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Peculiarities of the exciton scattering in double semiconductor quantum wells with disordered layers

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Abstract. Effects of the presence of isolated disordered layers on the exciton scattering by compositional fluctuations in double semiconductor quantum wells have been studied. In the structures containing both ordered and disordered layers, the probability of the scattering depends on the degree of the exciton wavefunction localization in the disordered layers, where it interacts with the fluctuations. For some parameters of the structure the exciton wavefunction can penetrate deeply into the ordered layers of the structure, which leads to a sharp drop of the probability of the scattering and, consequently, to the narrowing of the optical exciton bands. It has been shown that for heterostructures containing diluted magnetic semiconductor layers, the probability of the scattering can be tuned by external magnetic field.

Keywords: double quantum well, diluted magnetic semiconductor, exciton scattering.

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1. Introduction

The extensive use of semiconductor heterostructures in modern optoelectronic devices spurred to study factors influencing broadening the exciton bands in these systems [1-3]. In semiconductor quantum wells, the bandwidth is conditioned by various factors: fluctuations in the well thickness, interface roughness, various kinds of macroscopic inhomogeneities *etc*. In semiconductor alloys, like to $Cd_{1-x}Mn_xTe$, $Al_xGa_{1-x}As$, $Zn_{1-x}Mn_xSe$, in addition to these technological factors, there is another mechanism of the band broadening caused by the microscopic compositional disorder – the exciton scattering by fluctuations in the crystal composition. Ions of components of an alloy are randomly distributed across the crystal lattice, which creates rapid oscillations in the space potential for carriers. This potential arises from different values of electron densities of the substitutional atom and that of the crystal (for small contents of these atoms, one can say about "impurity atoms" and "host atoms"), deformation of the lattice in the vicinity of substitutional atoms and so on. This disorder is always present in the semiconductor alloys, and it is especially important for high-quality samples. It must be noted that calculations of the effect of this scattering mechanism on the bandwidth don't tolerate uncertainties related to unknown values of parameters, in contrast to mechanisms caused by technological defects. In diluted magnetic alloys, like to $Cd_{1-x}Mn_xTe$, $Zn_{1-x}Mn_xSe$, excitons scatter also by magnetic ion spin projection fluctuations. Calculations and experimental study demonstrate some interesting manifestations of this scattering: for example, the strong magnetic field dependence of the optical exciton bandwidths is observed in diluted magnetic semiconductors [4-7].

In the present paper, the exciton scattering by fluctuations in composition in double quantum well structures has been studied. Very often in such hetero-structures some layers are formed by semiconductor alloys, and others – by pure semiconductor crystals, for

example, CdTe/(Cd,Mn)Te, (Al,Ga)As/GaAs *etc.* It means that in these systems only some of the layers are essentially disordered, and the probability for exciton to be scattered by the fluctuations depends on the probability for carriers to be in the disordered layers or, in other words, on the spatial distribution of the exciton wavefunction over the ordered and disordered layers. It leads, for example, to extremely low broadening of exciton bands in shallow GaAs/(In,Ga)As/GaAs single quantum wells [3] due to strong penetration of the wavefunction from the disordered $In_{1-x}Ga_xAs$ region into the GaAs barriers, where compositional disorder is absent. In the case of double quantum wells, the spatial distribution of the wavefunction over the structure essentially depends on the parameters of the whole system, which, as it will be shown, causes some interesting peculiarities in the exciton scattering. Also, the magnetic field dependence of the probability of the exciton scattering in the structure with magnetic impurities in one of the quantum well layers has been considered.

2. Model of the system and methods of calculations

The methods used for calculating the probability of the exciton scattering by the fluctuations of distribution and spin projections of the impurities in diluted magnetic semiconductors are similar to those described in the work [7] in detail. So, in this paper, consideration will be confined to a short description of the basic theoretical methods and discussion of the obtained results.

Let us consider a double quantum well with the impurities localized in the well layers (Fig. 1). In the studied system, Hamiltonian of exciton can be written as

$$H = H_0 + H_{\text{int}}, \tag{1}$$

where H_0 is typical free exciton Hamiltonian, including the kinetic energy of electron, hole and Coulomb interaction; H_{int} – Hamiltonian of interaction between carriers and impurities.

Hamiltonian of exciton interaction with magnetic impurity ions H_{int} can be written as

$$H_{\text{int}} = \sum_{\vec{n}} \frac{1}{N_0} \left\{ \left(\Delta_e - J_e \vec{S}_e \vec{S}_{\vec{n}} \right) \delta\left(\vec{r}_e - \vec{n} \right) + \right.$$
$$\left. + \left(\Delta_h + J_h \vec{S}_h \vec{S}_{\vec{n}} \right) \delta\left(\vec{r}_h - \vec{n} \right) \right\} x_{\vec{n}} \,. \tag{2}$$

Here, N_0 is the concentration of cation lattice sites, $\vec{n}$ – coordinate of the cation lattice site, $\vec{r}_{e(h)}$ – position of electron (hole), $\Delta_{e(h)}$ – potential of the nonmagnetic interaction of electron (hole) with impurity ion, $x_{\vec{n}}$ describes occupation of cation sites by impurity ions: $x_{\vec{n}} = 0$ if there is host ion in the $\vec{n}$ lattice site, and $x_{\vec{n}} = 1$ if the site is occupied by substitutional ion, $J_{e(h)}$ – exchange integral for electron (hole), $\vec{S}_{e(h)}$ – spin of electron (hole), $\vec{S}_{\vec{n}}$ – spin of magnetic ion.

The numbers of the site occupation can be expressed as

$$x_{\vec{n}} = \bar{x} + \delta x_{\vec{n}}, \quad S_{z,\vec{n}} = \bar{S}_{z,\vec{n}} + \delta S_{z,\vec{n}} \,. \tag{3}$$

Here, $\bar{x}$ denotes the average value of the relative concentration of ions in a certain layer of the structure, $\bar{S}_z^{(1)}$ is the average value of the single spin projection on the direction of magnetic field, coinciding with the direction of the structure growth along the axis *z* (this average value can be easily obtained in the mean field approximation [9]), $\delta x_{\vec{n}}$ and $\delta S_{z,\vec{n}}$ denote the fluctuations of the corresponding values, which lead to the scattering of exciton.

To describe this scattering, perturbation Hamiltonian may be introduced:

$$\Delta H = H_{\text{int}} - \bar{H}_{\text{int}}, \tag{4}$$

Where $\bar{H}_{\text{int}}$ determines the profile of quantum wells for electron and hole in the mean field approximation (see [8, 9] for the detail description). For calculations, the following form of the variational wavefunction of exciton in the double quantum well was used:

$$\Psi_{\vec{k}}\left(\vec{r}_e, \vec{r}_h\right) = \frac{1}{\sqrt{S}} e^{i\vec{k}\vec{R}} f_e\left(z_e\right) f_h\left(z_h\right) \sqrt{\frac{2}{\pi\lambda^2}}\, e^{-\rho/\lambda}, \tag{5}$$

where $f_{e(h)}\left(z_{e(h)}\right)$ is the one-particle wavefunction of electron (hole) in the double quantum well, $\vec{r}_{e(h)} = \left(\vec{\rho}_{e(h)}, z_{e(h)}\right)$, $\vec{k}$ and $\vec{R}$ are the wave vector and position of the exciton center of masses in the plane of layers, *z* is the direction of crystal growth. The fluctuations lead to the elastic exciton scattering with the change of the two-dimensional wave vector $\vec{k}$. The reverse relaxation time can be calculated using the formula:

$$\frac{1}{\tau_{\vec{k}}} = \sum_{\vec{k}'} W_{\vec{k},\vec{k}'}, \tag{6}$$

where $W_{\vec{k},\vec{k}'}$ is the probability of the exciton scattering from $\vec{k}$ state to $\vec{k}'$ state calculated with the wave-function (5) and perturbation Hamiltonian (4) [7]. The obtained relaxation time was averaged with respect to the impurity concentration and spin projection distributions assuming the latter to be chaotic:

$$\left\langle \delta x_{\vec{n}}, \delta x_{\vec{m}} \right\rangle = x(1-x)\delta_{\vec{n},\vec{m}}, \left\langle \delta S_{z,\vec{n}}, \delta S_{z,\vec{m}} \right\rangle = \left\langle \delta S_z^2 \right\rangle \delta_{\vec{n},\vec{m}} \,. \tag{7}$$

The scattering of exciton should manifest itself in the broadening of exciton optical bands. The reverse relaxation time $\hbar/\tau_{E(\omega)}$, where $E(\omega)$ is the exciton energy on the frequency ω, determines the contribution of the scattering to the damping of the excitonic resonance and, consequently, the shape of the exciton absorption bands [10].

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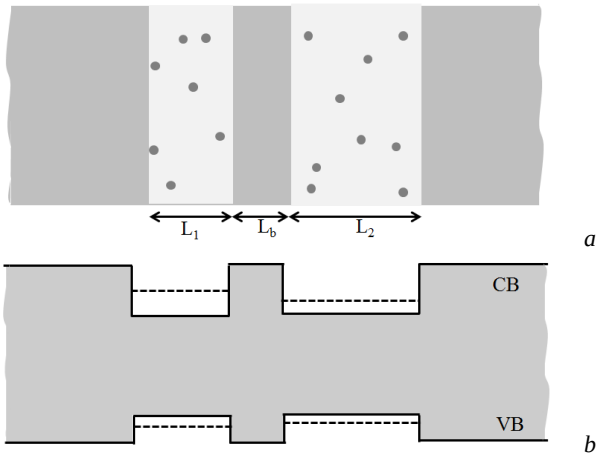

Fig. 1. A schematic illustration of the structure (*a*) and corresponding band edge profiles (*b*) of a double-well heterostructure containing ordered (dark grey) and disordered (light grey with circles) semiconductor layers. Impurity ions are placed in the layers forming potential wells for electrons and holes in the conduction and valence bands. Dashed lines depict one-particle energy levels in the quantum wells.

Calculations were performed for the ZnTe/ $Cd_{1-x}Mn_xTe$ /ZnTe/$Cd_{1-y}Mn_yTe$/ZnTe double quantum well. The following parameters were used [9, 11-13]: the total energy band gap for $Cd_{1-x}Mn_xTe$ $E_g(Cd_{1-x}Mn_xTe)$ = = $1.606 + dE_g^{Mn}(x)$ eV, $dE_g^{Mn}(x) = 1.592x$ eV, $\Delta_e = (1-\alpha)\frac{dE_g^{Mn}(x)}{dx}$, $\Delta_h = \alpha\frac{dE_g^{Mn}(x)}{dx}$, $\alpha = 0.4$, the total energy band gap for ZnTe E_g(ZnTe) = 2.35 eV, the valence band offset on the interfaces ZnTe/(Cd, Mn)Te was chosen to be equal to $\alpha' = 0.2$, the effective masses of electron and heavy hole were considered as the same for all layers and are equal to $m_e = 0.096m_0$, $m_{hh} = 0.6m_0$, where m_0 is the mass of free electron, the dielectric constant $\varepsilon = 9.7$, $J_e = 0.22$ eV, $J_h = -0.88/3$ eV, and the concentration of cation lattice sites $N_0 = 4/a_0^3$, where a_0 = 6.48 Å is the lattice parameter in CdTe.

The calculated dependence of the reverse relaxation time $\hbar/\tau_k$ for $k = 0$ on the barrier width for the quantum wells of the same width and concentration of impurities in ZnTe/$Cd_{1-x}Mn_xTe$/ZnTe/$Cd_{1-x}Mn_xTe$/ZnTe in the absence of external magnetic field ($H = 0$) is depicted in Fig. 2. The thick lines correspond to the ground exciton state 1*e* – 1*hh*, and the thin lines correspond to the excited state 2*e* – 2*hh*. To explain the obtained dependence for the ground state, we have to take into account distribution of the wavefunction over the layers of the structure containing and not containing the impurities. In single and double well structures with a very thin barrier, the wavefunctions of electron and hole are localized in the well layer, where the impurities are placed. For exciton that corresponds to a high probability to be scattered by concentration fluctuations of the impurities. As the thickness of the barrier layer rises, the wavefunction of the exciton begins to penetrate into the barrier layer, which leads to decrease in the probability of the scattering. When the barrier becomes thick enough, penetration of the wavefunction into the barrier layer becomes weaker, and the probability of the scattering rises a little. Regarding the excited state for very thin as well as for thick barriers, its wavefunction penetrates deeper into barriers than the function of the ground state, and the probability of the scattering for the excited state is less than for the lowest one. It can be seen that there is the region of barrier widths, where the probability to be scattered for the ground state decreases so essentially (due to penetration of the wavefunction into the ordered barrier layer) that it turns out to be less than that for the excited state.

In Fig. 3, the reverse relaxation time $\hbar/\tau_k$ for $k = 0$ for the same structure in the absence of external magnetic field and for the first well width L_1 =3.5 nm as a function of the second well width L_2 is shown for a few values of the barrier widths. The curves have a well-defined drop when the well widths are equal. This effect is also associated with the redistribution of the wavefunction between the layers containing and not containing the impurities. Again, the part of the wavefunction in the barrier layer (where impurities are absent) is maximal for the wells of the same width when localization of the particles in the disordered well layer is the weakest one.

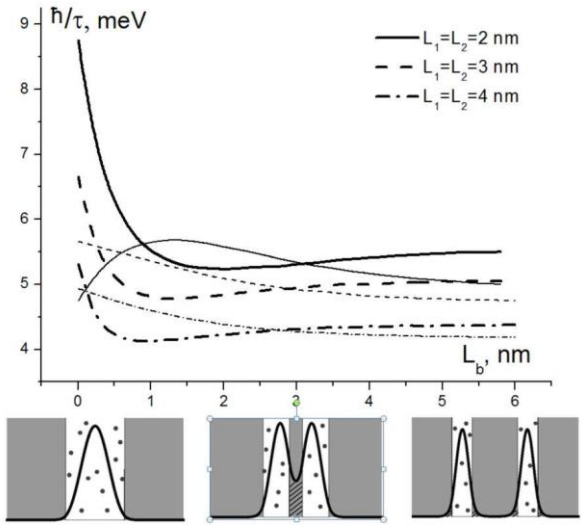

Fig. 2. The reverse relaxation time as a function of the barrier width for $k = 0$ and various values of the well widths in the symmetrical structure $L_1 = L_2$, $x = y = 0.03$, $H = 0$ for the ground state (thick lines) and excited (thin lines) exciton states. To illustrate, depicted at the bottom of the figure are schematic pictures of the one-particle wavefunction (solid curve) for the ground state of carriers in the structure with an absent barrier layer $L_b = 0$ (left), a thin barrier layer (centre) and thick (right) barrier layer. Dark grey with hatch line marks the regions of penetration of the wavefunction into the barrier layers (grey), where impurities are absent, which decreases the probability of the exciton scattering.

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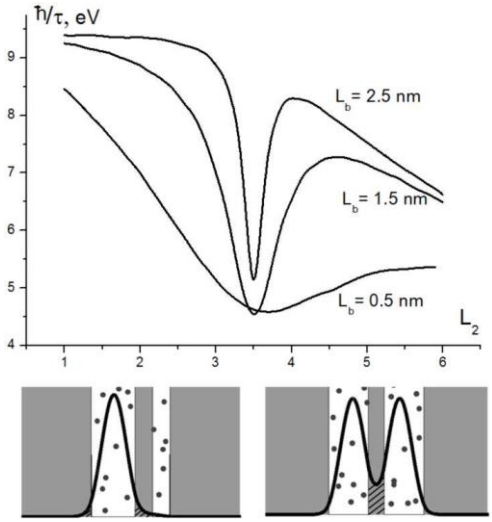

Fig. 3. The reverse relaxation time as a function of the right well width L_2 for $k = 0$ for the first well width $L_1 = 3.5$ nm, $x = y = 0.03$, and various values of the barrier widths. To illustrate, depicted at the bottom of the figure are schematic pictures of the one-particle wavefunction (solid curve) for the ground state of carriers in the structure with different (left) and equal (right) well widths. Dark grey line marks the regions of penetration of the wavefunction into the barrier layers. This penetration is much more essential in the case of equal wells (right).

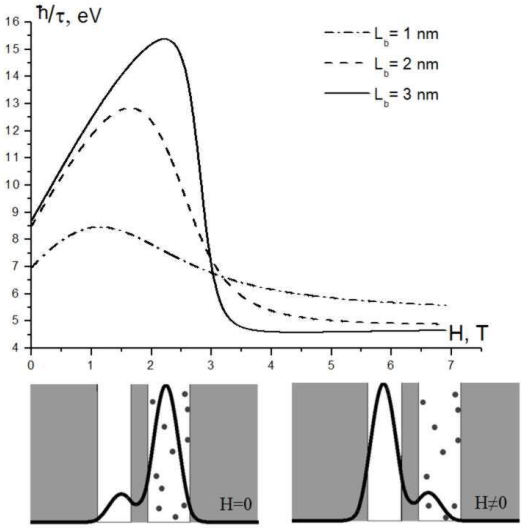

Fig. 4. The reverse relaxation time as a function of external magnetic field for $k = 0$ for the system with one magnetic well for a few values of the barrier widths. The left well is non-magnetic with the well width $L_1 = 2$ nm, and the right well is magnetic with the width $L_2 = 4$ nm and magnetic ion concentration $x = 0.03$, temperature $T = 4.2$ K. To illustrate, depicted at the bottom of the figure are schematic pictures of the one-particle wavefunction for the ground state of carriers in the structure without magnetic field (left) and under external magnetic field (right) for the σ^--transition. In the absence of magnetic field, the lowest state of carriers corresponds to localization of carriers in the wider well, where magnetic impurities are placed and, therefore, to the high probability of the scattering. Under high magnetic field, the band gap in the magnetic layer rises, which leads to transition of carriers to the non-magnetic layer and, respectively, to drop of the scattering.

Both the considered above effects should take place in similar structures formed by any semiconductor alloys, both magnetic and non-magnetic. At the same time, in diluted magnetic semiconductors, parameters of the structure can be tuned by external magnetic field. It is known [5, 6] that in diluted magnetic semiconductors, the bandwidth increases with increase of the magnetic field for the σ^--component of the exciton transition, while it decreases for the σ^+-component. Suppose, in contrast to the previous cases, only one of the quantum well layers contains magnetic ions. External magnetic field influences the depths of the quantum wells for electron and hole formed by the diluted magnetic layer. It can change drastically the wavefunction of the system, i.e. there is the probability for the carrier to be found in the certain layer of the structure. Suppose also that the magnetic layer is rather wide, and in the absence of external magnetic field the ground state of the system corresponds to the carriers localized in the magnetic layer (Fig. 4). Under magnetic field for the σ^--component of the exciton transition, the quantum well depths for both carriers decrease as the intensity of the field rises [9]. Simultaneously, the probability of exciton to be scattered by the fluctuations rises because of strengthening the magnetic part of interaction with ions. As it can be seen from Fig. 4, in our system the probabilty of the scattering also rises as the magnetic field rises in low fields. It takes place until the carriers are localized in the magnetic layer. When achieving a certain some value of the magnetic field, the potential wells become too shallow, and it becomes energetically advantageous for carriers to transit to the non-magnetic well, which results in sharp drop of the probability of the scattering.

3. Conclusions

In the paper, the exciton scattering in double quantum wells, some layers of which are formed by ternary semiconductor alloys, has been considered. In these disordered layers, the scattering is caused primarily by the interaction of carriers with fluctuations in the impurity concentration and (in the case of diluted magnetic semiconductors) fluctuations of magnetic ion spin projections. It has been shown that the probability of the scattering depends essentially on those of the system's parameters that determine the degree of the exciton wavefunction localization in the disordered layers. Particularly, the probability of the scattering in the system with quantum wells of equal widths essentially drops: in this case, penetration of the wavefunction in the ordered barrier layers of the structure is maximal, which decreases the effect of the fluctuations in the disordered layers and, as a result, decreases the excitonic optical bandwidth. The same effect can be reached by tuning one of the particle levels in the quantum wells by external magnetic field, which also leads to delocalization of the wavefunction and narrowing the optical bands.

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