

VILNIUS UNIVERSITY  
SEMICONDUCTOR PHYSICS INSTITUTE

**Aurimas Čerškus**

**EFFECT OF BERYLLIUM AND SILICON IMPURITIES  
ON RADIATION FROM GaAs/AlAs QUANTUM WELLS**

Summary of doctoral dissertation

Physical sciences, physics (02 P), semiconductor physics (P 265)

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The doctoral dissertation is available for review at the libraries of the Semiconductor Physics Institute and Vilnius University.

VILNIAUS UNIVERSITETAS  
PUSLAIDININKIŲ FIZIKOS INSTITUTAS

**Aurimas Čerškus**

**BERILIO IR SILICIO PRIEMAIŠŲ ĮTAKA GaAs/AlAs  
KVANTINIŲ ŠULINIŲ SPINDULIUOTEI**

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## Introduction

The semiconductor nanostructures are grown using modern technology methods. Such structures are grouped into two-dimensional (2D), named quantum wells (QWs), one-dimensional (1D), named quantum wires, and zero-dimensional (0D), named quantum dots. The investigation and application of quantum wells and superlattices are one of the most developing areas of solid-state physics. This thesis focus on the physical properties of GaAs/AlAs quantum wells. They differ from GaAs/Al<sub>x</sub>Ga<sub>1-x</sub>As quantum wells because they achieve a higher barrier height and thereby obtain maximum energy levels splitting in these quantum wells.

The properties of doped quantum wells differ from bulk crystals, where the impurity binding energy is strictly defined. Changing the width of the quantum well does not only change the quantum well energy spectra, but also change the impurity binding energy, thus providing more possibilities for creating various optoelectronic devices. Different energy levels for optical transition can be desinged using the fundamental properties of QW, such as changing its geometric size. This feature is applicable when making devices with various wavelength radiation, for example, lasers or photodetectors. Contrary to bulk crystal devices, quantum wells can have electron transition in the same band between subbands. This effect is used in the design of quantum well infrared photodetectors and quantum cascade lasers.

At present, both infrared and terahertz photodetectors and emitters are designed and developed within the research community, thus being dependent on the availability of a broadband or technologically variable parameter device. By taking advantage of charge carrier transitions through impurities that falls within this region, such impurity doped wells will realise the full potential of creating this kind of devices. Of the different types of quantum well infrared detectors that have been created, GaAs/Al<sub>x</sub>Ga<sub>1-x</sub>As, with  $x \leq 0.4$ , quantum wells technology is the most common. However, due to the promising nature of GaAs/AlAs QWs, the application of this technology in the development of these devices is being investigated.

This work have therefore focused on the research of the photoluminescence (PL) properties of undoped and Be acceptor or Si donor doped GaAs/AlAs QWs. We believe,

that the results obtained will aid both the design and device development that is dependant on the properties of impurities in quantum wells. The work will further help to understand the underlying processes found in impurity doped quantum wells.

### ***The aim of the work***

To investigate the influence of beryllium acceptor and silicon donor impurities on photoluminescence spectra of GaAs/AlAs multiple quantum wells (MQWs) from liquid helium to room temperature. To define the influence of the impurities type and concentration on radiation of different width GaAs/AlAs quantum wells.

### ***Goals of the work***

1. To determine the influence of the impurities on intrinsic radiation. To describe theoretically the excitonic radiation for different widths of the quantum wells. To compare the experimental results with theoretical calculations.

2. To analyse impurities related photoluminescence in GaAs/AlAs MQWs. To ascertain the dependence of the impurity related radiation line shape as a function of QW width and to describe it theoretically.

3. To research experimentally the influence of the phonons on impurities related radiation in GaAs/AlAs QWs. To ascertain the nature of phonon replicas and their relation with Huang-Rhys factor. To determine the value of Huang-Rhys factor in Be  $\delta$ -doped GaAs/AlAs MQWs and to compare these values to theoretical calculations.

4. To research the PL spectra peculiarities of highly  $\delta$ -doped GaAs/AlAs MQWs. To investigate the conditions and obtain the results of insulator-metal Mott transition in quantum wells.

### ***Scientific novelty***

The literature referring to experimental works on the optical properties of GaAs/AlAs MQWs are limited. The results presented in the dissertation do not only provide data about optical properties of GaAs/AlAs QW, but also presents new information about the influence of impurities on the optical properties. New facts about the interaction of impurities related radiation with lattice vibrations, such as longitudinal optical (LO) phonons that creates phonon replicas, have also been presented.

The asymmetry of impurity related radiation lineshapes has been determined from the fractional dimensional space approach. The dependence of Huang-Rhys factor on quantum well width has also been theoretically calculated using the same approach. The two-dimensional expression of the Huang-Rhys factor has been obtained.

This dissertation also presents experimental results about Mott transition in *p*-type QWs.

### ***Defended propositions***

The impurities do not only influence excitonic radiation but also generate their own asymmetric impurity related recombination spectra.

The interaction of impurities related radiation with longitudinal optical phonons will create phonon replicas. The Huang-Rhys factor describes the intensity of the phonon replicas. This factor increases when the width of the GaAs/AlAs quantum decreases.

Two-dimensional structures need higher concentration of impurities for triggering insulator-metal Mott transition to occur. A new structure of subbands forms in QW above the Mott transition.

### ***Approval and publication of the results***

Eleven presentations have been made on the topic of the dissertation: three at the national conference “Lithuanian National Conference of Physics” (2005, 2009) and eight at the international conferences “International symposium of Ultrafast Phenomena in Semiconductors” (2004, 2007), “Advanced optical materials and devices” (2005), “Modulated Semiconductor Structures” (2007), “Radiation interaction with material and its use in technologies” (2008). Six of them are included in the dissertation.

Thirteen scientific publications have been published on the topic of the dissertation, of which eight have been included in the dissertation. Eleven articles have been published in journals included in the database of the Institute of Scientific Information. Two articles have been published in revised journals from the list of international database approved by the Research Council of Lithuania.

## **Structure of doctoral dissertation**

The dissertation has been written in Lithuanian. It consists of 5 chapters. In total, there are 114 typewritten pages with 43 figures and 7 tables. The dissertation starts with introduction, literature overview, chapter about samples and measuring technique. The obtained experimental and theoretical results are discussed in three chapters with their own conclusions. The thesis ends with seven formulated main conclusions, list of references and scientific publications of the author on the topic of the dissertation.

## **Content of doctoral dissertation**

### **“Introduction”**

The motivation, aim and goals of the work, scientific novelty, defended propositions, approval and publication of the results are presented in this section.

### **Chapter 1. “Literature review”**

This chapter presents the review of scientific literature on GaAs/Al<sub>x</sub>Ga<sub>1-x</sub>As quantum wells. The main features of materials used to realise quantum structures, types of two-dimensional structures and the basic physical properties of GaAs and AlAs crystals are presented here. The main features and optical properties of GaAs/Al<sub>x</sub>Ga<sub>1-x</sub>As quantum wells, the properties of excitons and impurities are also discussed in this chapter.

### **Chapter 2. “Samples and measuring technique”**

The main characteristics of each sample is presented in the table 1. The investigated samples were grown by molecular beam epitaxy on semi-insulating (100) GaAs substrates. A buffer layer was grown prior to deposition of the multiple quantum wells. Each of the multiple quantum well structures contained the same 5 nm wide AlAs barrier layer, while every GaAs well layer was  $\delta$ -doped at the well centre with Be acceptor or Si donor atoms. A single epilayer of GaAs:Be and undoped MQWs were grown for reference samples.



**Table 1.** Characteristics of the samples:  $L_W$  – GaAs QW width,  $N$  –  $\delta$ -doped impurity concentration,  $T_S$  – temperature of substrate,  $N_{QW}$  – number of MQWs,  $L_B$  – AlAs barrier width.

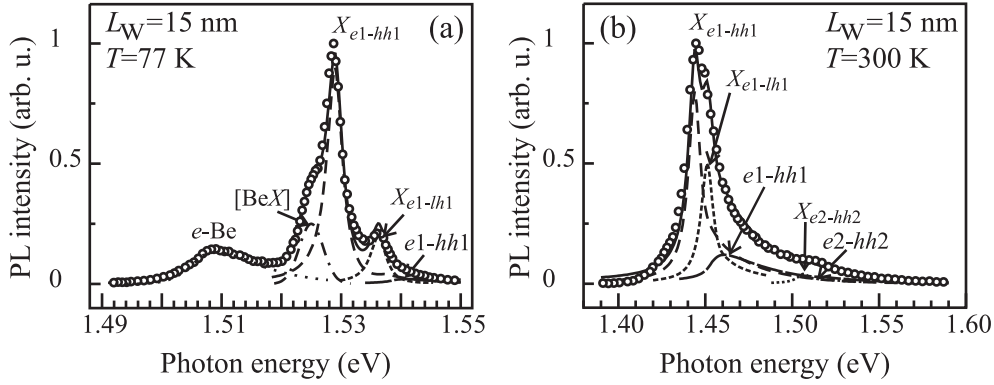
Sample	$L_W$ , nm	Impurity	$N$ , cm <sup>-2</sup>	$T_S$ , °C	$N_{QW}$	$L_B$ , nm	Buffer width, nm
<b><i>p</i>-type samples</b>							
S1807	20	Be	$5 \times 10^{10}$	550	100	5	500
S1392	20	Be	$2.5 \times 10^{12}$	540	40	5	500
S1303	15	Be	$2.5 \times 10^{12}$	540	50	5	500
S1794	10	Be	$5 \times 10^{10}$	550	200	5	500
S2068	5	Be	$5 \times 10^{10}$	550	300	5	500
S2071	5	Be	$5 \times 10^{12}$	550	300	5	500
L152	15	Be	$2.7 \times 10^{11}$	646	60	5	1000
L151	15	Be	$2.7 \times 10^{12}$	647	60	5	1000
L153	15	Be	$2.7 \times 10^{13}$	642	60	5	1000
L154	15	Be	$5.3 \times 10^{13}$	644	60	5	1000
<b><i>n</i>-type samples</b>							
L29	20	Si	$4 \times 10^9$	570	40	5	1000
L44	20	Si	$1 \times 10^{10}$	595	40	5	550
L30	20	Si	$1.4 \times 10^{11}$	570	40	5	1000
L45	20	Si	$1.4 \times 10^{11}$	595	40	5	550
L80	15	-	undoped	615	40	5	1000
L78	15	Si	$1.4 \times 10^{11}$	615	40	5	1000
L79	15	Si	$4 \times 10^{11}$	615	40	5	1000
<b>Bulk</b>							
S1796	5 $\mu$ m GaAs epilayer	Be	$2 \times 10^{16}$ cm <sup>-3</sup> uniform	550	-	-	500

The photoluminescence measuring technique is also presented in this chapter. Experiments were performed from liquid helium to room temperature. A continuous wave argon-ion laser was used to excite the PL, and the PL signal was then dispersed by a monochromator and detected by a cooled GaAs photomultiplier operating in the photon counting regime. An optical cryostat with liquid nitrogen was used for cooling, and after improvement, we used helium closed cycle refrigerator system from Janis.

### Chapter 3. “Investigation of photoluminescence spectra of weakly $\delta$ -doped GaAs/AlAs quantum wells”

This chapter presents the research results of the photoluminescence spectra of Be acceptor and Si donor impurities weakly  $\delta$ -doped GaAs/AlAs multiple quantum wells having different widths and doping levels. We have studied excitonic states and impurities induced effects.

Some results of Be  $\delta$ -doped GaAs/AlAs MQWs  $L_W = 15$  and 20 nm width at various temperatures and laser excitation intensities are shown in figures 1 and 2. A series of clearly resolved peaks can be seen in both figures. In MQWs with widths of  $L_W = 15$  and 20 nm, both heavy-hole  $X_{e1-hh1}$  and light-hole  $X_{e1-lh1}$  excitonic peaks are almost merged together at room temperature and comparisons can only be done after deconvolution of the spectra. These lines are separated in narrower QW or at low temperatures (see Fig. 1 (a)). A closer look at the room temperature spectra allows to discriminate the line  $X_{e2-hh2}$ , related to the second sublevel of excited electronic holes (see Fig. 1 (b)).



**Fig. 1.** The PL spectra of Be  $\delta$ -doped  $L_W = 15$  nm GaAs/AlAs MQWs (a) at liquid nitrogen and (b) room temperatures.  $X_{e1-hh1}$ ,  $X_{e2-hh2}$  and  $X_{e1-lh1}$  indicate heavy-hole and light-hole excitonic transition, [BeX] labels exciton bound-to-Be acceptor,  $e$ -Be designates electron-neutral Be acceptor transitions,  $e1-hh1$  and  $e2-hh2$  indicate electron-hole transitions. Dashed lines depict theoretical calculations; solid lines represent the sum of all recombination mechanisms.

At liquid nitrogen or lower temperatures (Figs. 1 (a) and 2), some additional lines appear in the spectra. The lower energy transitions, labelled as  $e$ -Be, are attributed to the recombination of free electrons and holes bound to Be acceptor, and so labelled as

[BeX], are attributed to excitons bound to acceptor impurity. Similar spectra were also given to Si donor  $\delta$ -doped GaAs/AlAs MQWs.

To analyse the excitonic PL spectra we have used a dimensionless absorption coefficient, which was theoretically deduced in fractional-dimensional space (FDS) approach [1]:

$$O(\hbar\omega) = O_0 \left[ \sum_{n=1}^{\infty} \frac{4Ry_X \Gamma(n + \alpha - 2)}{(n-1)! \left(n + \frac{\alpha-3}{2}\right)^{\alpha+1}} \delta(\hbar\omega - E_n) + \left| \Gamma\left(\frac{\alpha-1}{2} + i\gamma\right) \right|^2 e^{\pi\gamma} \frac{\gamma^{2-\alpha}}{\pi} \Theta(\hbar\omega) \right]. \quad (1)$$

$Ry_X$  is exciton Rydberg energy in three dimensional (3D) case,  $\Gamma(x)$  – Euler gamma function,  $\alpha$  – dimensionality, which changes from 2 in 2D case to 3 in 3D case,  $\delta(x)$  – Dirac delta function, coefficient  $\gamma = \sqrt{Ry_X / \hbar\omega}$ ,  $\hbar\omega$  is photon energy,  $\Theta(x)$  – Heaviside step function, and

$$O_0 = \frac{2^{2\alpha-3} e^2 |d_{cv}|^2 L^{\alpha-2} \left[ \Gamma\left(\frac{\alpha}{2}\right) \right]^2 \Gamma\left(\frac{\alpha-1}{2}\right)}{\pi^{(\alpha-3)/2} n_B c m_0^2 \omega a_{0X}^\alpha Ry_X [\Gamma(\alpha-1)]^3}, \quad (2)$$

where  $e$  is electronic charge,  $|d_{cv}|^2$  – conduction-to-valence squared matrix element,  $L$  – effective length of the active medium,  $n_B$  shows the refractive index of medium,  $m_0$  – free electron mass,  $\omega$  – the angular frequency of incident light,  $a_{0X}$  – 3D exciton Bohr radius.

The absorption coefficient of the interband optical transitions was calculated using the complex dielectric function from Ref. 2.

$$K_{b-b} = \frac{2^{3-\alpha} \pi^{2-\alpha/2} e^2 |d_{cv}|^2 L^{\alpha-2} \left(\frac{2\mu_{cv}}{\hbar^2}\right)^{\alpha/2}}{\Gamma\left(\frac{\alpha}{2}\right) n_B c m_0^2 \omega} \sum_v (\hbar\omega - E_{QW}^{vv})^{\alpha-1} \Theta(\hbar\omega - E_{QW}^{vv}), \quad (3)$$

where  $\mu_{cv} = m_c^* m_v^* / (m_c^* + m_v^*)$  is reduced effective mass of the electron and hole,  $E_{QW}^{vv}$  is energy gap between  $v$ th subbands of the conduction and valence band.

The measurable dimensionless absorption coefficient including Lorentzian line shapes with full width at half maximum  $w_L$  can be calculated:

$$K_X = \int_0^\infty O(\hbar\omega - E) \frac{2w_L}{\pi(4E^2 + w_L^2)} dE. \quad (4)$$

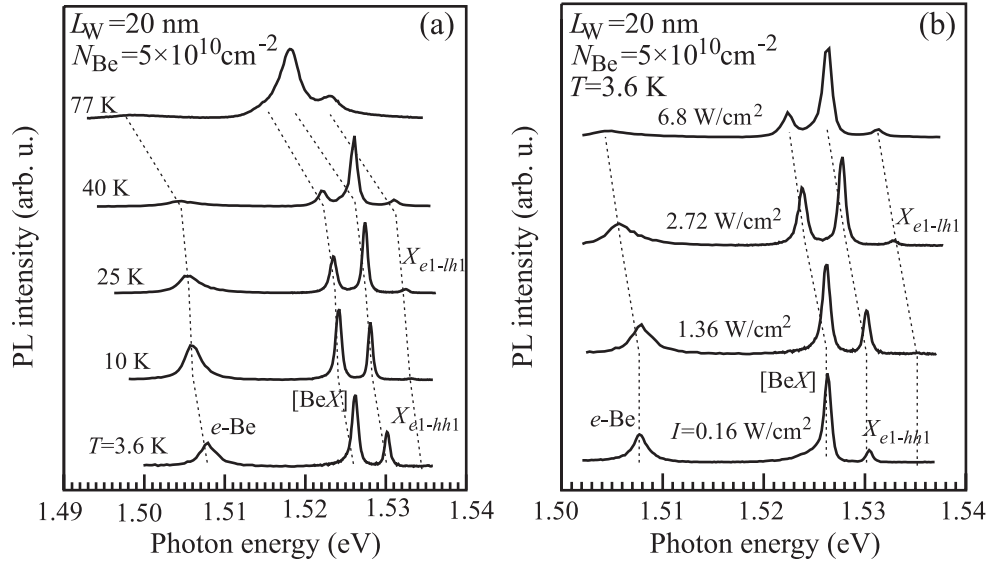
The luminescence intensity  $I_{PL}(E)$  is related to absorption coefficient  $K(E)$  and thermal function  $f(E)$  through energy balance relation

$$I_{PL}(E) \propto K(E)f(E). \quad (5)$$

The dimensionality has been determined directly from exciton binding energy calculated in FDS by using equation [3]:

$$E_n = Ry / \left( n + \frac{\alpha - 3}{2} \right)^2. \quad (6)$$

The calculated PL spectra results at liquid nitrogen and room temperatures are shown in Fig. 1 as lines. The line shape of bound excitons [BeX] was approximated by a Gaussian function.



**Fig. 2.** The PL spectra of Be  $\delta$ -doped  $L_W = 20$  nm GaAs/AlAs MQWs (a) at different temperatures and (b) at 3.6 K temperature for different laser excitation intensities. The notation is the same as in Fig. 1. The spectra are shifted vertically for clarity. Dotted lines indicate the shift of peaks for eyes.

Analysing Be  $\delta$ -doped  $L_w = 20$  nm width GaAs/AlAs MQWs, we found out that free exciton line full width at half maximum changes from 0.7 meV to 1.3 meV, when impurity concentration varies in range  $N_{\text{Be}} = 5 \times 10^{10} - 2.5 \times 10^{12} \text{ cm}^{-2}$ . In the modelling of the line shape, we assumed that broadening of the excitonic PL linewidth consists of two components: a homogeneous and an inhomogeneous parts [4]:

$$\Gamma = \Gamma_0 + aT + \frac{b}{e^{\frac{\hbar\omega_{\text{LO}}}{kT}} - 1}, \quad (7)$$

where  $\Gamma_0$  is the temperature  $T$  independent inhomogeneous width. Coefficients  $a$  and  $b$  represent the strengths of exciton scattering by acoustic and optical phonons. Values of these coefficients were evaluated from measurement results at different temperatures. For weakly doped samples, coefficients of acoustic scattering  $a \approx 10-11 \text{ } \mu\text{eV/K}$  and optical scattering  $b \approx 4-41 \text{ meV}$  conform others results and are smaller than in bulk GaAs case. Exciton scattering by optical phonon is weaker for Si donor than Be acceptor doped QW.

The knowledge of the transition energies allows to determine bound exciton binding energy  $E_b[\text{BeX}]$ , using the relation

$$E_b[\text{BeX}] = E(X_{e1-hh1}) - E[\text{BeX}]. \quad (8)$$

Here,  $E(X_{e1-hh1})$  and  $E[\text{BeX}]$  are the energies of the free  $X_{e1-hh1}$  and bound  $[\text{BeX}]$  excitons transitions. The measured binding energies of the excitons bound to acceptor or donor impurity are about twice as big as in GaAs case. For  $L_w = 5-20$  nm width Be acceptor  $\delta$ -doped GaAs/AlAs MQWs, they have values of 5.8–3.6 meV respectively.

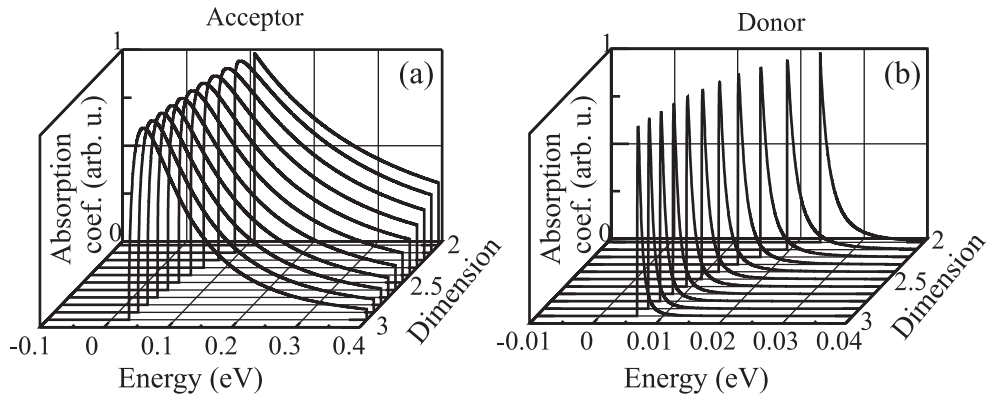
In the other part of the chapter, impurity related radiation is analysed. As can be seen from the spectrum in Fig. 1 (a), the  $e$ -Be line shape is asymmetric. In the dissertation we show that the line shape of impurity related radiation does not depend on the laser excitation intensity and impurity concentration up to  $N_{\text{Be}} = 2.5 \times 10^{12} \text{ cm}^{-2}$ , where they are considered as noninteracting. Line shape was analysed theoretically in the fractional-dimensional space approach. The absorption coefficient of the acceptor-conduction band transitions can be calculated using Eagles [5] or Dumke's [6] models.

Following the ideology of Lefebvre [7], we have calculated the dimensionless absorption coefficient:

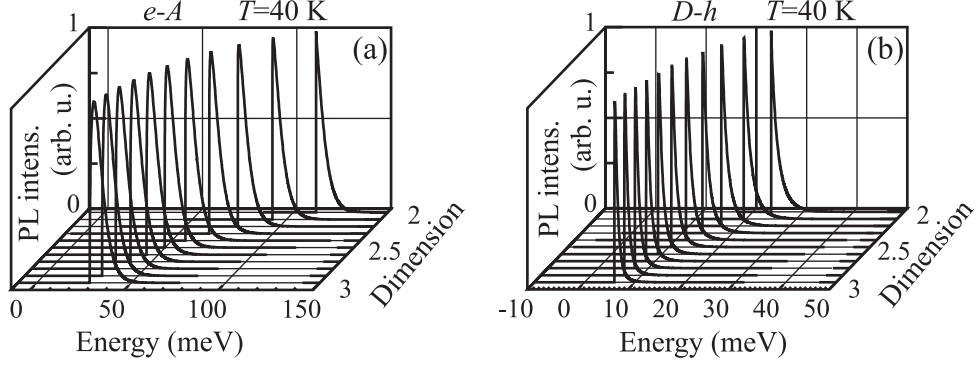
$$K = N_I g_I \frac{4\pi^2 e^2}{c n_B m_0^2 \omega} |d_{cv}|^2 \frac{2^{\alpha+1} \Gamma\left(\frac{\alpha+1}{2}\right)}{\pi^{1/2} \Gamma\left(\frac{\alpha}{2}\right)} \left(\frac{m_c^*}{m_p^*}\right) \frac{1}{Ry_I \left(\frac{2}{\alpha-1}\right)^2} \times \left[ \frac{m_c^*}{m_p^*} \frac{E}{Ry_I \left(\frac{2}{\alpha-1}\right)^2} \right]^{\frac{\alpha}{2}-1} \Theta(E) / \left[ 1 + \frac{m_c^*}{m_p^*} \frac{E}{Ry_I \left(\frac{2}{\alpha-1}\right)^2} \right]^{\alpha+1}, \quad (9)$$

here  $N_I$  and  $g_I$  are the impurity concentration in [ $1/\text{cm}^2$ ] and level degeneracy respectively,  $m_c^*$  is the electron effective mass in conduction band,  $m_p^*$  is the effective mass of hole related to impurities,  $Ry_I$  is the acceptor binding energy in the 3D case.

In the 3D case, we obtain absorption coefficient that consists with well-known results from literature [5, 6]. For the 2D case, the expression is in agreement with the calculations from Ref. 8. We have calculated the free-electron-acceptor, donor-valence-band absorption coefficients from Eq. (9) and the PL line shapes from Eq. (5) for the GaAs/AlAs QW with varying dimensionality. The calculated results are presented in Figs. 3 and 4. One can see that owing to the small ratio  $m_c^*/m_p^*$ , the absorption coefficient represents a slowly decreasing function of energy above the threshold.



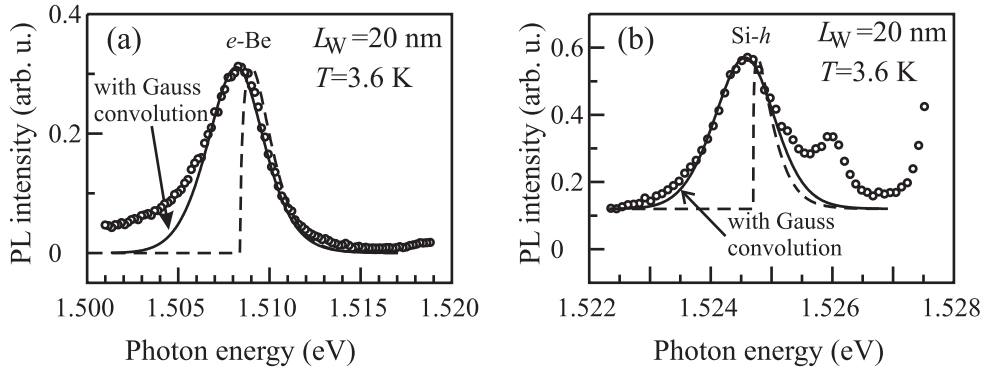
**Fig. 3.** The spectral shapes **(a)** of the electron-acceptor transition and **(b)** of the donor-hole transition absorption coefficients. The energetic scale is relative and shifted by the forbidden QW energy minus double impurity binding energy in all of the dimensionality cases.



**Fig. 4.** The calculated line shapes **(a)** of the electron-acceptor and **(b)** of the donor-hole photoluminescence intensity on the QW dimensionality at 40 K temperature. The energetic scale is relative and shifted by the forbidden QW energy minus double impurity binding energy in all of the dimensionality cases.

However, the PL line shape from the higher energy side is resolved by the Fermi-Dirac distribution function.

To describe the spectral shape of the observed impurity related transitions, we applied a Gaussian convolution in order to obtain a realistic fractional-dimensionality calculation which includes random distribution of impurities in their sheet. The modelling results and experimental data for the MQWs of 20 nm width at 3.6 K are presented in Fig. 5. It is clear that the use of Gaussian convolution provides an excellent agreement with the experimental results.



**Fig. 5.** The spectral shape of the **(a)** free-electron-acceptor ( $N_{\text{Be}} = 5 \times 10^{10} \text{ cm}^{-2}$ ) **(b)** donor-valence-band ( $N_{\text{Si}} = 4 \times 10^9 \text{ cm}^{-2}$ ) transition in  $L_{\text{W}} = 20 \text{ nm}$  width MQWs at 3.6 K temperature. Points show experimental data, lines denote theory: the dotted line is without and solid line with the Gaussian convolution.

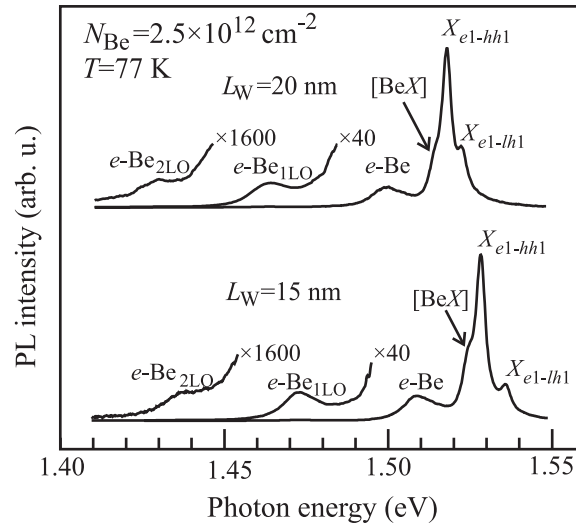
From transition energies, the impurity binding energy was estimated using the expression

$$E_{A,D} = E(X_{e1-hh1}) + E_b(X_{hh}) - E(e\text{-Be, Si-h}), \quad (10)$$

where  $E(X_{e1-hh1})$  and  $E(e\text{-Be, Si-h})$  are the energy of the  $X_{e1-hh1}$  and  $e\text{-Be, Si-h}$  lines, and  $E_b(X_{hh})$  is the binding energy of the heavy hole exciton and can be deduced from theoretical calculations [9]. For GaAs/AlAs QWs, the Be acceptor binding energy varies from about 30 meV for  $L_W = 20$  nm to 42 meV for  $L_W = 5$  nm. Varying quantum well width, it is possible to use GaAs/AlAs MQWs to design terahertz photodetectors and emitters in the range of 6.8–10.9 THz.

## Chapter 4. “Extension of radiation spectra in GaAs/AlAs quantum wells”

Two new low intensity lines were resolved from the lower energy side of the PL spectra of Be doped GaAs/AlAs QWs. They are designated as  $e\text{-Be}_{1LO}$  and  $e\text{-Be}_{2LO}$  in figure 6. From prima facie it was not clear to what transition one could attribute these lines. Therefore, the influence of the excitation intensity and impurity concentration on the PL spectra was investigated. The relative intensity and energetic position of the lines does not depend on the intensity of the laser excitation. Only at higher intensities, all the spectra lines are shifted a few meV towards the lower energy side. However, the relative distances between the lines remain the same. The impurity related PL intensities

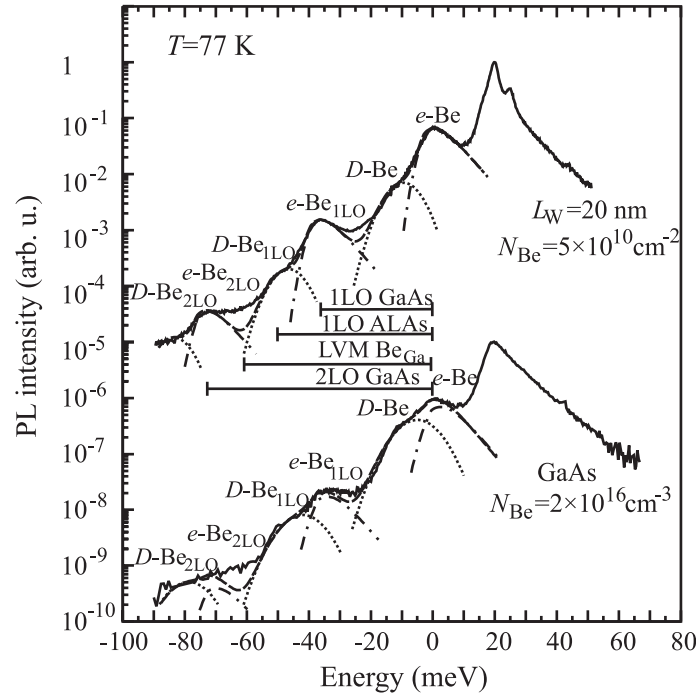


**Fig. 6.** The PL spectra of the Be  $\delta$ -doped  $N_{Be} = 2.5 \times 10^{12} \text{ cm}^{-2}$  GaAs/AlAs MQWs  $L_W = 15$  and 20 nm at liquid nitrogen temperature.  $e\text{-Be}_{1LO}$  and  $e\text{-Be}_{2LO}$  depict the first and second phonon replicas which are enlarged in factor of 40 and 1600, respectively. Other notations are the same as in Fig. 1.



becomes lower for weakly doped QWs in comparison with the highly doped structures, whereas the energetic positions of the lines is not influenced by the impurity concentration.

Having compared the PL spectra, we noticed that  $e\text{-Be}_{1\text{LO}}$  and  $e\text{-Be}_{2\text{LO}}$  lines are in the same position from impurity related transition  $e\text{-Be}$  line. This position does not change with QW width, and is the same as for QW and bulk GaAs. The PL spectra fixed at  $e\text{-Be}$  transition of Be  $\delta$ -doped  $N_{\text{Be}} = 5 \times 10^{10} \text{ cm}^{-2}$  GaAs/AlAs MQWs  $L_{\text{W}} = 20 \text{ nm}$  and Be doped  $N_{\text{Be}} = 2 \times 10^{16} \text{ cm}^{-3}$  bulk GaAs are shown in semi-logarithmic scale in Fig. 7. It is clear that the  $e\text{-Be}$  transition sidebands position will coincide with first longitudinal optical (1LO) and 2LO-phonon energy of GaAs. These energy values are presented as bars in the figure. The shoulder between 1LO and 2LO-phonon replicas, the energy of



**Fig. 7.** The relative PL spectra peaks positions of Be  $\delta$ -doped  $N_{\text{Be}} = 5 \times 10^{10} \text{ cm}^{-2}$  GaAs/AlAs MQWs  $L_{\text{W}} = 20 \text{ nm}$  and Be doped  $N_{\text{Be}} = 2 \times 10^{16} \text{ cm}^{-3}$  bulk GaAs at liquid nitrogen temperature. The origin of energy is shifted to  $e\text{-Be}$  transition peak maximum. Solid lines are experimental results, other types of lines depict theoretical calculations:  $e\text{-Be}$  transition and its phonon replicas are dash-dotted lines, residual donor-Be acceptor  $D\text{-Be}$  transition and its phonon replicas denoted as dotted lines, dashed line marks full calculated spectra in impurity related region. Bars are phonon energies: 1LO GaAs is LO phonon energy in GaAs, 1LO AlAs denotes LO phonon energy in AlAs, LVM  $\text{Be}_{\text{Ga}}$  labels local vibrational mode of Be atom, 2LO GaAs shows double phonon energy in GaAs.

which is close to the barrier AlAs 1LO-phonon energy, is attributed to the residual donor-Be acceptor transition 1LO-phonon replica. This shoulder is also typical for bulk GaAs which was grown from the same material and in the same conditions as QWs. Consequently, the main sideband lines are related to the first and second phonon replicas of the  $e$ -Be transitions, the energetic distance of which is equal to the bulk GaAs LO-phonon energy  $\hbar\omega_{LO} = 36.75$  meV [10].

The proposed model was illustrated using fractional dimensional space approach and Gaussian shape curve for  $e$ -Be and  $D$ -Be transitions (and its replicas) respectively.

The distribution of emission intensities  $I$  between phonon replicas and the main emission peak may be described in terms of the Huang-Rhys factor  $S$ . The Huang-Rhys factor was experimentally extracted from the ratios of second and first replicas. For example, the ratio  $I_{2LO}/I_{1LO}$  leads to

$$S = 2 \frac{I_{2LO}}{I_{1LO}}. \quad (11)$$

The theoretical analysis of Huang-Rhys factor was done from the point of view of the fractional dimensional space approach. Using adiabatic approximation and Frölich continuum theory, the Huang-Rhys factor in the FDS approach equals to

$$S_\alpha = \frac{e^2}{4\pi\epsilon_0\hbar\omega_{LO}} \left( \frac{1}{\epsilon_\infty} - \frac{1}{\epsilon_s} \right) \frac{\Gamma\left[\frac{\alpha-1}{2}\right]\Gamma\left[\frac{1}{2}+\alpha\right]}{\Gamma[1+\alpha]\Gamma\left[\frac{\alpha}{2}\right]} \frac{1}{a_0(\alpha-1)}, \quad (12)$$

where  $\epsilon_\infty$  and  $\epsilon_s$  are the high-frequency and static dielectric constant, respectively.  $a_0$  is impurity Bohr radius in the 3D case.

In 3D and 2D cases the Huang-Rhys factor equal

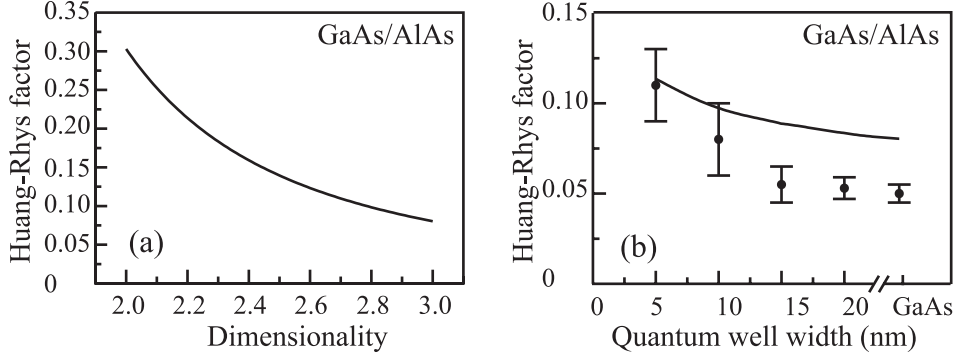
$$S_3 = \frac{e^2}{4\pi\epsilon_0\hbar\omega_{LO}} \left( \frac{1}{\epsilon_\infty} - \frac{1}{\epsilon_s} \right) \frac{5}{16a_0}, \quad (13)$$

$$S_2 = \frac{e^2}{4\pi\epsilon_0\hbar\omega_{LO}} \left( \frac{1}{\epsilon_\infty} - \frac{1}{\epsilon_s} \right) \frac{3\pi}{8a_0}. \quad (14)$$

The ratio between the 2D and 3D cases is equal to

$$S_2 / S_3 = 6\pi/5 \approx 3,77. \quad (15)$$

This show that phonons interaction is stronger in two dimensional structures than in bulk crystal.

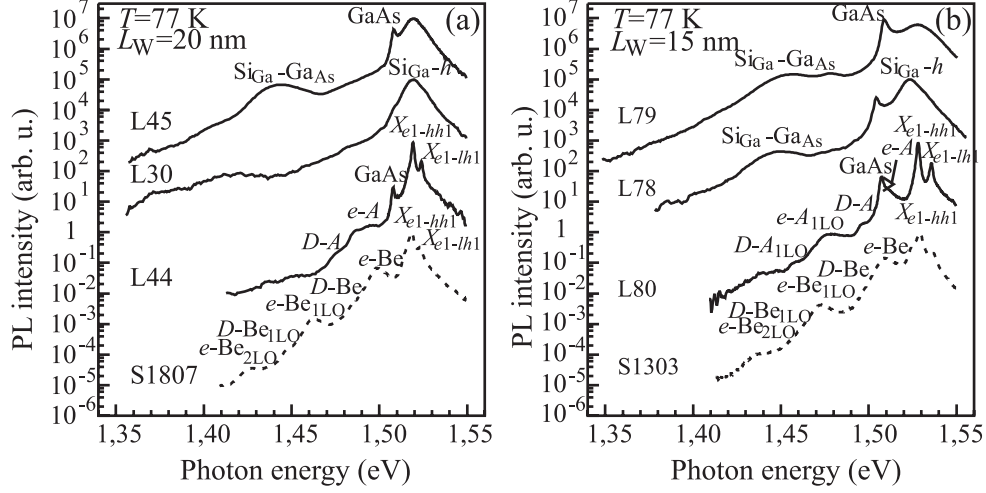


**Fig. 8.** Dependence of the calculated Huang-Rhys factor **(a)** on dimensionality, **(b)** on the GaAs/AlAs QW width. The points are experimental values and bars indicate their scattering.

The theoretical results calculated from (12) where the dimensionality  $\alpha$  was estimated from (6) are presented in Fig. 8. The experimental values are presented as points as well. The theoretical calculations were found to be in good agreement with the experimental results. For wide QWs, the Huang-Rhys factor for  $e$ -Be transitions  $S \approx 0.052$  is similar to the bulk GaAs value; however, for the narrow QWs this factor tends to increase.

The investigation of moderately Si donor doped samples showed that a new line appears in the lower energy side of PL spectra. The low energy tail of the PL spectra at liquid nitrogen temperatures for the Si  $\delta$ -doped GaAs/AlAs MQWs with  $L_w = 20$  and 15 nm are shown in Figs. 9 (a) and 9 (b), respectively. It is seen that for undoped and weakly Si  $\delta$ -doped samples the observed spectra are similar to Be  $\delta$ -doped samples. This indicates that excitonic transitions and transitions related to residual donors, acceptors and their phonon replicas prevail in the PL spectra. However, for highly Si  $\delta$ -doped samples, the low energy PL spectra change drastically: First, the PL emission is more intense in the low energy tail and the spectra lose their fine structure; second, one

observes new bands at energies of 1.438 eV for  $L_W = 20$  nm and 1.442 eV for  $L_W = 15$  nm. These bands are marked as  $\text{Si}_{\text{Ga}}\text{-Ga}_{\text{As}}$  and are related to Si donor-antisite defect transitions.



**Fig. 9.** The low energy tail PL spectra of undoped and Si  $\delta$ -doped GaAs/AlAs MQWs with widths: **(a)**  $L_W = 20$  nm and **(b)**  $L_W = 15$  nm at liquid nitrogen temperature.  $\text{Si}_{\text{Ga}}\text{-Ga}_{\text{As}}$  marks the Si donor-antisite defect related transitions.  $e\text{-Be}$  indicates the free electron-neutral acceptor transitions, and  $D\text{-A}$  the donor-acceptor transitions. GaAs is PL spectrum from GaAs buffer layer. For comparison the PL spectra of a Be  $\delta$ -doped GaAs/AlAs MQW samples are shown for (a) S1807 and (b) S1303. Here,  $e\text{-Be}$  and  $e\text{-Be}_{1\text{LO}}$ ,  $e\text{-Be}_{2\text{LO}}$  are the free electron-neutral Be acceptor and its first, second phonon replica transitions.  $D\text{-Be}$  and  $D\text{-Be}_{1\text{LO}}$  indicate donor-Be acceptor and its phonon replica transitions.

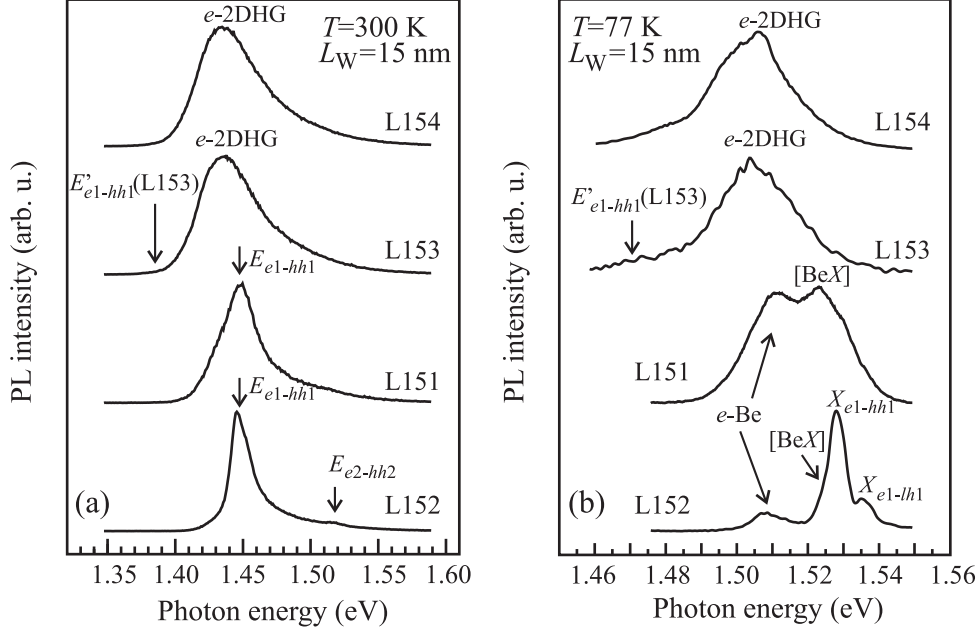
The energy position of the  $\text{Si}_{\text{Ga}}\text{-Ga}_{\text{As}}$  band does not depend on the laser excitation intensity. The inherent feature of this band is that it dominates in the PL spectrum at low excitation power, but quenches as the excitation power is increased. From our experimental data, we found that the deep acceptor type defect activation energy is about 79 meV. This energy is in agreement with 78 meV found for bulk Si doped GaAs [11] and also observed in molecular beam epitaxy grown Si-doped GaAs layers [12]. However, for one sample (L30), we did not observe a  $\text{Si}_{\text{Ga}}\text{-Ga}_{\text{As}}$  band in PL spectrum, see Fig. 9 (a). This could be related to the fact that this sample was grown at a lower temperature, since, generally, the formation of defects is generally sensitive to the growth conditions [12].

## Chapter 5. “Quantum well radiation near the Mott transition”

In this chapter the peculiarities of radiative recombinations near the Mott transition are studied. For the case of highly  $\delta$ -doped semiconductors or quantum wells, the nature of the impurity states changes drastically, and the interacting impurities form new states, which leads to the formation of a two-dimensional carrier gas and the occurrence of the dielectric-metal Mott transition [13, 14]. One can therefore introduce two critical concentrations  $N_{I\_B}$  and  $N_M$ . For heavily doped QWs ( $N_{I\_B} < N_I < N_M$ ), the impurities form a band that leads to a renormalization of the first conduction ( $n$ -type) or valence ( $p$ -type) subband edge. For very heavily  $\delta$ -doped QWs ( $N_I > N_M$ ) the impurity concentration corresponds to the metallic limit, triggering the formation of a V-shaped potential which transforms the whole QW sublevel system.

The PL spectra for the  $L_W = 15$  nm GaAs/AlAs MQW samples are shown in Figs. 10 (a) and 10 (b) at room and liquid nitrogen temperatures, respectively. The spectra for the higher doped samples (L151, L153, L154) are more complicated than for weakly doped sample L152. For example, the spectrum of L151 sample at room temperature is similar to that of the low doped sample. However, it is different and more complicated at liquid nitrogen temperature. Two peaks related to  $e$ -Be and [BeX] transitions are observed. In addition, two shoulders are present at energies  $X_{e1-hh1}$  and  $X_{e1-lh1}$  (Fig. 10 (b)). We assumed that QWs are nondegenerated, but the impurity concentration is close to the Mott transition ( $N_{I\_B} < N_I < N_M$ ) and acceptors form an impurity band.

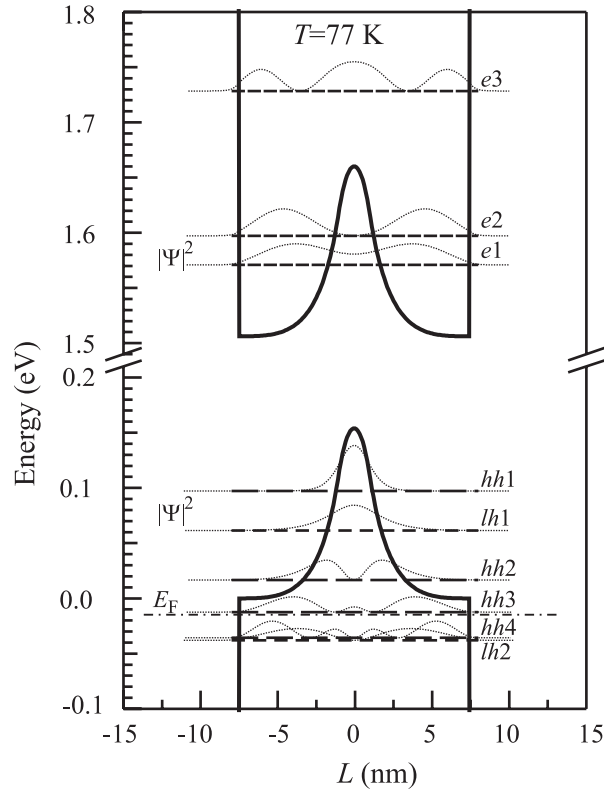
The spectra of heavily doped samples L153 and L154 differ strongly from the spectra of samples L151 and L152. First, changes in the fine structure of the spectra are seen. Second, the spectra are shifted to lower energy. It was shown that, in these cases, radiative recombination is related to the formation of a two-dimensional hole gas (2DHG). We showed experimentally that Mott transition occurs when  $N_{Be} \geq 3 \times 10^{12} \text{ cm}^{-2}$  for Be  $\delta$ -doped GaAs/AlAs MQWs  $L_W = 15$  nm and  $N_{Be} \geq 5 \times 10^{12} \text{ cm}^{-2}$  for  $L_W = 5$  nm. This correlates with theoretical predictions found applying a simple spherical symmetry model for impurities in QWs, and the concentration is higher compared with the  $N_{Be} = 2.2 \times 10^{12} \text{ cm}^{-2}$  in  $\delta$ -doped GaAs case.



**Fig. 10.** The PL spectra of Be  $\delta$ -doped GaAs/AlAs  $L_W = 15$  nm MQWs (for L152,  $N_{Be} = 2.7 \times 10^{11} \text{ cm}^{-2}$ , for L151,  $N_{Be} = 2.7 \times 10^{12} \text{ cm}^{-2}$ , for L153,  $N_{Be} = 2.7 \times 10^{13} \text{ cm}^{-2}$ , for L154,  $N_{Be} = 5.3 \times 10^{13} \text{ cm}^{-2}$ ) at (a) room and (b) liquid nitrogen temperatures.  $e$ -2DHG denotes optical transitions related to the 2D hole gas.  $E'_{e1-hh1}(L153)$  is the calculated energy difference between sublevels in the heavily doped sample L153.  $E_{en-hhn}$  and  $E_{en-lhn}$  (indicated by arrows) is the calculated energy difference between the  $n$ th electron and  $n$ th heavy-hole and light-hole energy levels, respectively. The other notations are the same as in Fig. 1.

To prove 2DHG formation and to quantitatively estimate the transformation of the energy-level structure that occurs at high doping level, we numerically calculated the valence- and conduction- band structure based on a self-consistent solution of the coupled Poisson-Schrödinger equations [15]. The simulated energy band diagram at 77 K for QWs L153 is shown in Fig. 11. The calculated energy  $E'_{e1-hh1}(L153)$  between  $e1$  and  $hh1$  energy levels is shown in Fig. 10 and fits well with the threshold of the PL band.

We finally briefly discussed some of the recombination anomalies: Fermi edge singularity [16] and  $F$ -type emission [17]. We haven't observed any transitions between spatially separated electrons and holes, the so-called  $F$ -type emission. The spectra of very heavily doped samples showed features, such as nonlinear change of the spectral shape with excitation, similar to those observed in the case of a Fermi edge singularity. However, in our case, we demonstrated that this phenomena is related to photoemission from the GaAs buffer layer.



**Fig. 11.** Diagram of the conduction and valence bands, together with the subband energies, for a 15 nm wide QW,  $\delta$ -doped with  $2.7 \times 10^{13} \text{ cm}^{-2}$  acceptor atoms, calculated at 77 K from self-consistent solution of the Poisson-Schrödinger equations. Dotted lines are wave functions squared  $|\Psi|^2$ .

## Conclusions

1. Besides impurity related radiation, the spectrum line of the exciton bound to the impurity is also observed in impurities doped quantum wells. The impurities are also increasing the width of heavy and light hole free excitonic spectrum lines.
2. It has been determined that the lineshape of impurity related radiation in GaAs/AlAs QWs is asymmetric. The asymmetry is more significant for acceptor impurities than donor impurities, and is related to the wider absorption spectrum of the acceptors.
3. Two extra peaks were found on the lower energy side of PL spectrum of Be  $\delta$ -doped GaAs/AlAs MQWs. These were identified as the first and second phonon replicas of impurities related radiation  $e$ -Be. It was determined that the

distance between the lines was equal to energy of GaAs longitudinal optical phonon  $\hbar\omega_{LO} = 36.75$  meV .

4. The strength of interaction of  $e$ -Be radiation with LO phonon which is described in terms of the Huang-Rhys factor has been measured experimentally and calculated theoretically. It was found that the Huang-Rhys factor increases when the quantum well narrows. This increase is associated with the confinement of carriers in the quantum well which changes the wave function.
5. It was shown that the Mott transition in 2D structures occurs under higher impurity concentration than in 3D case. From experimental observation the Mott transition can be observed in Be  $\delta$ -doped GaAs/AlAs quantum wells of  $L_W = 15$  nm width for  $N_{Be} \geq 3 \cdot 10^{12}$  cm<sup>-2</sup>, and  $L_W = 5$  nm width –  $N_{Be} \geq 5 \cdot 10^{12}$  cm<sup>-2</sup>. While in  $\delta$ -GaAs, it occurs when  $N_{Be} = 2.2 \cdot 10^{12}$  cm<sup>-2</sup>.
6. By changing the width of the QW, the binding energy of the Be impurity can be tuned from 28 meV to 45 meV. Meanwhile  $n$ -type Si donor binding energies can be varied in the range of 6–16 meV. Be acceptor impurities can be used for designing GaAs/AlAs photodetectors and emitters in the 6,8–10,9 THz range, whereas Si donor impurities in 1,4–3,8 THz range.
7. Heavily  $n$ -type Si  $\delta$ -doped  $N_{Si} = 4 \times 10^{11}$  cm<sup>-2</sup> quantum wells  $L_W = 15$  nm can be used to design 2DEG-free transitions detector in the 2.5 THz region.

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## **Short information about the author**

Aurimas Čerškus was born in Girbučiai vil., Kupiškis district on 31 October, 1977.

He left Alizava secondary-school and went to Physics and Technology Faculty of the Vilnius Pedagogical University in 1995. He finished the course of physics and astronomy speciality (higher education diploma) in 2000 and was given the qualification of physics and astronomy teacher. In 2002 he finished postgraduate studies of Vilnius Pedagogical University with honours degree. From 2005 to 2009 he has been a PhD student at Semiconductor Physics Institute.

From 1997 to 2003 he worked as a laboratory assistant in the Department of General Physics at Vilnius Pedagogical University. From 2000 to 2004 he worked as a physics teacher at the Karoliniškės gymnasium in Vilnius. From 2003 to 2008 – a assistant in the Department of General Physics, Vilnius Pedagogical University. From 2004 till now (brokenly) has been working as a junior research employee in Inhomogeneous Structures laboratory of Semiconductor Physics Institute. Also, from 2008 he has been working as a lecturer in the Department of General Physics, Vilnius Pedagogical University.

## Reziūmė

Disertacijoje pateikti akceptorinių Be ir donorinių Si priemaišų įtakos  $\delta$ -legiruotų GaAs/AlAs kartotinių kvantinių šulinių fotoluminescencijos spektrams nuo kambario iki skystojo helio temperatūros tyrimai. Matavimai buvo atliekami su skirtingo pločio ir įvairių legiravimo tankių kvantiniais šuliniais. Darbą sudaro įvadas, penki pagrindiniai skyriai. Disertacijos pabaigoje pateikti pagrindiniai darbo rezultatai ir išvados, sudaryti cituotos literatūros bei autoriaus mokslo publikacijų disertacijos tema sąrašai.

Temos aktualumo pagrindimas, pagrindinis darbo tikslas pateikiami **Įvade**. Taip pat formuluojami darbo uždaviniai, ginamieji teiginiai bei nurodomas gautų rezultatų mokslinis naujumas.

**Pirmajame skyriuje** pateiktos bendrosios GaAs ir AlAs fizikinės savybės. Trumpai apžvelgtos GaAs/Al<sub>x</sub>Ga<sub>1-x</sub>As kvantinių šulinių bei eksitonų ir priemaišų juose savybės.

**Antrasis skyrius** skirtas tirtų GaAs/AlAs bandinių sandaros ir nuostoviosios fotoluminescencijos matavimo technikos aprašymui.

Silpnai  $\delta$  legiruotų GaAs/AlAs kvantinių šulinių fotoluminescencijos spektrų tyrimų rezultatai pateikti **Trečiajame skyriuje**. Šio skyriaus pirmoje dalyje pateikiami eksperimentiniai fotoluminescencijos spektrai esant įvairioms temperatūroms, eksperimentiškai nustatytos su Be ir Si priemaiša surištųjų eksitonų ryšio energijos GaAs/AlAs kvantiniuose šuliniuose. Savitosios spinduliuotės teorinė analizė naudojantis trupmeninių dimensijų erdvės modeliu aptarta antrame poskyryje. Įvertintas priemaišomis legiruotų kvantinių šulinių eksitoninių linijų išplitimas bei eksitonų sąveika su akustiniais ir optiniais fononais. Trečiame poskyryje nagrinėjama priemaišinė spinduliuotė bei pateikiamos iš fotoluminescencijos spektrų nustatytos priemaišų aktyvacijos energijos. Taip pat teoriškai įrodoma priemaišinės spinduliuotės smailės asimetrija.

**Ketvirtasis skyrius** skirtas spinduliuotės tūšai GaAs/AlAs kvantinių šulinių fotoluminescencijos spektruose. Pirmame poskyryje pateikti Be legiruotų GaAs/AlAs kvantinių šulinių rezultatai, kuriuose pirmą kartą stebėtos priemaišinės spinduliuotės su optiniu fononu replikos. Eksperimentinės ir teorinės Huang-Rhys faktoriaus vertės

palygintos antrame poskyryje. Pirmą kartą teoriškai išvedama Huang-Rhys faktoriaus formulė dvimačiu atveju. Skyriuje taip pat pateikiami Si legiruotų bandinių spinduliuočių tūšos spektrų rezultatai, kuriuose stebėta papildoma priemaišinė juosta. Ši juosta susijusi su  $p$ -tipo  $\text{GaAs}$  pakaitinio defekto susidarymu.

$\text{GaAs}/\text{AlAs}$  kvantinių šulinių spinduliuotės arti dielektrikas-metalas arba Mott virsmo ypatumai aptarti **Penktajame skyriuje**. Pateikiami eksperimentiniai rezultatai iki Mott virsmo ir po jo. Apskaičiuoti akceptorinių ir donorių kriziniai tankiai, kuriems esant įvyksta dielektrikas-metalas virsmas.

### **Pagrindinės išvados:**

1. Į kvantinius šulinius įterpus priemaišų be joms būdingos priemaišinės spinduliuotės, FL spektruose stebima su priemaiša surištojo eksitono linija. Dėl įterptų priemaišų padidėja sunkiųjų ir lengvųjų skylių eksitoninių linijų plotis.
2. Nustatėme, kad  $\text{GaAs}/\text{AlAs}$  kvantinių šulinių priemaišinės spinduliuotės linijos forma yra asimetrinė. Asimetriškumas labiausiai pasireiškia akceptorinėms nei donorinėms priemaišoms. Tai susiję su platesniu akceptorinių sugerties spektru.
3. Be  $\delta$ -legiruotų  $\text{GaAs}/\text{AlAs}$  kvantinių šulinių FL spektro mažesnių energijų srityje atradome dvi papildomas smailes. Įrodėme, kad tai yra priemaišinės spinduliuotės  $e$ -Be pirmoji ir antroji fononinės replikos. Nustatėme, kad atstumas tarp linijų lygus  $\text{GaAs}$  išilginio optinio fonono energijai  $\hbar\omega_{\text{LO}} = 36,75 \text{ meV}$ .
4. Eksperimentiškai ir teoriškai nustatėme  $e$ -Be spinduliuotės sąveikos su LO fononu stiprį kurį išreiškia Huang-Rhys faktorius. Gavome, kad siaurėjant kvantiniame šuliniui Huang-Rhys faktorius didėja. Parodėme, kad padidėjimas yra susijęs su krūvininkų apribojimu kvantiniame šulinyje ir banginės funkcijos pasikeitimu.
5. Pademonstravome, kad dvimačiuose dariniuose Mott virsmas įvyksta prie didesnių priemaišų tankių nei trimačiu atveju. Eksperimentiškai parodėme, kad Be  $\delta$ -legiruotuose  $L_w = 15 \text{ nm}$  pločio kvantiniuose šuliniuose Mott virsmas

įvyksta kai  $N_{\text{Be}} \geq 3 \cdot 10^{12} \text{ cm}^{-2}$ , o  $L_{\text{w}} = 5 \text{ nm}$  pločio – kai  $N_{\text{Be}} \geq 5 \cdot 10^{12} \text{ cm}^{-2}$ . Tuo tarpu  $\delta$ -GaAs tai įvyksta kai  $N_{\text{Be}} = 2,2 \cdot 10^{12} \text{ cm}^{-2}$ .

6. Keičiant GaAs/AlAs kvantinių šulinių plotį, Be priemaišinių lygmenų energiją galima keisti nuo 28 meV iki 45 meV. Tuo tarpu,  $n$ -tipo Si priemaišinių lygmenų energiją galima keisti 6–16 meV intervale. Akceptorinės Be priemaišos taikytinos 6,8–10,9 THz, o donorinės Si priemaišos 1,4–3,8 THz srities GaAs/AlAs jutikliams ir emiteriams kurti.
7. Stipriai  $n$ -tipo Si  $\delta$ -legiruoti kvantiniai šuliniai, pavyzdžiui,  $L_{\text{w}} = 15 \text{ nm}$  ir  $N_{\text{Si}} = 4 \cdot 10^{11} \text{ cm}^{-2}$ , gali būti pritaikyti kuriant dvimatės elektronų dujos-laisvi elektronai šuolių detektorių, veikiantį 2,5 THz srityje.

**Literatūros sąrašė** pateikti darbai, kurių rezultatai buvo apžvelgti ir cituojami disertacijoje.

## **Trumpos žinios apie autorių**

Aurimas Čerškus gimė 1977 m. spalio 31 d. Girbučių kaime, Kupiškio raj.

1995 metais baigė Alizavos vidurinę mokyklą ir įstojo į Vilniaus pedagoginio universiteto (VPU) Fizikos ir technologijos fakultetą. 2000 metais baigė fizikos ir astronomijos specialybės kursą (aukštojo mokslo diplomas) ir buvo suteikta bendrojo lavinimo mokyklos fizikos ir astronomijos mokytojo kvalifikacija. 2002 m. su pagyrimu baigė VPU magistrantūros studijas bei įgijo fizikos magistro laipsnį ir mokytojo kvalifikaciją. 2005–2009 m. studijavo Puslaidininkų fizikos instituto doktorantūroje.

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