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Optical absorption in GaAs quantum well caused by donor-acceptor pair transitions

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1. Introduction. The investigation of properties related with impurity centers in semiconductor quantum well (QW) structures has not only fundamental interest, but also is of major importance in optoelectronic device applications (high electron mobility transistors, QW infrared photodetectors or emitters, etc.) [1].

In semiconductors of A^3B^5 group, the electrons that bound with doped impurities, form shallow energy states close to band gap edges. In particular, doping the bulk semiconductor simultaneously with both donor and acceptor impurities, form the shallow states near the band gap edges, making possible optical transitions between two clearly isolated energy levels. [2-4].

One of the first works related to investigations of donor-acceptor pair (DAP) transitions in above-mentioned semiconductors is Hopfield's work [2]. Later, detailed investigation of DAP transitions were made by Stoneham and Harker [3], where central-cell corrections were taken into account.

The investigation of hydrogenic impurities in GaAs QW was in details performed by Bastard [5]. Later investigations of impurity properties in QW was followed by several other, more detailed investigations. The energy spectrum of the ground state and the low-lying excited states for shallow impurities in QW structures, influence of dielectric constant mismatches at well interfaces, effects of spatially dependent screening, electron-phonon interactions, nonparabolicy of the conduction and valence band, etc. were in details performed by other authors (see for example Ref. [6])

Variations in the properties can be caused by changing the concentration of the dopant from uniform distributions within QW to concentrated sheet layers resulting in a so-called δ-doped profile. Energetic levels of an impurity are possible to tune in a controlled way by changing the doping profile. Understating the influence of impurities on the optical properties near the QW intrinsic transitions is of particular concern in order to optimize the design of optoelectronic devices.

The PL spectrum is an effective technique for characterizing doped QWs. In addition to free-excitonic transition, donor-bound exciton [7,8], acceptor-bound exciton [9], free electron to acceptor [10-12] and heavy hole to donor [10-12] transitions were also observed in p-type and n-type doped QWs.

Besides above-mentioned ones, acceptor-to-donor pair transitions in QWs are also possible. There are several experimental reports concerning observation of the DAP transition peak in the PL spectra. Ding et al [13] have reported an observation of an anomalously large blueshift of apparent

DAP transition peak in compensation-doped coupled QWs. The blueshift was observed in PL spectra while the excitation intensity increases from 0.54 to 423 W/cm^2. Authors proposed that the blueshift is due to the change of the Coulomb interaction energy between recombined donors and acceptors as their separation decreases. Later Guzman et al [14] performed an optical characterization of GaAs/GaAlAs single QW structures by interband PL spectroscopy. The peak in PL spectra at lower energy was observed and attributed to DAP transition. Samples were grown by molecular beam epitaxy (MBE) with two-dimensional doping concentration (Si) in the wells in the range of 0-10^{12} cm^{-2}. Si is related to acceptor, while C is related to residual donor, which is always present in samples grown by MBE. In this connection, one can assume that non-compensated QWs were considered. The dependence of DAP transition peak on different doping concentration was performed, and the blueshift was observed.

However, in above-mentioned experimental works, discussions about DAP transitions concerned only qualitative aspect of the subject. In this connection, it is important to have a quantitative model, which will describe aforementioned transitions that can give an opportunity to perform an essential comparison between theory and the experiment.

In this paper, we present a theoretical investigation of DAP transitions in the framework of non-compensated lightly doped GaAs infinite-barrier QW.

2. Theory. The impurity envelope functions are the solutions of Schrödinger equation with the effective Hamiltonian

$$\hat{H} = \frac{\hat{p}^2}{2m^*} + V(z) - \frac{e^2}{\kappa\sqrt{\rho^2 + (z - z_i)^2}}, \tag{1}$$

where m^* is the electron effective mass, κ - the dielectric constant (for GaAs $\kappa = 13.18$), z_i (i = D, A) is the impurity position along OZ axes, $V(z)$ - the confinement potential.

For definiteness we will only refer to the donor state, because it is clear that (1) also applies to the acceptor state, where m^* understood as the hole effective mass.

We present the envelope function of ground state as

$$\psi_0(\rho, z) = \varphi_0(\rho)\chi_0(z), \tag{2}$$

where $\varphi_0(\rho)$ is the function in QW plane and $\chi_0(z)$ is along the quantization axis OZ.

Taking into account the normalization condition for $\chi_0(z)$ we get two-dimensional Schrödinger equation for the function $\varphi_0(\rho)$

$$\left[\frac{\hat{p}_x^2 + \hat{p}_y^2}{2m^*} + V_{eff}(\rho)\right]\varphi_0(\rho) = (\varepsilon - E_0)\varphi_0(\rho), \tag{3}$$

where $V_{eff}(\rho)$ is the effective Coulomb potential in XOY plane:

$$V_{eff}(\rho) = -\frac{e^2}{\kappa}\int_{-L/2}^{L/2}\frac{|\chi|^2}{\sqrt{\rho^2+(z-z_i)^2}}dz. \quad (4)$$

The solution of Eq.(3) is found using the variational method, with the trial function of the ground state in the form [5]

$$\varphi_0(\rho) = \frac{1}{\lambda}\sqrt{\frac{2}{\pi}}e^{-\rho/\lambda}, \quad (5)$$

where λ is the variational parameter.

The ground state energy is obtained after the minimization of the function

$$\varepsilon(\lambda, z_i) = E_0 + \frac{\hbar^2}{2m^*\lambda^2} - \frac{2e^2}{\kappa\lambda}\int_0^{\infty} xe^{-x}dx\int_{-L/2}^{L/2}\frac{|\chi_0|^2 dz}{\sqrt{x^2+\frac{4}{\lambda^2}(z-z_i)^2}}. \quad (6)$$

The binding energy is equal to

$$E_{bind} = E_0 - \min_{\lambda}\varepsilon(\lambda, z_i). \quad (7)$$

Now we turn to the calculation of the absorption coefficient in considered structure, conditioned by transitions between ground states of DAP.

Let us consider lightly doped QW with concentration of acceptors n_A, so that $\bar{R} >> a_D, a_A$ conditions are satisfied ($\bar{R}$ is the average distance between acceptors and donors in the QW plane). In this case the main contribution into the transitions within the donor-acceptor system makes pairs satisfying to $R \geq a_D, a_A$ conditions, because the number of pairs with $R < a_D$ is not significant. For this case the coupling energy of the DAP can be taken equal to $e^2/\kappa R$ and considered as an acceptor energy level shift. The location of the donor is $(\vec{\rho}, z)$, and the acceptor is $(\vec{\rho} - (\vec{R}, z)$, where $\vec{\rho}$ is the radius vector and $\vec{R}$ is the distance between donor and acceptor in QW plane. Later we will assume that donor and acceptor are located in the center of QW.

The electron and hole ground eigenstates and eigenvalues are (measured from the maximum of valence band)

$$\psi_A = \frac{2}{\lambda_A}\sqrt{\frac{1}{\pi L}}\cos\left(\frac{\pi z}{L}\right)e^{-\frac{|\vec{\rho}-\vec{R}|}{\lambda_A}}u_{v,0}(\vec{\rho}-\vec{R}), \quad (8)$$

$$\psi_D = \frac{2}{\lambda_D}\sqrt{\frac{1}{\pi L}}\cos\left(\frac{\pi z}{L}\right)e^{-\frac{\rho}{\lambda_D}}u_{c,0}(\vec{\rho}), \quad (9)$$

$$E_A = -\min \varepsilon_A(\lambda_A) - \frac{e^2}{\kappa R}, \tag{10}$$

$$E_D = \min \varepsilon_D(\lambda_D) + \varepsilon_{gap}, \tag{11}$$

where λ_A, λ_D are variational parameters, $u_{v,0}$, $u_{c,0}$ - Bloch amplitudes in the center of the Brillouin zone (in the discussed structure zone extrema are on the center of Brillouin zone).

The light absorption coefficient is determined by the formula [15]

$$\alpha_R(\omega) = \frac{4\pi^2 c}{N\omega V} \frac{|M_{AD}|^2}{|A_0|^2} \delta(E_f - E_i - \hbar\omega), \tag{12}$$

where V is the sample volume, M_{AD} - the matrix element of "acceptor→donor" transition, N - the refractive index, A_0 is the vector potential amplitude of incident electromagnetic wave.

In the case of normal incident light the matrix element can be written as

$$M_{AD} = \frac{2e}{\pi m_0} (\vec{e}\,\vec{p}_{cv}) \frac{1}{\lambda_a \lambda_D} \frac{2}{L} \int_{L/2}^{-L/2} \frac{e^{iq_z z}}{\cos} \left(\frac{\pi z}{L} \right) \cos \left(\frac{\pi z}{L} \right) dz \times$$

$$\times \int_0^{2\pi} \int_0^{\infty} e^{-\left(\frac{1}{\lambda_A} \sqrt{\rho^2 + R^2 - 2\rho R \cos\varphi} + \frac{1}{\lambda_D}\rho \right)} \rho d\rho d\varphi = \frac{2e}{\pi m_0} (\vec{e}\,\vec{p}_{cv}) \frac{1}{\lambda_A \lambda_D} F(R)\xi(q_z L), \tag{13}$$

where $\vec{p}_{cv}$ is the matrix element conditioned by Bloch amplitudes, $\vec{e}$ is the incident light polarization, q_z is the photon wave vector in the z direction.

By F(R) and $\xi(q_z L)$ we denoted the following integrals

$$F(R) = \int_0^{2\pi} \int_0^{\infty} e^{-\left(\frac{1}{\lambda_A} \sqrt{\rho^2 + R^2 - 2\rho R \cos\varphi} + \frac{1}{\lambda_D}\rho \right)} \rho d\rho d\varphi,$$

$$\tag{14}$$

$$\xi(q_z L) = \frac{2}{L} \int_{-L/2}^{L/2} e^{iq_z z} \cos \left(\frac{\pi z}{L} \right) \cos \left(\frac{\pi z}{L} \right) dz.$$

In discussed case of shallow impurities Eq.(13) can be simplified, if we take into consideration the fact, that for GaAs $\tilde{\varepsilon}_g \gtrsim \varepsilon_g \sim 1$ eV (the expression for $\tilde{\varepsilon}_g$ see below) and for QW width we have $L \sim 10^{-6}$ cm (~ 100 Å), which makes the parameter $q_z L << 1$. This allows us to take $\xi(q_z L)$ approximately equal to 1.

As it follows from Eq. (12) such transitions are possible only between those DAPs, the distances between which can be determined from the energy conservation law

$$R_1 \equiv R = \frac{e^2}{\kappa(\hbar\omega - \tilde{\varepsilon}_g)}, \tag{15}$$

where

$$\tilde{\varepsilon}_g = \varepsilon_g + E_D^0 + E_A^0, \quad E_A^0 = \min_{\lambda_A} \varepsilon_A(\lambda_A), \quad E_D^0 = \min_{\lambda_D} \varepsilon_D(\lambda_D). \tag{16}$$

Considering R as changing continuously when $n_A >> n_D$, let us write the expression for the absorption coefficient [4]

$$\alpha(\omega) = N_D \int_0^\infty \alpha_R(\omega) W(R) dR, \tag{17}$$

where N_D - number of donors, W(R) - distribution function by R values.

As DAPs distribution function we take the adjacent-neighbor distribution [4], and taking W(R) not dependent on z:

$$W(R) = 2\pi R n_A \exp\{-\pi R^2 L n_A\}, \tag{18}$$

where n_A is the bulk concentration of acceptors.

After averaging over the distribution (18) for the absorption coefficient of DAP transition we obtain the following expression

$$\alpha_{DAP}(\omega) = \frac{2^5 \pi N n_A^- n_D^+}{L\omega \lambda_A^2 \lambda_D^2 c m_0^2} \left|\vec{e}\vec{p}_{cv}\right|^2 \left|\xi(q_z L)\right|^2 \left|F(R_1)\right|^2 R_1^3 \{-\pi R_1^2 n_A^-\}, \tag{19}$$

where n_A^- and n_D^+ are two dimensional surface concentrations of acceptors and donors, respectively.

3. Discussion. Fig. 1 shows the dependencies of the absorption coefficient on the energy of incident light at different values of QW width (L = 50 Å, 65 Å, 100 Å). As it follows from figure, with the increase of L the effective width of the forbidden band decreases and therefore the absorption threshold shifts to the smaller energies (smaller frequencies), as a result of size-quantization weakening. Also small reduction of the absorption coefficient value is observed. Calculations are made at the value of dominant impurity (acceptors) concentration equals to $n_A^- = 10^{11}$ cm^{-2}, and at k = 0.05 compensation value ($k = n_D^+ / n_A^-$). The numerical values of parameters in

the absorption coefficient (19) in the GaAs structures are: ε_{gap} = 1.519 eV, $m_v = 0.34m_e$, m_c = $0.067m_e$, N = 3.6.

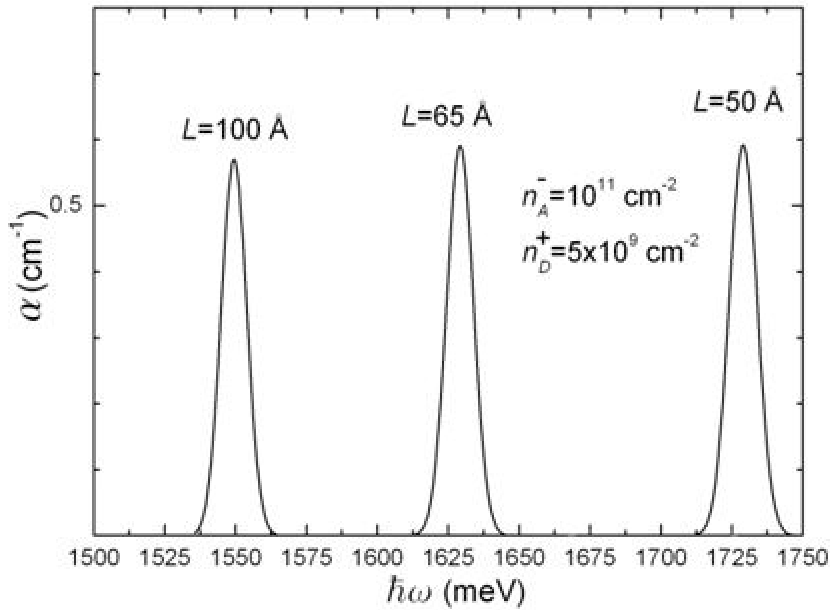

Fig.1. Absorption coefficient dependence on incident light frequency at different widths of QW

Fig. 2 presents the absorption coefficient dependencies on the incident light frequency at different values of dominant impurity concentration ($n_A^- = 5 \times 10^{10}$ cm^{-2}, $n_A^- = 10^{11}$ cm^{-2}, $n_A^- = 2 \times 10^{11}$ cm^{-2}, $n_A^- = 5 \times 10^{11}$ cm^{-2}). With the increase of the impurity concentration the absorption coefficient growth occurs, as well as threshold frequency slightly increases (i.e. the blueshift is observable).

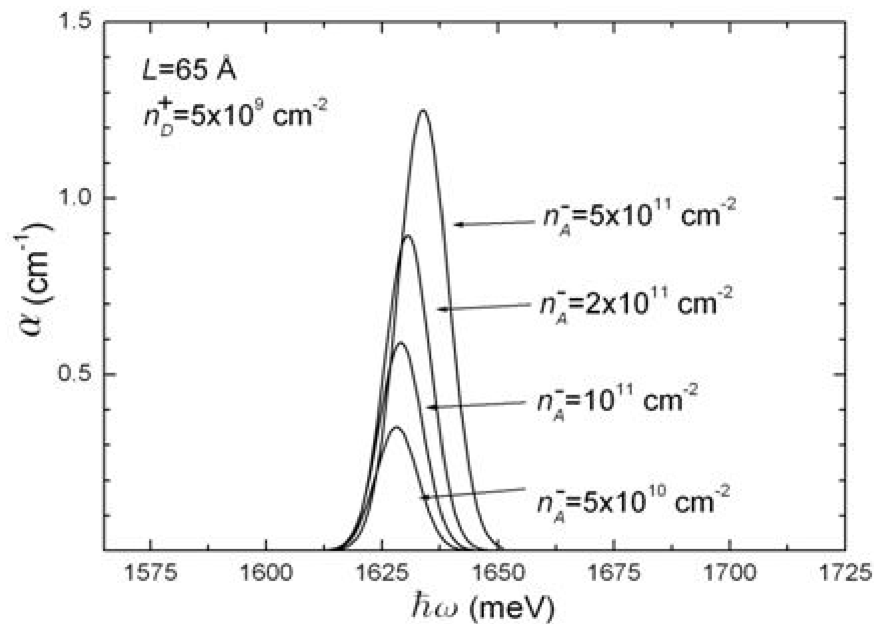

Fig.2. Absorption coefficient dependence on incident light frequency at different concentrations of dominant impurity

Fig. 3 shows the blueshift dependences on different values of two-dimensional concentrations of

dominant impurity (acceptor). There is a significant difference between the experimental and theoretical data for the lightly doped samples.

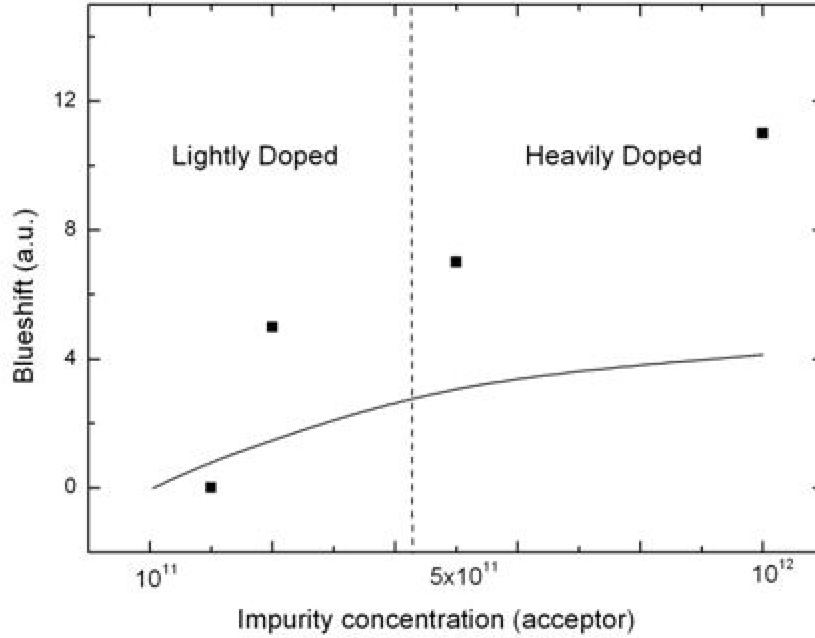

Fig.3. The blueshift dependence on dominant impurity (acceptor) concentration: squares - experimental results29, solid line - result of calculations, left - region of low concentrations, right - region of high concentrations

The blueshift can be presented as

$$\Delta E_{shift} = \varepsilon_g - E_{bD} - E_{bA} + \frac{q_1 q_2}{R} \tag{20}$$

where E_{bD} and E_{bA} are donor and acceptor binding energies, respectively; the fourth item in Eq.(20) is the Coloumbian term. When acceptor concentration is increasing (e.g. concentration of Si atoms [14]), donors (e.g. residual C atoms [14]) and acceptors become spatially closer, the blueshift in the acceptor-donor transition peak should take place, as a result of the Coloumbian term increase [13], [14]. So the growth of doping level should be the reason of blueshift increase. Such a result is obtained in our theoretical model.

In Ref.[14] the blueshift of DAP transition peak was observed with respect to e1-hh1 peak (transition between first conduction subband and first heavy-hole subband) in GaAs/AlGaAs QW infra-red detector structures. The considered samples with different concentrations of impurities were grown at different runs via MBE. In the reported results fluctuations of QW thicknesses (appearing due to different runs) introduce certain variation into blueshift growth tendency along with impurity concentration growth in the lightly doping samples. The comparison of our theoretical results with the experimental data shows that in the lightly doped samples the mentioned technological fluctuations significantly affect on the blueshift growth tendency along

with the impurity concentration increase from sample to sample. As it is seen from Fig. 1, even small differences in well thicknesses can result in significant shift of the absorption threshold (peak position).

4. Conclusion. We have presented the theoretical model for donor-acceptor pair transitions in non-compensation doped GaAs QW. These transitions are taking place between different impurity atoms' levels. The developed model enables in the frames of simple theoretical model to simulate blueshift behavior in doped QW structures.

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Դոնոր-ակցեպտոր անցումներով պայմանավորված օպտիկական կլանումը GaAs-ից քվանտային փոսում

Տեսականորեն հետազոտված է օպտիկական կլանումը GaAs-ից քվանտային փոսում՝ պայմանավորված դոնոր-ակցեպտորային անցումներով: Արդյունարար զանգվածի մոտավորությամբ վարիացիոն եղանակով ուսումնասիրված են դոնորի և ակցեպտորի հիմնական վիճակների ալիքային ֆունկցիաները և էներգետիկ մակարդակները: Հաշվի է առնված կլանման կորի լայնացումը՝ պայմանավորված միջխառնուրդային հեռավորությունների միջինացմամբ: Հետազոտված է կլանման գործակցի՝ քվանտային փոսի լայնությունից և խառնուրդների կոնցենտրացիայից կախման բնույթը: Ուսումնասիրված է կլանման սպեկտրի կապույտ շեղումը, և կատարված է համեմատություն փորձնական արդյունքների հետ:

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Оптическое поглощение в квантовой яме из GaAs, обусловленное донор-акцепторными переходами

Теоретически исследовано оптическое поглощение в квантовой яме из GaAs, обусловленное донор-акцепторными переходами. В приближении эффективной массы вариационным методом изучены волновые функции и энергетические уровни основных состояний донора и акцептора. Учтено уширение кривой поглощения, обусловленное усреднением по межпримесным расстояниям. Исследован характер зависимости коэффициента поглощения в зависимости от толщины квантовой ямы и от концентрации примесей. Изучено синее смещение в спектре поглощения и проведено сравнение с имеющимися экспериментальными данными.