences on the sample temperature as well as on the bias voltage have been investigated. The low-frequency band and the "bulk-related" one have been shown to be of different nature. According to the calculation results on the binding energies of confined acceptors, the low-frequency band has been shown to result from the photoexcitation of acceptors in SiGe quantum wells.

12. M.S. Kagan, G.M. Min'kov, N.G. Zhdanova, E.G. Landsberg, I.V. Altukhov, K.A. Korolev, R. Zobl, E. Gornik. *Weak Localization of Holes in Acceptor-Doped SiGe Quantum Well* Proc.11th Int. Symp. "Nanostructures: Physics and Technology", St.Petersburg, Russia, 2003, PP. 135-136

Negative magnetoresistance is observed in boron-doped SiGe/Si quantum-well structures. The effect of a random potential caused by charged boron delta-layers in barriers on quantum corrections to the conductivity is found. Elastic and inelastic scattering times of holes as well as the magnitude of the random potential are determined.

13. J. Kolodzey, T.N. Adam, R.T. Troeger, I.N. Yassievich, and M.S. Kagan. *TeraHertz Sources and Detectors Based on SiGe Nanostructures*. Proc.11th Int. Symp. "Nanostructures: Physics and Technology", St.Petersburg, Russia, 2003, PP. 210-211

THz luminescence was produced by three different types of sources: intersubband transitions in SiGe quantum wells, resonant-state transitions in boron-doped strained quantum wells, and impurity transitions in doped Si layers. THz absorption was observed in SiGe quantum wells with heavy-hole to light-hole intersubband transitions. The devices were grown by MBE, fabricated by dry etching, and characterized by FTIR spectrometry. These results suggest that SiGe nanotechnology is attractive for THz device applications.

14. M.S. Kagan, I.V. Altukhov, E.G. Chirkova, V.P. Sinis, R.T. Troeger, S.K. Ray, and J. Kolodzey. *THz Lasing due to Resonant Acceptor States in Strained p-Ge and SiGe Quantum-Well Structures*. Phys. Stat. Sol. (b), 2003, V. 235, PP. 293-296.

An intense THz emission was observed from strained SiGe/Si quantum-well structures under strong pulsed electric field. The p-type structures were MBE-grown on n-type Si substrates and δ-doped with boron. Lines with wavelengths near 100 microns were observed in the emission spectrum. The modal structure in the spectrum gave evidence for the stimulated nature of the emission. The origin of the THz emission was attributed to intra-centre optical transitions between resonant and localized boron levels similar to that in compressed p-Ge.

15. M.S. Kagan, *THz Lasing of Strained p-Ge and Si/Ge Structures*. In: "Towards the first silicon laser", edited by L. Pavesi, S. Gaponenko, L. Dal Negro, Kluwer Academic Publishers, Dordrecht, The Netherlands (2003).

Stimulated THz emission was observed from uniaxially compressed p-Ge and strained SiGe/Si quantum-well structures doped with shallow acceptors. The origin of the THz emission was attributed to intra-center optical transitions between resonant and localized acceptor levels.

16. M.S. Kagan, G.M. Min'kov, N.G. Zhdanova, E.G. Landsberg, I.V. Altukhov, K.A. Korolev, R. Zobl, and E. Gornik. *Weak localization of holes in acceptor-doped SiGe quantum wells.* Physica B, 2003, V. 340-342, PP. 827-830.

Negative magnetoresistance is observed in boron-doped SiGe/Si quantum-well structures. The effect of a random potential caused by charged boron δ-layers in barriers on quantum corrections to the conductivity is found. Elastic and inelastic scattering times of holes as well as the magnitude of the random potential are determined.

17. V.Ya. Aleshkin, V.I. Gavrilenko, D.V. Kozlov, Z.F. Krasil'nik, D.N. Lobanov, A.V. Novikov. *Impurity photoconductivity in SiGe/Si:B multi-quantum-well heterostructures.* Physica B, 2003, V.340-342, PP. 1065-1068.

A new theoretical method for calculation of acceptor energy spectra in Si /SiGe quantum well heterostructures, taking into account the anisotropy effects has been developed. The impurity photoconductivity spectra in strined SiGe/ Si:B quantum well heterostructures have been studied experimentally. In addition to the photoconductivity band resulting from the photoionization of boron acceptors in the bulk Si a new low-frequency band has been discovered. According to the calculation results the low-frequency band is attributed to the photoexistation of acceptors in SiGe quantum wells.

18. I.V. Altukhov, E.G. Chirkova, V.P. Sinis, M.S. Kagan, R.T. Troeger, S.K. Ray, J. Kolodzey, A.A. Prokofiev, M.A. Odnoblyudov, and I.N. Yassievich. *Effect of potential and doping profiles on excitation of stimulated THz emission of SiGe/Si quantum-well structures.* Physica B, 2003, V. 340-342, PP. 831-834.

Studies of stimulated THz emission from boron-doped $Si/Si_{1-x}Ge_x$./ n-Si quantum-well (QW) structures of various potential and doping profiles are presented. In the single-QW structures with the optical resonator, the stimulated THz emission is observed only for Ge content x= 0.07,0.1,0.15. Two different regimes for excitation of the emission are observed in the same depending on charging the surfaceand thermal ionizationof donors in the substrate.

19. Yu.N. Drozdov, L.V. Krasilnikova, D.N. Lobanov, A.V. Novikov, M.V. Shaleev, M.V. Stepikhova, N.V. Vostokov, A.N. Yablonskii, Z.F. Krasilnik, A.N. Ankudinov, M.S. Dunaevskii, I.P. Soshnikov, A.N.Titkov, V.Dzhagan, V.U. Yukhymchuk and M.Ya. Valakh. *Self-assembled GeSi nanoislands on Si(001)*. NATO Advanced Research Workshop «Quantum Dots: Fundamentals, Applications and Frontiers», Crete (2003).

The results of investigations into the growth and optical properties of single and multilayer Ge(Si)/Si(001) structures grown at different Ge deposition temperatures are presented. It is

shown that the sizes and surface density of the islands can be varied in a wide range by altering the Ge deposition temperature (T_g): from nanometer scale islands for high T_g to small quantum dots with a height of ~ 1 nm and a surface density of > 10^{11} cm^{-2}. The GeSi alloy formation in islands grown at T_g > 580^{0}C was observed by X-ray diffraction, Raman scattering and selective etching. The alloy formation is caused by a strain-driven Si diffusion in islands. The dependence of island composition on T_g was experimentally measured and found to drastically affect the sizes and shape of the islands.

20. M.S. Kagan, I.V. Altukhov, V.P. Sinis, E.G. Chirkova, I.N. Yassievich, and J. Kolodzey. *Stimulated Terahertz Emission of Strained p-Ge and SiGe/Si Structures.* Journal of Communications Technology and Electronics, 2003, V. 48, PP. 1047-1054.

The origin and properties of stimulated terahertz (THz) emission of uniaxially compressed p-Ge and strained SiGe/Si structures doped with shallow acceptors are discussed. This emission is associated with the stimulated optical transitions between resonant and localized acceptor states.

21. M.S. Kagan, I.V. Altukhov,.V.P. Sinis, E.G. Chirkova, I.N. Yassievich, and J. Kolodzey. *Stimulated Terahertz Emission of Strained p-Ge and SiGe/Si Structures.* Proc. Russian Conf. "Photonics-2003", Novosibirsk, Russia, 2003.

The origin and properties of stimulated terahertz (THz) emission of uniaxially compressed p-Ge and strained SiGe/Si structures doped with shallow acceptors are discussed. This emission is associated with the stimulated optical transitions between resonant and localized acceptor states.

22. M.A. Odnoblyudov, A.A. Prokofiev, I.N. Yassievich, I.V. Altukhov, V.P. Sinis, M.S. Kagan. *Resonant Impurity States Semiconductor THz Lasers.* Proc. IRMMW2003, Otsu, Japan, 2003.

Comprehensive theoretical study of CW operation mode of the Resonant State THz lasers on the basis of strained p-Ge is performed. The conditions for population inversion are analyzed and calculation of THz gain is performed.

23. P.-C. Lv, R.T. Troeger, T.N. Adam, S. Kim, J. Kolodzey, I.N. Yassievich, M.A. Odnoblyudov, and M.S. Kagan. *Electroluminescence at 7 terahertz from phosphorus donors in silicon.* Appl. Phys. Lett, 2004, V. 85, PP. 22-24.

Terahertz (THz) emissions corresponding to intracenter transitions of phosphorus impurities in silicon have been observed up to 30 K. Electrical pulses (250 ns) with a repetition rate of 413 Hz were used for excitation, and the peak power was calculated to be ~20 mW/facet for a 190*120 μm^2 device with a peak pumping current of 400 mA at 12 K. THz emission intensity increased linearly with pumping current and quenched when the sample temperature was above 30 K. The current-voltage characteristics suggested a conduction and excitation mechanism by injection of electrons from a Schottky barrier followed by impact ionization of the neutral impurities.

24**.** S.P. Svetlov, V.Yu. Chalkov, V.G. Shengurov, V.I. Gavrilenko, M.N. Drozdov, Yu.N. Drozdov, Z.F.Krasil'nik. *Growth of epitaxial multiplayer S/Si$_{1-x}$Ge$_x$ delta-doped structures using sublimation MBE of Si in GeH$_4$.* Proc. Russian Ac. Sci. (Izv. Acad. Nauk), Physics, 2004, PP. 32-34 (in Russian).

The conditions for growth of multilayer epitaxial structures with sharp hetero-interfaces containing selectively doped layers of SiGe solid solution by sublimational MBE of Si in german environment are discussed. By means of electro-chemical profiling and SIMS, the widths of the grown thin (20-35 nm) Si and SiGe layers are shown to be repeated with high accuracy and contained δ layers of boron and gallium.

25. A.V. Andrianov, A.O. Zakhar'in, I.N. Yassievich, N.N. Zinov'ev. *Terahertz electroluminescence in conditions of breakdown of shallow acseptors in germanium.* JETP Letters, 2004, V. 79(8), PP. 448-451.

The spectrum of spontaneous THz electroluminescence was obtained near the breakdown threshold of a shallow acceptor (Ga) in Ge. The emission spectrum exhibits narrow lines with maxima at ~1.99 THz (8.2 meV) and ~2.36 THz (9.7 meV), corresponding to the optical transitions of non-equilibrium holes from the excited states to the ground state of impurity. A broad line with a maximum at ~3.15 THz (13 meV) corresponding to the hole transitions from the valence band to the impurity ground state is also seen in the spectrum. The contribution of hole transitions from the valence band increases with the increase in electric field. Simultaneously, the optical transitions of non-equilibrium holes between the subbands of the valence band appear in the emission spectrum. The integral terahertz-emission power is ~17 nW at 1 W of the input power.

26. M.A. Odnoblyudov, A.A. Prokofiev, I.N. Yassievich, and K.A. Chao. *Theory of p-Ge THz Laser.* Phys. Rev. B 70, 115209 (2004).

A theory of a strained p-Ge resonant-state THz laser is developed. A comprehensive study of the processes leading to the stimulated THz emission in strained p-Ge under an electric field applied is presented. The distribution functions of light and heavy holes are found. The scattering by optical and acoustic phonons, as well as resonant scattering by charged impurities are taken into account. The steady-state hole distribution functions are used to calculate the generation-recombination coefficients which enter into the system of rate equations for the localized states populations. The populations of localized and resonant acceptor states are found. The conditions for population inversion are investigated. The optical gain calculation is carried out taking into account main optical transitions in the THz spectrum range.

27. P.-C. Lv, R.T. Troeger, S. Kim, K.W. Goossen, J. Kolodzey, I.N. Yassievich, M.A. Odnoblyudov, M.S. Kagan. *Terahertz Emission From Electrically Pumped Gallium Doped Silicon Devices.* Appl. Phys. Lett, 2004, V. 85, PP. 3660-3662.

THz emission due to intracenter transitions of Ga acceptors in silicon have been observed up to 30 K. The peak power was 12 µW per facet at a pumping current of 400 mA. The spectra occurred in two distinct series at 7.9-8.5 THz, and at 13.2-13.8 THz. The emission was attributed to the hole transitions from the split sublevels of the $1\Gamma_8$ excited state to the $1\Gamma_8^+$ and the $1\Gamma_7^+$ states.

28. M.A. Odnoblyudov, A.A. Prokofiev, I.N. Yassievich, I.V. Altukhov, V.P. Sinis, M.S. Kagan. *Hot carrier effect on resonant state THz laser operation.* Semicond. Sci. Technol. 2004, V. 19, PP. 1-3.

A comprehensive theoretical study of operation of the strained hot hole p-Ge RSL is performed. Hot hole kinetics in strained p-Ge under an applied electric field is studied and heavy and light hole distribution functions are found as a solution to the Boltzmann kinetic equation, which includes interactions with acoustic and optical phonons, as well as resonant and non-resonant ionized impurity scattering. Non-equilibrium population of the localized acceptor states is obtained as a solution to system of rate equations within the two-level model for an impurity level structure. Conditions for the formation of the intra-center population inversion are studied as a function of the electric field and external strain. We have observed that the population inversion is formed in a wide range of electric fields and, therefore, could be easily achieved. Net gain at the THz frequencies is calculated using the non-equilibrium hot hole distribution function

and the localized states population. Possibility to achieve net THz gain in semiconductors by injection of hot carriers into impurity resonant state is demonstrated.

29. V.Ya. Aleshkin, A.V. Antonov, V.I. Gavrilenko, Z.F. Krasil'nik, A.V. Novikov, M.V. Shaleev, E.A. Uskova. *Negative mid IR photoconductivity in selectively doped SiGe/Si:B QW heterostructures with two-dimensional hole gas.* Proc. "Nanophotonics" workshop. N. Novgorod,. 2004, PP. 307-309 (in Russian).

THz photoconductivity of $Si_{1-x}Ge_x/Si$ (x=0.12-0.3) single-QW structures with δ-doped barriers has been studied. The doped region in the selectively doped structures was 50 nm wide. It was separated by 20 nm Si spacer layer from the QW interface. The sheet boron concentration was $4*10^{12}$ cm^{-2}. A low-frequency photoconductivity band in the range of $210 \div 330$ cm^{-1} related to boron ionization in the SiGe QW was observed, as well as the photoconductivity in the range of $330 \div 700$ cm^{-1} related to boron ionization in bulk Si. In addition to the impurity bands in the photoconductivity spectra, a wide band with spectral position being depended on Ge content in QW was found. The high-frequency photoconductivity band is supposed due to hole transitions from QW into long-living states in Si barriers, which leads to the negative photoconductivity.

30. A.A. Prokofiev, M.A. Odnobludov, V.M. Chistyakov, I.N. Yassievich, D.V. Kozlov. *Influence of short-range potential on energies of shallow acceptors states in strained semiconductors.* Proc. "Nanophotonics" workshop. N.Novgorod. 2004. PP. 342-345 (in Russian).

Effect of central-cell corrections (chemical shift) on the eigenenergy of the lowest resonant acceptor state in iniaxially stressed Ge has been studied. The acceptor wavefunction has been expanded in termes of hole wavefunctions in the absence of the acceptor Coulomb potensial (plane waves). Resonant states in the energy continuum have been separated by finding a maximum of an upper subband share in the acceptor wavefunction expansion. The chemical shift has been taken into account via additional model potential of the spherically symmetric quantum well, the well radius and depth being the fitting parameters. The central-cell potential effect on resonant states is shown to be much larger than for excited localized states, whose eigenenergies being practically unchanged.

31. A.V. Antonov, V.Ya. Aleshkin, V.I. Gavrilenko, Z.F. Krasil'nik, A.V. Novikov, E.A. Uskova, and M.V. Shaleev. *MID IR photoconductivity in delta-doped GeSi/Si:B heterostructures with 2D holes gas.* Proc.12th Int. Symp. "Nanostructures: Physics and Technology", St. Petersburg, Russia, 2004, PP. 304-305

A new theoretical method for calculation of acceptor energy spectra in Si/SiGe quantum well heterostructures, taking into account the anisotropy effects has been developed. The impurity photoconductivity spectra in strained SiGe/Si:B quantum well heterostructures have been studied experimentally. In addition to the photoconductivity band resulted from the photoionization of boron acceptors in the bulk Si a new low-frequency band has been discovered. According to the calculation results the low-frequency band is attributed to the photoexcitation of acceptors in SiGe quantum wells.

32. Ya.E. Pokrovskiy, K.A. Khvalkovskiy. *A Spectoscopic Study of Ga-doped Ge, under Uniaxial Pressure.* JETP Letters, 2004, V. 80, PP. 581-584.

To identify optical transitions responsible for the excitation of a long wave stimulated radiation in a unaxially compressed Ga-doped Ge, the optical absorption and photoconductivity spectra of the material were investigated in a wide range of the pressure in [111] and [001] directions. The dependence of the valence band splitting between the branches of light and heavy holes in Ge as

a function of the applied pressure was found. Constants of deformation potential for valence band were determined.

33. N.S. Averkiev, A.E. Zhukov, Yu.L. Ivanov, P.V. Petrov, K.S. Romanov, A.A. Tonkikh, V.M. Ustinov, G.E. Zyrlin. *Energy structure of A$^+$ centers in quantum wells.* Semiconductors, 2004, V. 38, PP. 222-227.

In frames of zero radius potential method, a method of calculation of wave functions and binding energy for acceptor centers in quantum wells based on cubic semiconductors has been developed. In particular, an observed dependence of ground state energy of the positively charged deep acceptor in the AlGaAs QW is perfectly described by the proposed theory. Typical dimensions of wave functions of the localized states have been calculated. A charge carrier density distribution has been constructed for the deep acceptors localized near the surface. It has been shown that the non-spherically symmetrical charge distribution, observable in STM is conditioned by the initial cubic defect symmetry rather than by the casual deformations or electric fields.

34. Ya.E. Pokrovskiy, K.A. Khvalkovskiy. Spectroscopy of Ga-doped germanium under uniaxial compression. Semiconductors, 2005, V. 39, PP. 197-203.

The photoconductivity (due to photo-thermo impurity excitation) and absorption spectra of uniaxially stressed p-Ge were obtained with FTIR spectrometer. The spectra contain several lines corresponding to optical transitions between the ground and several excited acceptor states. The pressure dependence of acceptor states energies is determined.

35. V.Ya. Aleshkin, I.V. Erofeeva, V.I. Gavrilenko, A.V. Ikonnikov, D.V. Kozlov, O.A. Kuznetsov, D.V.Veksler *THz Spectroscopy of extremely Shallow Acceptors States in Ge/GeSi Multiple Quantum-Well heterostructures.* Acta Physica Polonica, 2005, V. 107, PP. 137-141.

New shallow acceptor magnetoabsorption lines in THz range have been discovered under bandgap photoexcitation in strained Ge/GeSi multiple-quantum well heterostrutures. It is shown both theoretically and experimentally, that the resonant absorption results from the photoionization of A$^+$-centers and from 1s-2p$_+$-type transitions from the ground state of the barrier-situated A^0 –centers into excited states in the 1st and 2nd electronic subbands. The shallowest discovered ground acceptor states (E$_B$ < 0.5 mev) are attributed to the :"barrier-spaced" acceptors (a hole bound with an acceptor ion in the neighboring Ge quantum well)**.**

36. A.V. Andrianov, A.O. Zakhar'in, I.N. Yassievich, N.N. Zinov'ev. *Spontaneous Terahertz Emission under Electrical Breakdown of a Shallow Acceptor in Ge.* Acta Physica Polonica, 2005, V. 107, PP. 142-146.

First measurements of spectra of the THz emission occurring under impact ionization of a shallow acceptor (Ga) in Ge are reported. The experiments were carried out at T= 5.5—5.7 K on p-Ge with N_A-N_D ~ 4x10^{14} cm^{-3}. The spectra were measured using a Fourier spectrometer. At the electric field close to the threshold of impurity breakdown, the electroluminescence spectrum shows two narrow emission lines with the maxima at 1.99 THz (8.2 meV) and 2.36 THz (9.7 meV), which correspond to the optical transitions between the excited states and the ground state of the acceptor. The spectrum contains also a broad emission band at ~ 3.15 THz (13 meV). This band is attributed to the optical transition of hot holes from the valence band to the ground state of acceptor. The contribution of these transitions increases with electric field. In addition, the optical transitions of holes between the states of heavy and light holes within the valence band appear in the spectrum at high electric fields. The quantum yield of THz spontaneous emission

of a sample 7x1.5x1.5x6 mm^3 is at the level of 10^{-8}. The results show that p-Ge can be used as the active media for THz electronic devices in 2 THz spectral region

37. M.S. Kagan, I.V. Altukhov, E.G. Chirkova, S.K. Paprotskiy, V.P. Sinis, I.N. Yassievich, J. Kolodzey. *Transient Characteristics of SiGe/Si QW Structures at Stimulated THz Emission.* Proc. "Nanophysics and nanoelectronics" Workshop, N.Novgorod, Russia, 2005, PP. 328-329 (in Russian).

It is shown that the stimulated THz emission in SiGe/n-Si QW structures is excited with the carrier injection through contacts in the case of low voltages or from the n-type Si substrate in the case of high voltages. The mechanism of intra-center population inversion in SiGe/Si structures is supposed to be due to acceptor ground state depopulation, which is in this case the result of either sweep-out of majority carriers or minority carrier injection.

38. I.V. Antonova, M.S. Kagan, V.I. Polyakov, L.L. Golik, and J. Kolodzey. *Effect of interface states on population of the quantum wells in SiGe/Si structures*. Phys. Stat. Sol., 2005, V. 2, PP. 1924-1928.

Recharging of electrically active defects in MBE-grown SiGe/Si heterostructures with both one and three SiGe quantum wells under applied voltage was studied. Based on measurements of capacitance–voltage and current–voltage characteristics and deep level transient spectroscopy, the electrically active centers and population of quantum wells were characterized as a function of Ge content.

39. I.V. Antonova, V.I. Obodnikov, M.S. Kagan, R.T. Troeger, S.K. Ray and J. Kolodzey. *Capacitance study of selectively doped SiGe/Si heterostructures*. Semicond. Sci. Technol. 2005, V. 20, PP. 335-339.

Capacitance studies of $Si/Si_{1-x}Ge_x/Si$ heterostructures with three $Si_{1-x}Ge_x$ layers selectively doped with boron are presented. A surface charge and carrier distributions in $Si_{1-x}Ge_x/Si$ heterostructures were found as a function of Ge content. The large positive charge observed at the surface of p-$Si/SiGe/Si$ heterostructures was shown to result from the surface segregation of Ge during the epitaxial growth. The effects of native oxide and additional annealing in hydrogen ambient on this charge were also found. It was found that population of quantum wells strongly increased after exposure of the $SiGe/Si$ structures under voltage

40. A.V. Antonov, V.Ya. Aleshkin, V.I. Gavrilenko, Z.F. Krasil'nik, A.V. Novikov, E.A. Uskova, M.V. Shaleev. *Negative Photoconductivity of Selectively Doped SiGe/Si : B Heterostructures with a Two-Dimensional Hole Gas in the Middle-Infrared Range*. Physics of the Solid State, 2005, V. 47, PP. 74-80.

The spectra of lateral photoconductivity in selectively doped SiGe/Si : B heterostructures with a two-dimensional hole gas are analyzed. It is revealed that the lateral photoconductivity spectra of these heterostructures exhibit two signals opposite in sign. The positive signal of the photoconductivity is associated with the impurity photoconductivity in silicon layers of the heterostructures. The negative signal of the photoconductivity is assigned to the transitions of holes from the SiGe quantum well to long-lived states in silicon barriers. The position of the negative photoconductivity signal depends on the composition of the quantum well, and the energy of the low-frequency edge of this signal is in close agreement with the calculated band offset between the quantum-confinement level of holes in the quantum well and the valence band edge in the barrier.

41. M.S. Kagan, I.V. Altukhov, E.G. Chirkova , S.K. Paprotskiy, V.P. Sinis, I.N. Yassievich, J. Kolodzey. *Transient Characteristics of SiGe/Si QW Structures at THz Lasing.* Proc 13th Int. Symp. "Nanostructures: Physics and Technology" St. Petersburg, Russia, 2005, PP. 242-243

Transient characteristics of SiGe-QW laser structures were studied. The excitation of stimulated THz emission is shown to be the result of carrier injection through contacts. The mechanism of intra-center population inversion caused by carrier injection is suggested.

42. E.E. Orlova, D.V. Kozlov, A.V. Antonov, J.N. Hovenier, T.O. Klaassen, A.J.L. Adam, M.S. Kagan, I.V. Altukhov, Q.V. Nguyen, D.A. Carder, P.J. Phillips, and B. Redlich. *Perspectives of acceptor lasing in strained SiGe structures.* Proc.13th Int. Symp. "Nanostructures: Physics and Technology" St. Petersburg, Russia, 2005, PP. 110-111.

The possibility of inverse population and lasing on acceptor transitions in strained SiGe structures is investigated. Intra-acceptor relaxation is studied using pump-probe method and the life time of the first excited state of boron acceptor in silicon is found to be about 0.5 ns. Acceptor spectrum in strained silicon is calculated. Strain values providing depletion of 1s state split off the ground state due to fast phonon assisted transitions and corresponding range of frequency tuning are determined.

43. A.M. Monakhov, K.S. Romanov, I.E. Panaiotti, N.S. Averkiev. *Spatial Structure of an individual deep acceptor in a cubic crystal.* International Journal of Nanoscience, 2006 (in print)

A method of calculation of wave functions and binding energy for acceptor centers in quantum wells in cubic semiconductors based on zero-radius potential method has been developed. Typical dimensions of wave functions of the localized states have been calculated. A charge carrier density distribution has been constructed for the deep acceptors localized near the surface.

44. M.S. Kagan, I. V. Altukhov, E. G. Chirkova , S. K. Paprotskiy, V. P. Sinis, I.N. Yassievich, J. Kolodzey. *Transient Characteristics of SiGe/Si QW Structures at THz Lasing.* International Journal of Nanoscience, 2006 (in print)
Transient characteristics of SiGe-QW laser structures were studied. The excitation of stimulated THz emission is shown to be the result of carrier injection through contacts. The mechanism of intra-center population inversion caused by carrier injection is suggested.

45. P.-C. Lv, X. Zhang, J. Kolodzey, M.A. Odnoblyudov, and I.N. Yassievich. *The effects of uniaxial compressive stress on the terahertz emission from phosphorus-doped silicon devices.* J. Appl. Phys., 2005, V. 98, P. 103511.

The effects of uniaxial compressive stress on the terahertz electroluminescence from P-doped silicon devices have been studied. A shift by ~0.5 THz in the emission peaks of donor state transitions: $2p_0$-$1s(E)$ and $3p_{+/-}$-$1s(E)$ has been observed for a stress of ~0.1 GPa along the [100] direction. Transitions from excited states to the strain split states of $1s(E)$ showed a pronounced polarization effect. Transitions involving the $1s(T_1)$ ground state, however, showed no polarization effect. These results suggest that it may be possible to realize a tunable impurity-doped silicon terahertz emitter by externally applied stress.

46. P.-C. Lv, R.T. Troeger, X. Zhang, T.N. Adam, J. Kolodzey, M.A. Odnoblyudov, and I.N. Yassievich. *Hot hole redistribution in impurity states of boron-doped silicon terahertz emitters.* J. Appl. Phys., 2005, V. 98, P. 093710.

The relative intensities of emission peaks from boron-doped silicon terahertz sources have been measured under various pumping conditions. These data have been analyzed to determine the hole occupations in the excited states. As the pumping current increased, the hole concentrations

increased approximately linearly. The hole population increased faster in the lower energy $1\Gamma^-_8$ state than in other excited states. At a fixed pumping current, the hole population decreased as temperature increased, but the decrease was slower for the $1\Gamma^-_8$ lower-energy state. These results suggest that to achieve terahertz emission at high temperatures it would be best to use dopants with transitions that have a strong oscillator strength from the lowest-energy excited state.

47. Towards Resonant-State THz Laser Based on Strained p-Ge and SiGe QW Structures/ First Annual Report on ISTC Project #2206p Moscow. IRE RAS.

48. Towards Resonant-State THz Laser Based on Strained p-Ge and SiGe QW Structures/ Second Annual Report on ISTC Project #2206p, Moscow, IRE .RAS.

49. Towards Resonant-State THz Laser Based on Strained p-Ge and SiGe QW Structures/ Third Annual Report on ISTC Project #2206p, Moscow, IRE RAS.

50. Towards Resonant-State THz Laser Based on Strained p-Ge and SiGe QW Structures/ Final Report on ISTC Project #2206p, Moscow, IRE RAS.

List of presentations at conferences and meetings with abstracts.

1. V.Ya. Aleshkin, V.I. Gavrilenko, D.V. Kozlov. *Shallow acceptors in Si/SiGe quantum well heterostructures*. 10th Int. Conf. on Shallow-Level Centers in Semiconductors. Warsaw, Poland, July 2002. Poster.

New shallow acceptor magnetoabsorption lines in THz range have been discovered under bandgap photoexcitation in strained Ge/GeSi multiple-quantum well heterostrutures.

2. V.Ya. Aleshkin, A.V. Gavrilenko, V.I. Gavrilenko, D.V. Kozlov, A.T. Dalakjan, V.N. Tulupenko. *On the impurity photoconductivity of uniaxially stressed p-Ge*. 10th Int. Conf. on Shallow-Level Centers in Semiconductors. Warsaw, Poland, July 2002. Poster.

Far infrared photoconductivity of stressed p-Ge in the high frequency spectral range corresponding to transitions from the acceptor ground state to the split-off subband has been observed for the first time. The theoretical approach for calculation of the energies and wave function of localized, resonant and the continuum states of shallow acceptors in the uniaxially compressed Ge was developed.

3. V.Ya. Aleshkin, A.V. Antonov, V.I. Gavrilenko, D.V. Kozlov, Z.F. Krasil'nik, D.N. Lobanov, A.V. Novikov. *Impurity photoconductivity in SiGe/Si:B quantum well heterostructures*. "Nanophotonics" Workshop, Nizhny Novgorod, Russia, March 2003. Oral.

The photoconductivity spectral measurements carried out at different temperatures and different bias voltages have shown that the discovered low-frequency photoconductivity band is connected with the photoionization of boron acceptors in GeSi QWs.

4. S.V. Svetlov, V.Yu. Chalkov, V.G. Shengurov, V.I. Gavrilenko, M.N. Drozdov, Yu.N. Drozdov, Z.F. Krasil'nik. *Growth of multilayer $Si/Si_{1-x}Ge_x$ structures with δ–doped layers by sublimational MBE of Si in german environment*. "Nanophotonics" Workshop, Nizhny Novgorod, Russia, March 2003. Poster.

The growth conditions of multilayer structures containing thin (20-35 nm) layers of SiGe solid solution selectively doped with B or Ga by sublimational MBE of Si in german environment have been investigated.

5. I.N. Yassievich. *Donor states in modulation-doped Si/SiGe heterostructures*. "Nanophotonics" Workshop, Nizhny Novgorod, Russia, March 2003. Oral.

Non-variational method for calculation of resonant as well as localized donor states parameters has been developed. It can be also used for evaluation of wavefunctions of the donor states and calculation of optical absorption spectrum for Si/Si_xGe_{1-x}.

6. I.V. Altukhov, E.G. Chirkova, V.P. Sinis, M.S. Kagan, R.T. Troeger, S.K. Ray, J. Kolodzey. *Effect of Potential and Doping Profiles on Excitation of Stimulated THz Emission of SiGe/Si Quantum Well Structures*. "Nanophotonics" Workshop, Nizhny Novgorod, Russia, March 2003. Oral.

The stimulated THz emission is shown to be excited in $Si/Si_{1-x}Ge_x/Si$ quantum-well structures with Ge content in SiGe alloy x=0.07, 0.1, and 0.15. In the structures with x=0.26, 0.32, and 0.48, the stimulated THz emission did not arise. The energy of lines observed in the emission spectra depends on the Ge content in SiGe alloy increasing with increasing x. Two different regimes for excitation of the emission in the same sample are observed.

7. V.Ya. Aleshkin, A.V. Antonov, V.I. Gavrilenko, D.V. Kozlov, Z.F. Krasil'nik, D.N. Lobanov, A.V. Novikov. *Impurity photoconductivity in SiGe/Si:B multi-quantum-well heterostructures*. 11th Int. Symp. "Nanostructures: Physics and Technology", St.Petersburg, Russia, June 2003. Oral.

The impurity photoconductivity spectra in strained SiGe/Si:B quantum well structures have been studied experimentally at $T \geq 4.2$ K. In addition to the photoconductivity band resulted from the photoionization of boron acceptors in the bulk Si the new low-frequency band has been found.

8. M.S. Kagan, G.M. Min'kov, N.G. Zhdanova, E.G. Landsberg, I.V. Altukhov, K.A. Korolev, R. Zobl, E. Gornik. *Weak Localization of Holes in Acceptor-Doped SiGe Quantum Wells*. 11th Int. Symp. "Nanostructures: Physics and Technology", St.Petersburg, Russia, June 2003. Poster.

Negative magnetoresistance is observed in boron-doped SiGe/Si quantum-well structures. The effect of a random potential caused by charged boron delta-layers in barriers on quantum corrections to the conductivity is found. Elastic and inelastic scattering times of holes as well as the magnitude of the random potential are determined.

9. J. Kolodzey, T.N. Adam, R.T. Troeger, I.N. Yassievich, and M.S. Kagan. *TeraHertz Sources and Detectors Based on SiGe Nanostructures*. 11th Int. Symp. "Nanostructures: Physics and Technology", St.Petersburg, Russia, June 2003. Invited.

THz luminescence was produced by three different types of sources: intersubband transitions in SiGe quantum wells, resonant-state transitions in boron-doped strained quantum wells, and impurity transitions in doped Si layers. These results suggest that SiGe nanotechnology is attractive for THz device applications.

10. Yu.N. Drozdov, L.V. Krasilnikova, D.N. Lobanov, A.V. Novikov, M.V. Shaleev, M.V. Stepikhova, N.V. Vostokov, A.N. Yablonskii, Z.F. Krasilnik, A.N. Ankudinov, M.S. Dunaevskii, I.P. Soshnikov, A.N. Titkov, V. Dzhagan, V.U. Yukhymchuk, and M.Ya. Valakh. *Self-assembled GeSi nanoislands on Si(001)*. NATO Advanced Research Workshop «Quantum Dots: Fundamentals, Applications and Frontiers», Crete, June 2003. Oral.

The results of investigations into the growth and optical properties of single and multilayer Ge(Si)/Si(001) structures grown at different Ge deposition temperatures are presented. It is shown that the sizes and surface density of the islands can be varied in a wide range by altering the Ge deposition temperature (T_g): from nanometer scale islands for high T_g to small quantum dots with a height of ~ 1 nm and a surface density of $> 10^{11}$ cm^{-2}. The GeSi alloy formation in islands grown at $T_g > 580^0$C was observed by X-ray diffraction, Raman scattering and selective etching. The alloy formation is caused by a strain-driven Si diffusion in islands. The dependence

of island composition on T_g was experimentally measured and found to drastically affect the sizes and shape of the islands.

11. M.A. Odnoblyudov, A.A. Prokofiev, I.N. Yassievich. *Hot Carriers Effect on Strained p-Ge Resonant State Laser Operation.* 13th International Conference on Nonequilibrium Carrier Dynamics in Semiconductors, Modena, Italy, July, 2003. Poster

Hot hole kinetics in strained p-Ge under an applied electric field is studied and heavy and light hole distribution functions are found as a solution to the Boltzmann kinetic equation, which includes interactions with acoustic and optical phonons, as well as resonant and non-resonant ionized impurity scattering. Non-equilibrium population of the localized acceptor states is obtained as a solution to system of rate equations within the two-level model for an impurity level structure. Conditions for the formation of the intra-center population inversion are studied as a function of the electric field and external strain. We have obtained that the population inversion is formed in a wide range of electric fields. Net gain at the THz frequencies is calculated using the non-equilibrium hot hole distribution function and the localized states population.

12. M.A. Odnoblyudov, A.A. Prokofiev, I.N. Yassievich, I.V. Altukhov, V.P. Sinis, M.S. Kagan. *Hot carrier effect on resonant state THz laser operation.* 13th International Conference on Nonequilibrium Carrier Dynamics in Semiconductors, Modena, Italy, July, 2003. Poster

Hot-hole kinetics in uniaxially strained p-Ge has been investigated theoretically. Calculated distribution functions of holes in valence band have been used to determine localized and resonant acceptor states populations. Optical gain spectrum in THz band has been obtained. It has been shown than the positive gain at the intraband transition frequency occurs when electric field strength is in the range 1-5 V/cm. The results are in good agreement with experimental data.

13. I.V. Altukhov, E.G. Chirkova, V.P. Sinis, M.S. Kagan, R.T. Troeger, S.K. Ray, J. Kolodzey, A.A. Prokofiev, M.A. Odnoblyudov, and I.N. Yassievich. *Effect of potential and doping profiles on excitation of stimulated THz emission of SiGe/Si quantum-well structures.* 13th International Conference on Nonequilibrium Carrier Dynamics in Semiconductors, Modena, Italy, July, 2003. Poster

Studies of stimulated THz emission from boron-doped $Si/Si_{1-x}Ge_x/n$-Si quantum-well structures of various potential and doping profiles are presented. In the single-QW structures with the optical resonator, the stimulated THz emission is observed only for Ge content x=0.07, 0.1, and 0.15. Two different regimes for excitation of the emission are observed in the same sample depending on charging the surface and thermal ionization of donors in the substrate.

14. I.V. Altukhov, E.G. Chirkova, V.P. Sinis, M.S. Kagan, R.T. Troeger, S.K. Ray, J. Kolodzey, A.A. Prokofiev, M.A. Odnoblyudov, and I.N. Yassievich. *Effect of Potential and Doping Profiles on Excitation of Stimulated THz Emission of SiGe/Si Quantum Well Structures.* 22nd International Conference on Defects in Semicond., Aahrus, Denmark, July, 2003. Poster.

The conditions and regimes of excitation of stimulated THz emission in $Si/Si_{1-x}Ge_x/Si$ quantum-well structures with different Ge content (0.07 to 0.48) and potential profile (single and triple QWs) are investigated.

15. M.S. Kagan, G.M. Min'kov, N.G. Zhdanova, E.G. Landsberg, I.V. Altukhov, K.A. Korolev, R. Zobl, E. Gornik. *Weak Localization of Holes in Acceptor-Doped SiGe Quantum Wells.* 22nd International Conference on Defects in Semicond., Aahrus, Denmark. July, 2003. Poster.

Negative magnetoresistance is observed in boron-doped SiGe/Si quantum-well structures. The effect of a random potential caused by charged boron delta-layers in barriers on quantum corrections to the conductivity is found. Elastic and inelastic scattering times of holes as well as the magnitude of the random potential are determined.

16. V.Ya. Aleshkin, V.I. Gavrilenko, D.V. Kozlov, Z.F. Krasil'nik, D.N. Lobanov, A.V. Novikov. *Impurity photoconductivity in SiGe/Si:B multi-quantum-well heterostructures.* 22nd International Conference on Defects in Semicond., Aahrus, Denmark, July, 2003. Poster.

A new theoretical method for calculation of acceptor energy spectra in Si /SiGe quantum well heterostructures, taking into account the anisotropy effects has been developed. The impurity photoconductivity spectra in strined SiGe/ Si:B quantum well heterostructureshave been studied experimentally. In addition to the photoconductivity band resulting from the photoionization of boron acceptors in the bulk Si a new low-frequency band has been discovered. According to the calculation results the low-frequency band is attributed to the photoexistation of acceptors in SiGe quantum wells

17. V.Ya. Aleshkin, A.V. Antonov, V.I. Gavrilenko, D.V. Kozlov, Z.F. Krasil'nik, D.N. Lobanov, A.V. Novikov. *Localized and resonant states of shallow acceptors in SiGe/Si:B quantum well heterostructures*. 6th Russian. Conf. Phys. Semicond., St.Petersburg, October 2003. Poster.

Far infrared photoconductivity of stressed p-Ge in the high frequency spectral range corresponding to transitions from the acceptor ground state to the split-off subband has been observed for the first time. The theoretical approach for calculation of the energies and wave function of localized, resonant and the continuum states of shallow acceptors in the uniaxially compressed Ge was developed.

18. I.V. Antonova, M.S. Kagan, R.T. Troeger, S.K. Ray, and J. Kolodzey. *Capacitance Study of Multilayered SiGe/Si Heterostructures*. 6th Russian. Conf. Phys. Semicond., St.Petersburg, October 2003. Oral.

Capacitance study of $Si_{1-X}Ge_X$/Si heterostructures with three $Si_{1-X}Ge_X$ layers (x value was varied in range of 0.15 – 0.25) selectively doped with boron has been made. A surface charge and carrier distributions in the structures were found as a function of Ge content. The effects of surface oxide and additional annealing in hydrogen ambient were also investigated. The large positive charge observed at the surface of the p-SiGe/Si heterostrucrures is shown to result from the surface segregation of Ge during epitaxial growing. It was found that population of quantum wells can be increased by exposure of the SiGe/Si structures under high voltage.

19. M.S. Kagan, I.V. Altukhov, E.G. Chirkova, V.P. Sinis, R.T. Troeger, S.K. Ray, J. Kolodzey, A.A. Prokofiev, M.A. Odnoblyudov, and I.N. Yassievich. *Stimulated Terahertz Emission of Strained p-Ge and SiGe/Si Structures.* 6th Russian. Conf. Phys. Semicond., St.Petersburg, October 2003. Invited.

The origin and properties of stimulated terahertz (THz) emission of uniaxially compressed p-Ge and strained SiGe/Si structures doped with shallow acceptors are discussed. This emission is associated with the stimulated optical transitions between resonant and localized acceptor states.

20. M.S. Kagan, I.V. Altukhov, V.P. Sinis, E.G. Chirkova, I.N. Yassievich, and J. Kolodzey. *Stimulated Terahertz Emission of Strained p-Ge and SiGe/Si Structures.* Russian Conf. "Photonics-2003", Novosibirsk, Russia, August 2003. Invited.

The origin and properties of stimulated terahertz (THz) emission of uniaxially compressed p-Ge and strained SiGe/Si structures doped with shallow acceptors are discussed. This emission is associated with the stimulated optical transitions between resonant and localized acceptor states.

21. M.A. Odnoblyudov, A.A. Prokofiev, I.N. Yassievich, I.V. Altukhov, V.P. Sinis, M.S. Kagan. *Resonant Impurity States Semiconductor THz Lasers.* IRMMW2003, Otsu, Japan, September, 2003. Oral.

Comprehensive theoretical study of CW operation mode of the Resonant State THz lasers on the basis of strained p-Ge is performed. The conditions for population inversion are analyzed and calculation of THz gain is performed.

22. A.V. Novikov, O.A. Kuznetsov, Yu.N. Drozdov, V.A. Perevoshchikov, M.V. Shaleev, N.V. Vostokov, and Z.F. Krasilnik. " *The relaxed $Si_{1-x}Ge_x/Si(001)$ buffer layer with low surface roughness*". 5th International Russian-Ukrainian seminar "Nanophysics and nanoelectronics", June 2004, St. Petersburg, Russia. Oral.

The relaxed compositionally graded $Si_{1-x}Ge_x/Si(001)$ buffer layer with low threading dislocations density have been grown by chemical vapor deposition method. The roughness of surface of the grown structures has been reduced by the chemical mechanical polishing down to values compared with the roughness of Si(001) substrates. It is shown that the fabricated $Si_{1-x}Ge_x/Si(001)$ buffer layers with low threading dislocations density and smooth surface can be used as "artificial substrates" for growth of Ge/Si heterostructures by molecular beam epitaxy method.

23. A.V. Antonov, V.Ya. Aleshkin, V.I. Gavrilenko, Z.F. Krasil'nik, A.V. Novikov, E.A. Uskova, and M.V. Shaleev. *MID IR photoconductivity in delta-doped GeSi/Si:B heterostructures with 2D holes gas*. 12th Int. Symp. "Nanostructures: Physics and Technology", St. Petersburg, Russia, June 2004. Poster.

A new theoretical method for calculation of acceptor energy spectra in Si/SiGe quantum well heterostructures, taking into account the anisotropy effects has been developed. The impurity photoconductivity spectra in strained SiGe/Si:B quantum well heterostructures have been studied experimentally. In addition to the photoconductivity band resulted from the photoionization of boron acceptors in the bulk Si a new low-frequency band has been discovered. According to the calculation results the low-frequency band is attributed to the photoexcitation of acceptors in SiGe quantum wells.

24. V.Ya. Aleshkin, A.V. Antonov, V.I. Gavrilenko, Z.F. Krasil'nik, A.V. Novikov, M.V. Shaleev, E.A. Uskova. *Negative mid IR photoconductivity in selectively doped SiGe/Si:B QW heterostructures with two-dimensional hole gas*. "Nanophotonics Workshop, IPM RAS, Nizhny Novgorod, May 2004. Oral.

THz photoconductivity of $Si_{1-x}Ge_x/Si$ (x=0.12-0.3) single-QW structures with δ-doped barriers has been studied. The doped region in the selectively doped structures was 50 nm wide. It was separated by 20 nm Si spacer layer from the QW interface. The sheet boron concentration was $4*10^{12}$ cm^{-2}. A low-frequency photoconductivity band in the range of $210 \div 330$ cm^{-1} related to boron ionization in the SiGe QW was observed, as well as the photoconductivity in the range of $330 \div 700$ cm^{-1} related to boron ionization in bulk Si. In addition to the impurity bands in the photoconductivity spectra, a wide band with spectral position being depended on Ge content in QW was found. The high-frequency photoconductivity band is supposed due to hole transitions from QW into long-living states in Si barriers, which leads to the negative photoconductivity.

25. A.A. Prokofiev, M.A. Odnobludov, V.M. Chistyakov, I.N. Yassievich, D.V. Kozlov. *Influence of short-range potential on energies of shallow acceptors states in strained semiconductors.* "Nanophotonics Workshop, IPM RAS, Nizhny Novgorod, May 2004. Oral.

Effect of central-cell corrections (chemical shift) on the eigenenergy of the lowest resonant acceptor state in iniaxially stressed Ge has been studied. The acceptor wavefunction has been expanded in termes of hole wavefunctions in the absence of the acceptor Coulomb potensial (plane waves). Resonant states in the energy continuum have been separated by finding a maximum of an upper subband share in the acceptor wavefunction expansion. The chemical shift has been taken into account via additional model potential of the spherically symmetric quantum well, the well radius and depth being the fitting parameters. The central-cell potential effect on resonant states is shown to be much larger than for excited localized states, whose eigenenergies being practically unchanged.

26. I.V. Altukhov, E.G. Chirkova, V.P. Sinis, M.S. Kagan, R.T. Troeger, S.K. Ray, J. Kolodzey, A.A. Prokofiev, M.A. Odnoblyudov, and I.N. Yassievich. *Stimulated Terahertz Emission of Strained p-Ge and SiGe/Si Structures.* XV Ural International Winter School on Phys. Semicond. February, 2004, Ekaterinburg, Russia. Invited.

The stimulated THz emission of uniaxially compressed p-Ge and strained SiGe/Si structures doped with shallow acceptors is discussed. The stimulated emission is explained by a population inversion of a resonant acceptor state with respect to the impurity states in the gap. 27. I.V. Antonova, M.S. Kagan, V.I. Polyakov, L.L. Golik and J. Kolodzey. *Effect of interface states on population of the quantum wells in SiGe/Si structures.* Phys. Stat.Sol. C, 2(6), 1924-1928 (2005). Int. Conf. on Extendeing Defects in Semiconductors (EDS2004), June 2004, Chernogolovka, Moscow Distr., Russia. Oral.

Recharging of electrically active defects in MBE-grown SiGe/Si heterostructures with both one and three SiGe quantum wells under applied voltage was studied. Based on measurements of capacitance–voltage and current–voltage characteristics and deep level transient spectroscopy, the electrically active centers and population of quantum wells were characterized as a function of Ge content.

28. M.S. Kagan, I.V. Altukhov, V.P. Sinis, E.G. Chirkova, R.T. Troeger, S.K. Ray, J. Kolodzey, M.A. Odnoblyudov, A.A. Prokofiev, I.N. Yassievich. *Stimulated THz Emission of Strained p-Ge and SiGe/Si Structures.* Ultrafast Phenomena in Semiconductors (UFPS-12), Vilnius, Lithuania, August 2004. Invited.

Studies of the emission spectra for boron-doped $Si/Si_{1-x}Ge_x/Si$ quantum well structures of various potential and doping profiles are presented. We also present evidence that the lasing is due to population inversion between resonant and localized acceptor states similar to bulk *p*-Ge. Conditions for continuous-wave operation of RSL are discussed.

29. I.N. Yassievich, M.A. Odnoblyudov, A.A. Prokofiev. *Polaron Effects for Shallow Centers in Semiconductors.* Ultrafast Phenomena in Semiconductors (UFPS-12), Vilnius, Lithuania, August 2004. Oral.

The results of the theoretical consideration of polaron effects for shallow Coulomb centers induced by the interaction of bound carriers with both acoustic and optical phonons is presented. The calculations of polaron energy shift have been carried out for ground states of donors and acceptors in Si, ZnSe and GaN. The values obtained for acceptor are of the order of 3 meV in Si and 30 meV for ZnSe. The results obtained have been used to analyze recent experimental data on frequency dependence of the donor-acceptor luminescence in ZnSe as well as its quenching by THz radiation.

30. A.V. Andrianov, A.O. Zakhar'in, I.N. Yassievich, N.N. Zinov'ev. *Spontaneous Terahertz Emission under Electrical Breakdown of a Shallow Acceptor in Ge*. Ultrafast Phenomena in Semiconductors (UFPS-12), Vilnius, Lithuania, August 2004. Poster.

First measurements of spectra of the THz emission occurring under impact ionization of a shallow acceptor (Ga) in Ge are reported.

31. V.Ya. Aleshkin, I.V. Erofeeva, V.I. Gavrilenko,A.V. Ikonnikov, D.V. Kozlov, O.A. Kuznetsov, D.V. Veksler. *THz Spectroscopy of extremely Sallow Acceptors States in Ge/GeSi Multiple Quantum-Well heterostructures*. Ultrafast Phenomena in Semiconductors (UFPS-12), Vilnius, Lithuania, August 2004. Poster.

New shallow acceptor magnetoabsorption lines in THz range have been discovered under bandgap photoexcitation in strained Ge/GeSi multiple-quantum well heterostrutures.

32. A.V. Andrianov, A.O. Zakharin, I.N. Yassievich, N.N. Zinov'ev. *Far Infrared Electroluminescence under Impact Ionization of a Shallow Acceptor in Ge*. 6th Int. Conf. "Mid-Infrared Optoelectronics Materials and Devices", St. Petersburg, June, 2004. Oral.

Spontaneous THz emission under the electric breakdown of a shallow acceptor (Ga) in Ge have been studied. Narrow lines with maxima at ~1.99 THz (8.2 meV) и ~2.36 THz (9.7 meV) which correspond to the optical transitions of holes from excited states of the impurity to the ground state. A broad emission band with the maximum at 3.15 THz (13 meV) is observed also. This band corresponds to the optical transitions of hot holes (an effective temperature is ~26 K) from valence band to the impurity ground state. The maximum in the electroluminescence coincides with the threshold of the photoconductivity signal.

33. N.V. Agrinskaja, N.S. Averkiev, Yu.L. Ivanov, K.S. Romanov, P.V. Petrov, V.M. Ustinov. *Photoluminescent and kinetic properties of A^+ centers in quantum well*. 27th Int. Conf. on the Phys. of Semicond. (ICPS -27), Flagstaff, Arisona, USA, 2004. Poster.

Experimental and theoretical studies of A^+ centers in GaAs/AlGaAs QW structures are presented. Transport and far-IR optical properties are studied.

34. M.S. Kagan, I.V. Altukhov, E.G. Chirkova, S.K. Paprotskiy, V.P. Sinis, I.N. Yassievich, J. Kolodzey. *Transient Characteristics of SiGe/Si QW Structures at Stimulated THz Emission*. "Nanophysics and nanoelectronics" workshop, N.Novgorod, Russia, March 2005. Poster.

Transient characteristics of SiGe-QW laser structures were studied. The excitation of stimulated THz emission is shown to be the result of carrier injection through contacts. The mechanism of intra-center population inversion caused by carrier injection is suggested.

35. M. S. Kagan, I. V. Altukhov, E. G. Chirkova , S. K. Paprotskiy, V. P. Sinis, I. N. Yassievich, J. Kolodzey. *Transient Characteristics of SiGe/Si QW Structures at THz Lasing*. 13th Int. Symp. "Nanostructures: Physics and Technology" St. Petersburg, Russia, June 2005. Poster.

The cause and conditions for excitation of THz emission in SiGe structures in the low-current regime were studied. The mechanism of intra-center population inversion caused by carrier injection is suggested.

36. E.E. Orlova, D.V. Kozlov, A.V. Antonov, J.N. Hovenier, T.O. Klaassen, A.J.L. Adam, M.S. Kagan, I.V. Altukhov, Q.V. Nguyen, D.A. Carder, P.J. Phillips, and B. Redlich. *Perspectives of acceptor lasing in strained SiGe structures*. 13th Int. Symp. "Nanostructures: Physics and Technology" St. Petersburg, Russia, June 2005. Poster.

The possibility of inverse population and lasing on acceptor transitions in strained SiGe structures is investigated. Intra-acceptor relaxation is studied using pump-probe method and the

life time of the first excited state of boron acceptor in silicon is found to be about 0.5 ns. Acceptor spectrum in strained silicon is calculated. Strain values providing depletion of 1s state split off the ground state due to fast phonon assisted transitions and corresponding range of frequency tuning are determined.

37. I.V. Antonova, L.L. Golik, M.S. Kagan, V.I. Polyakov, A.I. Rukavischnikov, N.M. Rossukanyi and J. Kolodzey. Q*uantum well related conductivity and deep traps in SiGe/Si structures*. Int. Conf. "Gettering and defect engineering in semiconductor physics" (GADEST-2005), Nice, France, July 2005. Poster.

Studies of vertical electrical transport and traps in SiGe/Si QW structures of low background doping level are presented. Temperature activation of holes from a quantum well was found to determine the vertical current through Si/SiGe/Si structures at T > 160 K. At lower temperatures (T < 130 K), the current mechanism is attributed to a thermally activated tunneling of holes from quantum well. Deep traps of high concentration (10^{11} – 10^{12} cm^{-2}) are observed in the Si/SiGe/Si structures. Traps are most likely as recombination centers at the QW interface.

38. M.S. Kagan. "*Stimulated Terahertz Emission of Strained p-Ge and SiGe/Si Structures*". Russian-French Workshop on Nanosciences and Nanotechnologies, August 2005, Lille, France. Oral.

The origin and properties of stimulated terahertz emission of uniaxially compressed p-Ge and strained SiGe/Si quantum-well structures doped with shallow acceptors are discussed. The THz emission is associated with the stimulated optical transitions between resonant and localized acceptor states. Spectra of the emission are presented. The regimes of emission excitation and possibility of cw operation are examined.

39. M.S. Kagan. "*Stimulated Terahertz Emission of Strained p-Ge and SiGe/Si Structures*". International Conference on MEMS and Semiconductor Nanotechnology, December 2005, Kharagpur, India. Oral.

The results on THz lasing in strained p-Ge and SiGe/Si QW structures are presented. The origin of population inversion is discussed. The lasing is attributed to the population inversion of strain-induced resonant-states.

40. M.S. Kagan, I.V. Altukhov, S.K Paprotskiy, V.P Sinis, I.N Yassievich, and J. Kolodzey. *Carrier Injection as a Cause of THz Lasing Excitation in SiGe/Si QW Structures.* 28th Int. Conf. Phys. Semicond. (ICPS 2006), Vienna, Austria, July 2006. Poster, accepted.

The mechanism of THz emission excitation in boron-doped strained SiGe/n-Si structures is suggested consisted of two steps: non-stationary electron injection through contacts into n-Si substrate and, in turn, electron injection from the substrate into SiGe layer resulting in a depopulation of acceptor states in SiGe QW and invertion population of acceptor resonant states.

41. M.S. Kagan, I.V. Altukhov, S.K Paprotskiy, V.P Sinis, I.N Yassievich, and J. Kolodzey. *Carrier Injection as a Cause of THz Lasing Excitation in SiGe/Si QW Structures.* 12th Int. Conf. on High Pressure Semiconductor Physics (HPSP-12), August 2006, Barcelona Spain. Oral, accepted.

The evolution of THz emission and current along the SiGe layer of SiGe/Si QW structure at the leading front of voltage pulse was studied. The contact related phenomena observed are explained in terms of excitation of space-charge waves. The essential role of the injection was confirmed by means of probe measurements. The mechanism of THz emission excitation in boron-doped strained SiGe/n-Si structures is suggested.

42. M.S. Kagan, I.V. Altukhov, V.P. Sinis, E.G. Chirkova, S.K. Paprotskiy, I.N. Yassievich, M.A. Odnoblyudov, A. A. Prokofiev, and J. Kolodzey. *Stimulated THz Emission of Strained p-Ge and SiGe/Si Quantum-Well Structures Doped with Shallow Acceptors.* 2nd International "SiGe & Ge: Materials, Processing, and Devices" Symposium (2006 ECS confs) Cancun, Mexico, October 29-Nov. 3, 2006. Invited, accepted.

The data on the stimulated THz emission in uniaxially compressed p-Ge and strained SiGe structures doped with shallow acceptors are presented. It is shown that the emission is the result of electric field-induced population inversion of strain-split acceptor states. The necessary condition for the inversion is the resonant state appearance. For p-Ge, the possibility of a strong frequency tuning by stress is demonstrated. It is also shown that SiGe structures δ-doped with boron are promising for realization of resonant-state laser (RSL) operating in THz region. Spectra of the emission are presented. The regimes of emission excitation and possibility of cw operation are examined.