

## BEHAVIOUR OF OPTICAL TRANSITIONS IN GaAs/AlAs WITH HIGHLY Be $\delta$ -DOPED MQWs

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We present the photoluminescence properties of highly Be  $\delta$ -doped GaAs/AlAs multiple quantum wells at liquid nitrogen and room temperatures. Possible mechanisms of carrier recombination focusing on peculiarities of excitonic and free-carriers–acceptor photoluminescence are discussed. It is estimated that for Be  $\delta$ -doped GaAs/AlAs quantum wells ( $L_W = 5$  nm) the Mott transition should occur at acceptor concentration  $N_{Be}$  some greater than  $5 \cdot 10^{12}$  cm<sup>-2</sup>.

**Keywords:** Be  $\delta$ -doped GaAs/AlAs quantum wells, photoluminescence, 2D Mott transition

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### 1. Introduction

The properties of quantum well structures are strongly influenced by the presence of doping impurities. The investigation of impurity properties in quantum wells has a fundamental importance and potential for novel device applications such as quantum well infrared photodetectors [1–3].

So far the basic research has been focused on barrier-doped quantum wells. There have been no in-depth studies performed on doped quantum wells, in particular acceptor doping. Impurities in quantum wells (QWs) may be distributed smoothly or concentrated in sheet – so called  $\delta$ -doping. The structure of the impurity energy spectrum depends on quantum well width, barrier height, impurity position, and concentration in QWs [4, 5]. In the case of highly  $\delta$ -doped semiconductors or quantum wells the impurity spectra reduce drastically and interacting impurities form a new state, leading to two-dimensional carrier gas [6].

As a rule, higher doping levels are required to improve quantum efficiency for emission from impurity-related states. However, in the case of high impurity concentrations, the broadening of photoluminescence (PL) lines becomes limiting and the recombination lines can merge obscuring those in the PL spec-

trum. Experimentally this problem cannot be resolved by reducing the lattice temperature. The line broadening is determined not only by phonons, but also by randomly distributed impurities in the lattice, and also by the quality of quantum well interface that affects narrow quantum wells more strongly.

During the years doped QWs have been investigated over a very broad doping range [7–13], however the question of the formation of impurity bands and two-dimensional subbands in highly  $\delta$ -doped quantum wells still remains open.

In this article we present results of an investigation into the PL properties of highly Be  $\delta$ -doped GaAs/AlAs multiple QWs at liquid nitrogen and room temperatures. The possible mechanisms of carrier recombination are discussed paying special emphasis on excitonic and free-carriers–acceptor impurity PL.

### 2. Samples and experimental conditions

Two multiple quantum well (MQW) structures were grown using MBE technique on semi-insulating GaAs substrates, containing  $N = 300$  wells with the width of  $L_W = 5$  nm, and were separated by  $L_B = 5$  nm wide AlAs barriers. Quantum wells were  $\delta$ -doped with Be

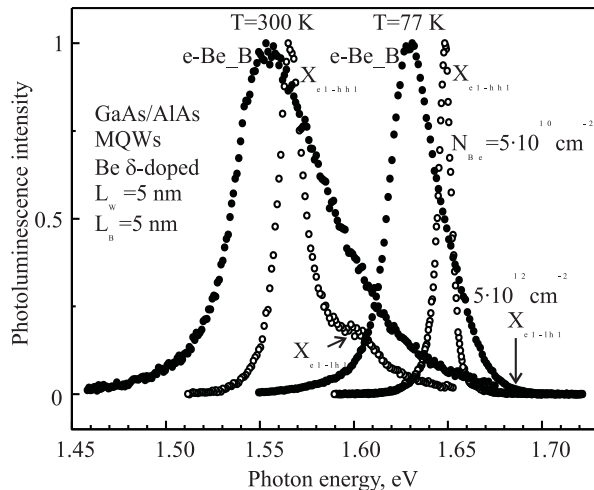


Fig. 1. The PL spectra of the Be  $\delta$ -doped GaAs/AlAs  $L_W = 5$  nm two MQWs ( $N_{Be} = 5 \cdot 10^{12} \text{ cm}^{-2}$  – closed circles and  $5 \cdot 10^{10} \text{ cm}^{-2}$  – open circles) at room and liquid nitrogen temperatures.  $X_{e1-hh1}$  and  $X_{e1-lh1}$  indicate heavy hole and light hole excitonic transitions. The arrow shows calculated energetic position  $X_{e1-lh1}$  at 77 K. Labels e-Be<sub>B</sub> mark PL associated with Be acceptor impurity band.

acceptors at the centre of the well. The doping spike width was 2 nm. The first investigated sample was highly doped with density of  $N_{Be} = 5 \cdot 10^{12} \text{ cm}^{-2}$ , whereas the next, so-called reference sample, was only weakly doped,  $N_{Be} = 5 \cdot 10^{10} \text{ cm}^{-2}$ .

A continuous wave argon ion laser was used to excite the PL. The PL excitation intensity was in the range of  $1 - 10 \text{ W/cm}^2$ . The PL signal was dispersed by a monochromator and detected by a cooled GaAs photomultiplier operating in the photon counting regime.

### 3. Experimental results

The PL spectra for two MQW samples at room and nitrogen temperatures are shown in Fig. 1. Since the investigated MQWs were heavily doped with Be acceptor impurities, it was important to identify the influence of doping upon the structure of QW energy levels and peculiarities of the PL spectra.

Firstly, we discuss PL spectra of the reference sample. At liquid nitrogen temperature we observe a single intensity peak, which is associated with heavy hole  $X_{e1-hh1}$  excitonic PL transitions. For narrow quantum wells the light hole excitonic transitions in PL spectra at low temperatures are not observed; this is because there is not sufficient thermal energy to excite holes into the light hole energy sublevel. The calculated position of this particular transition is shown by an arrow  $X_{e1-lh1}$  in Fig. 1. It is important to notice that in the PL spec-

tra the transitions associated with Be acceptors have not been observed, too. The radiative recombination of free electrons with acceptors (e-Be) is characteristic of Be doped MQWs [14]. The absence of this line could be due to the weak doping of the reference sample. For the narrow QWs with high potential barriers, the exciton oscillator strength is very large, which causes the excitonic transitions to be relatively more efficient than the e-Be transitions. In contrast, at room temperature, it is possible to resolve two kinds of peaks: the heavy hole  $X_{e1-hh1}$  and light hole  $X_{e1-lh1}$  excitons.

The spectra of highly doped sample are more complicated. At liquid nitrogen temperature we observe one peak at photon energy  $\hbar\omega = 1.63 \text{ eV}$ . On the higher energy side of this transition there is a shoulder at a position coinciding with the heavy hole excitonic line  $X_{e1-hh1}$  ( $\hbar\omega = 1.649 \text{ eV}$ ) of the reference sample. Consequently, we deduce that the spectra consist of several constituents caused by acceptor-related transitions and excitonic emission. Similar PL spectra are observed at room temperature. The band at energy  $\hbar\omega = 1.55 \text{ eV}$  is very broad and possibly consists of two components. A shoulder is resolved at  $\hbar\omega = 1.6 \text{ eV}$ . Its position coincides with the light hole excitonic line  $X_{e1-lh1}$  of the reference sample. The last comparison is, however, misleading; clarification of the bands origin can be made by performing simulations, which show a significant role played by band-to-band transitions (see discussion below). The lines of various PL transitions are merged and this requires a more detailed model for analysis.

### 4. Model

Impurities are a fundamental factor determining the electronic, optical, and transport properties of QWs. Most of these properties depend on the doping level. The properties of weakly doped QWs may be explained by a model assuming noninteracting impurities. However, as the impurity concentration increases, a situation is reached where a single-impurity theory is no longer valid as the overlap of impurity wave functions becomes significant. Such concentrations cause the formation of an impurity band (I<sub>B</sub>) and the tail in the first conduction or valence subband edge for *n*-type or *p*-type doping, respectively. Very high dopant concentration causes an overlap of the broadened I<sub>B</sub> with the free-carrier continuum. This threshold corresponds to transition from insulating to metallic behaviour of carriers (Mott transition [15]). A detailed understanding of this electronic phase change, which takes place at

very high doping concentrations in QWs, is not available yet.

A more complicated situation is observed in  $\delta$ -doped QWs, where the impurity concentration is above the metallic limit. In an ideal case, impurities begin to form a V-shaped potential well with a new two-dimensional subband structure. For  $n$ -type doped QWs the sublevel system is of one kind, whereas for  $p$ -type ones it has two kinds: heavy hole and light hole sublevels [6–8, 12]. This transformation affects the whole quantum well sublevel system. It can also change the wave function symmetry from even to odd, which influences the probability of optical transitions by changing the quantum transition matrix elements.

In the following discussion we introduce two critical concentrations,  $N_{I\_B}$  and  $N_M$ . When the impurity concentration  $N_I$  is less than  $N_{I\_B}$ , the impurities can be interpreted as noninteracting. For heavily doped QWs ( $N_{I\_B} < N_I < N_M$ ), the impurities form a band and cause the renormalization of the first conduction (valence) subband edge. For heavily uniformly doped QWs ( $N_I > N_M$ ), the impurity concentration corresponds to the metallic limit, which leads to renormalization of the first conduction (valence) subband and induces pinning of the Fermi level above the subbands. In the heavily  $\delta$ -doped case, formation of a V-shaped potential and transformation of the QW sublevel system occurs.

By analysing the heavily  $\delta$ -doped GaAs/AlAs MQWs ( $N_{Be} = 5 \cdot 10^{12} \text{ cm}^{-2}$ ) we assume that the quantum wells are nondegenerate, and their impurities are close to the Mott transition and under the level for the formation of an impurity band, in the region  $N_{I\_B} < N_I < N_M$ . To justify this model, several arguments will be put forward. Firstly, we observe shoulders in PL spectra, which are consistent with excitonic transitions in the reference weakly doped sample. This indicates that the transformation of the sublevel system of the QW is insignificant. The reported experimental results from Si-doped and Be-doped quantum wells show that the excitons continue to dominate in the radiative recombination at doping levels up to metallic limit [9, 11]. Also, the inclusion of just the energy level renormalization and neglect of the excitonic effects for acceptor-doped QWs at similar doping levels leads to problems of line identification in the excitonic region PL spectra. Secondly, the acceptor binding energy (or acceptor band centre energy  $E_{A\_B}$ ) can be determined from experimental data using the relation  $E_{A\_B} = E(X_{e1-hh1}) + E(X_{hh}) - E(e - Be\_B)$ , where  $E(X_{e1-hh1})$  and  $E(e - Be\_B)$  are the energies

of the  $X_{e1-hh1}$  and  $e-Be\_B$  lines, respectively, and  $E(X_{hh})$  is the binding energy of the heavy hole exciton, which can be deduced from theoretical calculations. For GaAs/AlAs QW with  $L_W = 5 \text{ nm}$  the heavy hole exciton binding energy  $E(X_{hh})$  is 15 meV [16]. Knowing the  $E(X_{e1-hh1})$  from the reference sample we deduce that  $E_{Be\_B} = 34 \text{ meV}$  at 77 K and  $E_{Be\_B} = 32 \text{ meV}$  at 300 K, which are close to the calculated Be impurity binding energy  $E_{Be} \approx 38 \text{ meV}$  in identical QWs [17]. The highest intensity bands can be attributed to the recombination of electrons with an acceptor impurity band as indicated in Fig. 1 by the label  $e-Be\_B$ . In weakly doped MQWs the influence of impurity recombination in the PL spectra at room temperature is negligible [14]. Because the binding energy of acceptors is high enough, not all acceptors are ionized at room temperature. The residual neutral acceptors for heavily doped QWs create competing centres for  $e-Be\_B$  recombination, which can be also contributed by the collective interaction of impurities.

## 5. Discussion

It is expected that at very low temperatures, where the exciton–phonon scattering is not efficient, or for highly doped QWs at strong exciton interaction with impurities or interface defects, the excitonic PL spectra is mostly inhomogeneously broadened and has a Gaussian shape, while the PL lineshape for pure QWs becomes more like a Lorentzian at higher temperatures.

To obtain the PL spectrum, the main task is to calculate the absorption coefficient  $K(\hbar\omega)$ . The luminescence intensity  $I_{PL}(\hbar\omega)$  is related to the absorption coefficient  $K(\hbar\omega)$  through the energy balance relation  $I_{PL}(\hbar\omega) \propto K(\hbar\omega)f(\hbar\omega)$ , where  $f(\hbar\omega)$  is a suitable thermal function. In the limit of a nondegenerate carrier density, the  $f(\hbar\omega)$  is approximated by a Boltzmann distribution function. The excitonic and band-to-band transitions for the weakly doped reference sample were calculated within fractional dimensional space (FDS) formalism, where a single parameter, dimensionality, contains the whole information on the confinement system [18, 19]. The Lorentzian lineshape convolution was also included into these calculations. However, for highly doped samples the  $e-Be\_B$  and excitonic PL bands were approximated with a Gaussian lineshape, and band-to-band transitions were calculated adapting the FDS formalism with a Gaussian lineshape convolution. This approximation is consistent with the PL spectra if some fraction of the excitons are bound to acceptor impurities at low temperatures [14]. The calcu-

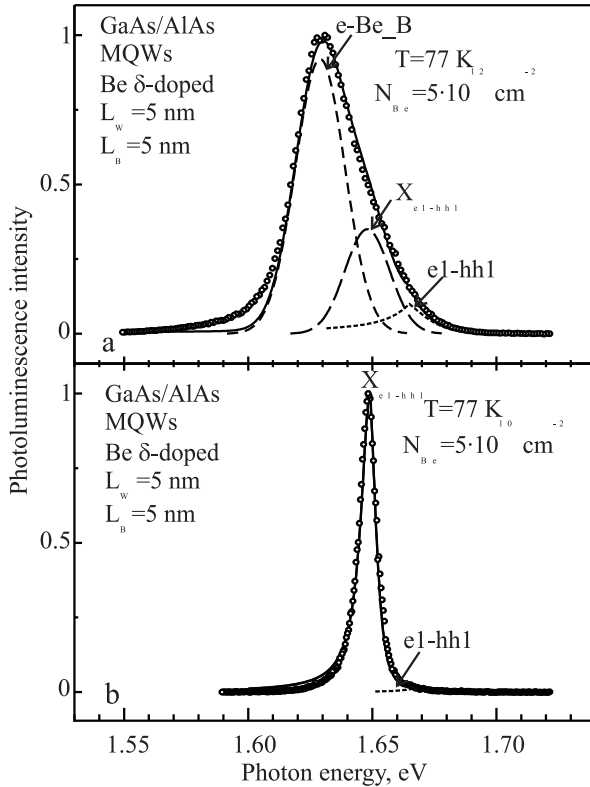


Fig. 2. Dots are experimental data, lines are calculated spectra of (a) heavily doped and (b) weakly doped reference MQWs at liquid nitrogen temperature. Label  $e\text{-Be}_B$  indicates free electron transitions from first conduction subband to Be impurity band.

lated spectra at liquid nitrogen and room temperatures are shown in Fig. 2 and Fig. 3. It has to be mentioned that band-to-band transitions are significant for heavily doped MQWs at room temperature. The energy of these transitions coincides with the light hole exciton dissociation energy position (see Fig. 3(a)).

The Mott transition is defined as the doping limit  $N_M$  over which the population of free carriers in the doped material no longer depends on temperature. Below this limit, impurity and conduction or valence bands are separated in energy, while above this limit, the material is semi-metal: the impurity and conduction bands are degenerate. For the 3D case, the Mott transition satisfies the relation [15]

$$N_M^{1/3} a_B \approx 0.2, \quad (1)$$

where  $N_M$  is critical doping concentration [ $1/\text{cm}^3$ ], and  $a_B$  is impurity Bohr radius [cm]. This transition occurs at the doping levels around  $2 \cdot 10^{16} \text{ cm}^{-3}$  and  $2 \cdot 10^{18} \text{ cm}^{-3}$  in bulk  $n$ - and  $p$ -GaAs, respectively.

In  $\delta$ -doped semiconductors and quantum wells with increasing impurity concentration, the impurity bound states are expected to broaden into impurity bands. In

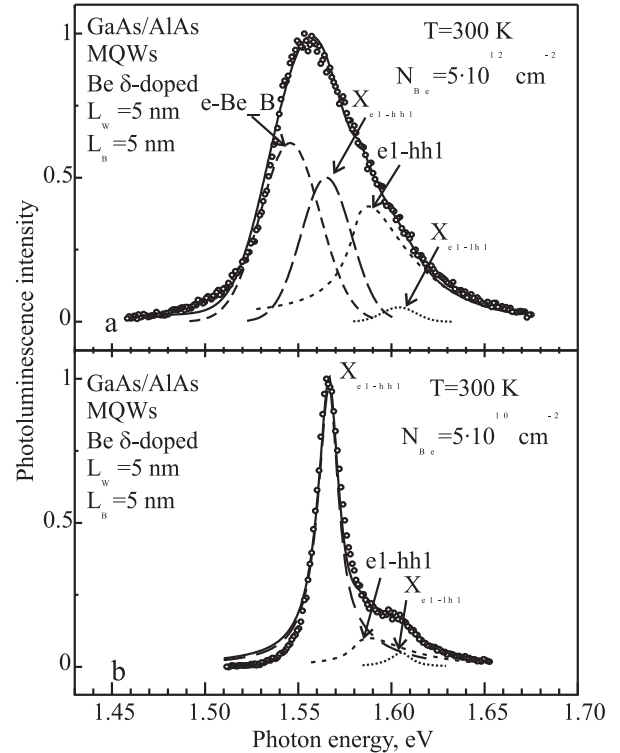


Fig. 3. Dots are experimental data, lines are calculated spectra of (a) heavily doped and (b) weakly doped reference MQWs at room temperature. Label  $e\text{-Be}_B$  indicates free electron transitions from first conduction subband to Be impurity band.

the high density limit, the electrons (holes) are confined to the ionized sheet of the impurities and form a two-dimensional electron (hole) gas with a two-dimensional subband structure. The critical concentration for the insulator–metal transition and formation of subband structure for the  $\delta$ -doped with Si impurity in GaAs can be estimated from relation [20]

$$N_1^{1/2} a_B \approx 0.31, \quad (2)$$

where  $N_1$  is the critical 2D doping concentration. Mott transition within the  $\delta$ -plane in  $n$ -GaAs is calculated to occur at the critical concentration  $N_{Si} \approx 10^{11} \text{ cm}^{-2}$ . Applying a simple spherical symmetry model for acceptor impurities in GaAs, when activation energy  $E_{Be} = 28 \text{ meV}$ , then  $a_{Be} = 2.1 \text{ nm}$ , consequently, the critical concentration for  $\delta$ -doped  $p$ -GaAs is found to be  $N_{Be} = 2.2 \cdot 10^{12} \text{ cm}^{-2}$ .

In QWs the impurity binding energy becomes larger than in the 3D case, whereas the effective Bohr radius decreases. For example, in  $\text{Al}_{0.3}\text{Ga}_{0.7}\text{As}/\text{GaAs}$  with  $L_W = 5 \text{ nm}$ , the donor activation energy  $E_D$  equals to 13 meV [4]. This corresponds to  $a_D \approx 4.5 \text{ nm}$  and the critical concentration  $N_D$  equals to  $4.8 \cdot 10^{11} \text{ cm}^{-2}$ , which is higher than in the 3D case and close to the

experimental value. It has been found that in  $n$ -type doped QWs the Mott transition occurs in the range  $N_D = 2 \cdot 10^{11} - 4 \cdot 10^{11} \text{ cm}^{-2}$  [21].

For GaAs/AlAs with  $L_W = 5 \text{ nm}$ , the acceptor binding energy is  $E_{Be} = 38 \text{ meV}$  and  $a_{Be} = 1.54 \text{ nm}$ . This leads to an insulator–metal transition at  $N_{Be} = 4 \cdot 10^{12} \text{ cm}^{-2}$ . Taking into account that this estimation is not rigorous, we can conclude that the heavily doped MQWs under study are not degenerate and only acceptors form the impurity band. This assumption allows one to explain the features observed in the PL spectra. It should be observed that for narrower quantum wells the increasing impurity binding energy and decreasing effective Bohr radius requires a higher doping level in order to reach the level at which the overlap of wave functions and the Mott transition occur.

## 6. Summary

The photoluminescence spectra of heavily ( $5 \cdot 10^{12} \text{ cm}^{-2}$ ) Be  $\delta$ -doped GaAs/AlAs MQWs at liquid nitrogen and room temperatures are explained by excitonic recombination and free electron–Be impurity band optical transitions. The estimation shows that the critical concentration for insulator–metal transition and the formation of subband structure with Be  $\delta$ -doped GaAs/AlAs quantum wells ( $L_W = 5 \text{ nm}$ ) occurs at acceptor concentration  $N_{Be}$  near or larger than  $5 \cdot 10^{12} \text{ cm}^{-2}$ .

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## OPTINIŲ ŠUOLIŲ SAVYBĖS STIPRIAUSIAI Be $\delta$ -LEGIRUOTUOSE GaAs/AlAs KARTOTINIUOSE KVANTINIUOSE ŠULINIUOSE

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### Santrauka

Kvantiniai šuliniai su įterptomis priemaišomis yra įdomūs ne vien tik fundamentinės, bet ir taikomosios fizikos požiūriu, pavyzdžiui, kuriant infraraudonosios spinduliuotės jutiklius. Geram prietaisui jautriai pasiekti reikalingas didelis priemaišų tankis. Toks tankis pasiekiamas naudojant vadinamąjį  $\delta$  legiravimą, kai priemaišos sukaupiamos ploname kvantinio šulinio sluoksnyje. Pasiekus tam tikrą tankį, priemaišos ima sąveikauti ir pasikeičia jų savybės: jos gali sukurti priemaišinę juostą ar net papildomus energijos lygmenis, kurių dalį užpildo laisvieji 2D krūvininkai. Tokį vyksmą apibrėžia dielektriko–metalo Mott'o virsmas.

Pateikti molekulių pluoštelių epitaksijos būdu išaugintų, akceptorinėmis Be priemaišomis  $\delta$  legiruotų GaAs/AlAs kartotinių  $L_W = 5$  nm pločio kvantinių šulinių fotoluminescencijos (FL)

ypatumai. Tam tikslui pasiekti buvo naudojami dviejų rūšių bandiniai: tiriamieji bandiniai, kuriuose priemaišų tankis siekė  $N_{Be} = 5 \cdot 10^{12} \text{ cm}^{-2}$ , ir etaloniniai, kuriuose  $N_{Be} = 5 \cdot 10^{10} \text{ cm}^{-2}$ . Palyginus tiriamųjų ir etaloninių bandinių FL spektrus, padaryta išvada, kad, esant Be priemaišų tankiams  $5 \cdot 10^{12} \text{ cm}^{-2}$ , yra svarbi laisvųjų elektronų rekombinacija su Be priemaišomis, kurios yra suformavusios priemaišinę juostą. Nustatyta, kad priemaišinės juostos centras yra apie 32–34 meV nutolęs nuo sunkiųjų skylių pirmojo energijos lygmens. Taip pat ištirta, kad FL spektre išlieka svarbi ir eksitoninė spinduliuotė. Įvertinta, kad GaAs/AlAs kvantiniuose  $L_W = 5$  nm pločio šuliniuose akceptorinėms priemaišoms Mott'o virsmas turėtų įvykti, esant šiek tiek didesniems nei  $5 \cdot 10^{12} \text{ cm}^{-2}$  tankiams  $N_{Be}$ .