INTERFACE EFFECTS IN THE MODEL OF δ-POTENTIAL FOR DILUTED MAGNETIC SEMICONDUCTOR QUANTUM STRUCTURES

F. V. KYRYCHENKO, Yu. G. SEMENOV[1]

Institute of Physics, Polish Academy of Sciences
(*Al. Lotnikow 32/46, 02668, Warsaw, Poland*),
[1]Institute of Semiconductor Physics, Nat. Acad. Sci. of Ukraine
(*45, Nauky Prosp., Kyiv 03028, Ukraine*)

UDC 539

‰ 2001

We further develop the recently proposed model of interface δ-potential in nonmagnetic/semimagnetic semiconductor heterostructures. We calculate the parameters of the δ-potential (applied to the description of the interface paramagnetic enhancement effect) using a smooth approximation of the interface potential. We propose useful analytic approximations of the magnetic field, temperature, and magnetic ion concentration dependences of the δ-potential intensity for the $CdTe/Cd_{1-x}Mn_xTe$-interface. Our calculations have proved the recent hypothesis about a Brillouin-like magnetic field dependence of the intensity of the δ-potential. It is shown that the approach allows one to satisfactorily describe the interface effects in diluted magnetic semiconductor quantum structures in terms of only one free parameter, the interface width ΔL_{if}. The obtained formulas are used to describe some experimental results from the present literature. It is shown that our theory provides good agreement with experimental data.

Introduction

It is known that realistic interface profiles in semiconductor heterostructures are not perfectly sharp. This is either due to non-ideality of technology or due to diffusion processes at the interface region. On the other hand, the interface effects play an important role in the formation of electronic states in semiconductor quantum wells (QW). For example, the asymmetry of interface potentials in QW results in the possibility of observation of forbidden optical transitions due to the breaking of a potential symmetry (see [1, 2]).

In the case of diluted magnetic semiconductor (DMS) quantum structures, the interface can be responsible for some other effects. One of them is the effect of paramagnetic enhancement of giant spin splitting (GSS) of excitonic spectra in QW with semimagnetic barriers (see [3] and references therein). This is due to the fact that non-ideality of interface leads to increasing in local magnetization in the interface region, which, in turn, gives rise to an enhancement of the effective exchange field $\mathbf{G}_{e(h)}$ acting on the spin of the electron (hole) comprising an exciton. The contribution of this additional magnetization to the spin-splitting of excitonic states is comparable with the total excitonic GSS.

So, generally speaking, if we deal with DMS quantum structures, we need to take into account the interface effects. To do this, one have to solve a $1D$ Schrödinger equation. Since the interface potential is not of a simple form, only a numerical solution is possible. In the case of hole states in DMS QW for the arbitrary magnetic field **B** orientation, we need to solve the system of four Luttinger equations. Once more, only a numerical solution is possible. The latter problem is, of course, very computer-intensive. The simple model of δ-potential has been proposed in [4, 5] to describe the contribution of a non-ideal interface to the Hamiltonian of the system. This model is based on the assumption that the characteristic length of the interface potential ΔL_{if} is much smaller than the QW width L_w. It allows one to approximate the interface contribution to the electron (hole) energy by the δ-potential and to calculate the characteristics of electron and hole states in QWs with DMS barriers analytically both for $\mathbf{B} \| \mathbf{C}$ and $\mathbf{B} \perp \mathbf{C}$, where **C** is the QW growth direction. Some parameters of the δ-potential introduced in [4, 5] were considered as fitting ones.

In the present paper, the parameters of the δ-potential are calculated in terms of a smooth approximation of interface potential. A useful analytic approximation of the magnetic field dependence of the intensity of the δ-potential is proposed in the case of $CdTe/Cd_{1-x}Mn_xTe$-interface. The obtained formulas are shown to provide a quantitative description of experimental results.

Calculation of Interface Potential

The possibility to introduce the interface δ-potential is based on the following speculation. Consider $\Psi(z)$ as an exact wave function of the appropriate Schrödinger equation for an electron in QW of width L_w. Then, the contribution of the interface potential $U_{\text{if}}(z)$ to the electron energy is expressed by

$$E_{\text{if}} = \int_{-\infty}^{\infty} |\Psi(z)|^2 U_{\text{if}}(z) dz. \qquad (1)$$

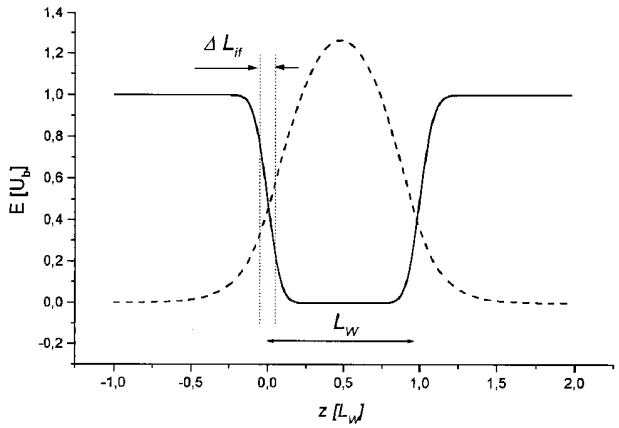

Fig.1. Potential energy and wave function of the electron ground state in a non-ideal rectangular quantum well with error function profile of interfaces. Model of interface δ-potential is based on the assumption that $\Delta L_{\rm if} << L_w$

If the typical electron (hole) localization length in a QW growth direction (z-direction) L_w is longer than $\Delta L_{\rm if}$ (see Fig.1), $\Psi(z)$ can be expanded in the vicinity of the interface at the point $z = L_w/2$. The first non-vanishing term of this expansion in Eq.(1) reads

$$E_{\rm if}^{(0)} = A_{\rm if} |\Psi(L_w/2)|^2, \quad A_{\rm if} = \int_{-\infty}^{\infty} U_{\rm if}(z)dz. \tag{2}$$

It is seen that $E_{\rm if}^{(0)}$ exactly corresponds to the contribution of the interface Hamiltonian

$$\hat{H}_{\rm if} = A_{\rm if}\,\delta(z - L_w/2) \tag{3}$$

which is proportional to the δ-function. The factor $A_{\rm if}$ is a function of magnetic field **B** and depends on a specific distribution of magnetic ions at the interface region. The magnetic field dependence of $A_{\rm if}$ was assumed in [4, 5] to be in the form of a modified Brillouin function with two free parameters $T_{\rm if}$ and $S_{\rm if}$. Below we do not use this assumption. Rather, we calculate the amplitude $A_{\rm if}$ for different values of temperature T and magnetic field **B** in terms of the model (developed in [3]) taking the interface spread into account. The main task of this work is to determine the magnetic field dependence of the factor $A_{\rm if}$ and to check the validity of the assumption of the Brillouin-like dependence of $A_{\rm if}$ used in [4, 5].

First, we need to determine a specific spatial distribution of magnetic ions in the vicinity of the interface. For definiteness, we consider the $CdTe/Cd_{1-x}Mn_xTe$-interface. In the present literature, there is no consent about the profile of the Mn ions distribution at the interface region. The exponential profile (described by segregation) and the error function profile (determined by diffusion processes) were discussed most commonly (see [3]). We choose the error function profile to describe the local concentration of Mn ions:

$$x(z) = \frac{x_0}{2}\left[\mathrm{erf}\left(\frac{z}{2\Delta L_{\rm if}}\right) + 1\right] \equiv$$

$$\equiv \frac{x_0}{2}\left[\frac{2}{\sqrt{\pi}}\int_0^{z/(2\Delta L_{\rm if})} \exp(-t^2)dt + 1\right]. \tag{4}$$

Here, x_0 denotes the molar concentration of Mn ions in the barrier far from interface region.

In the mean field approximation, the Hamiltonian of an electron (hole) in the DMS quantum structure has the form

$$\hat{H}_{e(h)} = \hat{T}_{e(h)} + V_{e(h)} + \mathbf{G}_{e(h)}\mathbf{S}_{e(h)}, \tag{5}$$

where the first and second terms describe (respectively) the electron (hole) kinetic and potential energies, while the last term represents the Zeeman energy of a carrier in the exchange field $\mathbf{G}_{e(h)} = J_{e(h)}x(z)\langle\mathbf{S}_{\rm Mn}\rangle$. Here, $J_{e(h)}$ and $\mathbf{S}_{\rm Mn}$ are the exchange constant and spin of Mn^{2+} ions, respectively. In the case of $\mathbf{B}||\mathbf{C}$, the term with exchange interaction is actually an additional potential for an electron (hole) with spin projection σ:

$$U_{e(h)}(\sigma, z) = V_{e(h)}(z) + \sigma G_{e(h)}(z). \tag{6}$$

We obtain (for each value of magnetic field) the interface potential $U_{\rm if}(z)$ needed to calculate $A_{\rm if}$ according to Eq.(2), by subtracting the ideal interface potential $U_{\rm ideal}(z)$ (step function) from the real interface potential profile $U_{\rm real}(z)$ (see, Fig.2). The real potential profile was calculated in the spirit of [3] by taking (at each point $z = z_0$) the values of the potential $U_{\rm real}(z_0)$ for a bulk $Cd_{1-x}Mn_xTe$ crystal with $x = x(z_0)$. The position of the step function $U_{\rm ideal}(z) \sim \Theta(z - z_{\rm if})$ was determined from the condition $A_{\rm if}(B = 0) = 0$. In the case of the Mn distribution described by Eq.(4), this procedure results in $z_{\rm if} = 0$.

The calculations are performed for the set of parameters $\Delta L_{\rm if}$, x_0 and temperature T. As an example, we plot the magnetic field dependence of the parameter $A_{\rm if}^e$ for the $CdTe/Cd_{0.85}Mn_{0.15}Te$-interface with $\Delta L_{\rm if} = 1$ Å for three different temperatures $T = 1$, 2.5, and 8 K (solid lines) in Fig.3.

In [4, 5], the magnetic field dependence of $A_{\rm if}$ was approximated by the modified Brillouin function $B_{5/2}$ with two free parameters $\Delta l = \Delta L_{\rm if}S_{\rm if}$ and $T_{\rm if}$.

$$A_{\rm if}^{e(h)} = J_{e(h)}S_{e(h)}\,x_0\Delta L_{\rm if}S_{\rm if}B_{5/2}\left(\frac{(5/2)\,g\,\mu_{\rm B}B}{k_{\rm B}(T + T_{\rm if})}\right). \tag{7}$$

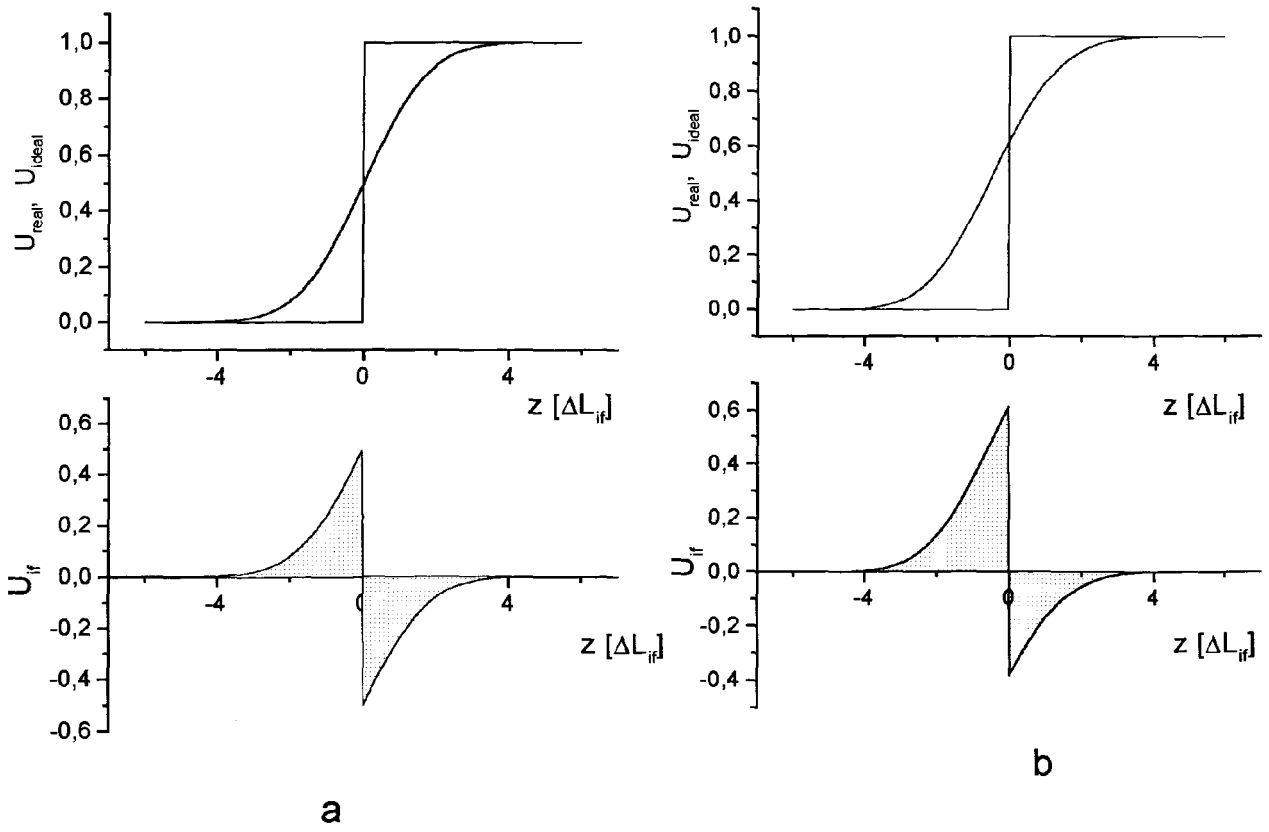

Fig.2. Typical shape of the interface potential $U_{if}(z)$ obtained by subtracting the ideal interface potential $U_{ideal}(z)$ (step function) from the real interface potential profile $U_{real}(z)$, *a* – without magnetic field (that corresponds to $A_{if} = 0$), *b* – in the magnetic field ($A_{if} \neq 0$)

Here, $J_e = 220$ meV and $J_h = -880$ meV are the carrier-magnetic ion exchange constants for $Cd_{1-x}Mn_xTe$ DMS, respectively, $S_{e(h)} = \pm \frac{1}{2}$ are electron (heavy hole) spin projections. The parameters S_{if} and T_{if} in Eq.(7) denote the effective spin and temperature of magnetic ions at the interface. We have to calculate S_{if} and T_{if} to reduce the number of free parameters in Eq.(7). It is easy to see that the Mn distribution in the vicinity of the interface in form (3) simply results in the relation $A_{if} \sim \Delta L_{if}$. The form of Eq.(7) also provides the explicit temperature and magnetic field dependence of the parameter A_{if}. This allows us to consider the effective parameters S_{if} and T_{if} as functions of Mn concentration in the barrier x_0 only. Our analyses show that these dependences can be represented by:

$$S_{if} = x_0[19.63 \exp(-27.81x_0) + 8.955 \exp(-4.474x_0) + 0.217], \quad (8)$$

$$T_{if} = \begin{cases} 0, & x_0 < 0.13, \\ 3.687 \tanh[3.112(x_0 - 0.13)], & x_0 \geq 0.13. \end{cases} \quad (9)$$

The dashed lines in Fig.3 represent the results of calculation of A_{if}^e using Eqs. (7) – (9). It is seen that the approximated curves differ slightly from those obtained according to Eq.(2) (solid lines). Note also that the remaining free parameter ΔL_{if} in Eq.(7) uniquely determines the interface profile via Eq.(3). This situation is opposite to the case of Refs. [4, 5] where ΔL_{if} represents the characteristic length of interface potential only.

However, the differences between the results of numerical integration and analytic expressions (Eqs. (7) – (9)) are noticeable in Fig.3. It can be shown that the difference of two modified Brillouin functions (one of them corresponds to bulk GSS) approximates the obtained magnetic field dependence of A_{if} more accurately:

$$A_{if}^{e(h)} = J_{e(h)} S_{e(h)} x_0 \Delta L_{if} \left[S_{eff} B_{5/2} \left(\frac{(5/2)\, g\, \mu_B B}{k_B (T + T_{eff})} \right) - \right.$$

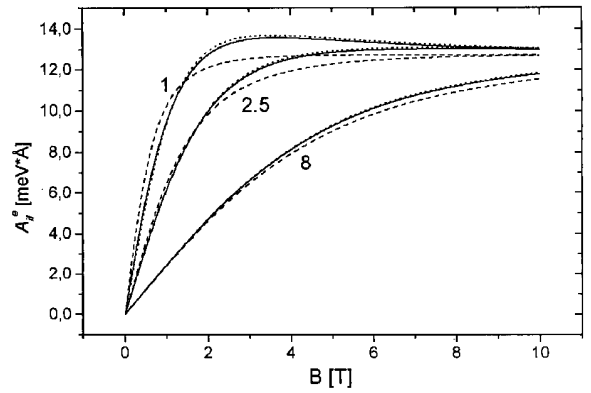

Fig.3. Magnetic field dependence of the parameter $A_{\rm if}^e(S_e = +1/2)$ for $CdTe/Cd_{0.85}Mn_{0.15}Te$-interface with $\Delta L_{\rm if} = 1$ Å for three different temperatures $T = 1, 2.5$, and 8 K. Solid lines are calculated using Eq.(2), dashed ones correspond to the analytic approximation by Eqs. (7) – (9). Dotted lines present the analytic approximation using Eqs.(10) – (12)

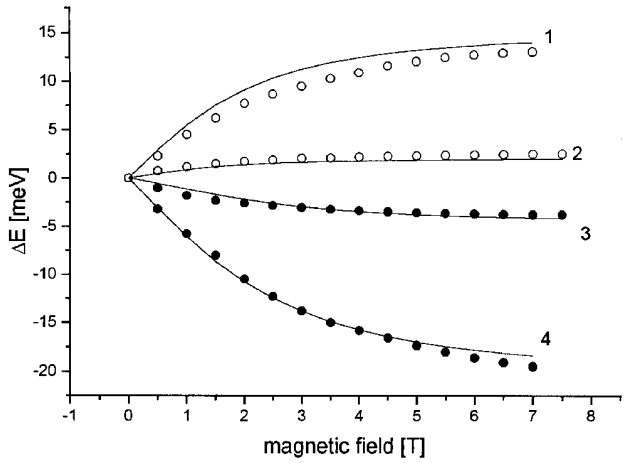

Fig.4. GSS of heavy hole exciton energies in the Faraday configuration for 30 Å-wide $Cd_{0.82}Mn_{0.18}Te/CdTe$ (curves *1*, *4*) and 88 Å-wide $Cd_{0.78}Mn_{0.22}Te/CdTe$ (curves *2*, *3*) quantum wells (from [6]). Open symbols correspond to σ^+ polarization and solid symbols to σ^- one. Lines are the calculations in the model of interface δ-potential using Eqs. (10) – (12) with $\Delta L_{\rm if} = 7.2$ Å for wide QW and $\Delta L_{\rm if} = 3.4$ Å for narrow QW

$$- S_0 B_{5/2}\left(\frac{(5/2) g \mu_B B}{k_B (T + T_0)}\right)\Bigg]. \qquad (10)$$

Here, the parameters $S_0 = S_0(x_0)$ and $T_0 = T_0(x_0)$ describe the magnetization of a bulk $Cd_{1-x}Mn_xTe$ crystal with molar fraction on Mn ions $x = x_0$. In our calculations, we use the expressions for $S_0(x_0)$ and $T_0 = T_0(x_0)$ from [3]. The effective parameters $S_{\rm eff}$ and $T_{\rm eff}$ in Eq.(10) depend only on x_0 (similar to $S_{\rm if}$ and $T_{\rm if}$ in Eq. (7)) and can be represented in the form:

$$S_{\rm eff} = \frac{0.466}{x_0}[1 - \exp(-5.29213\, x_0)] - 0.19227, \qquad (11)$$

and

$$T_{\rm eff} = 3.5 \tanh(3.2353\, x_0). \qquad (12)$$

The result of calculation of $A_{\rm if}^e$ using Eqs. (10) – (12) is reported in Fig.3 by dotted lines.

Comparison with Experiment

As was mentioned above, the model of interface δ-potential allows one to analytically describe the interface contribution to electron and hole Zeeman splitting in the DMS QWs both for $\mathbf{B} \| \mathbf{C}$ and $\mathbf{B} \perp \mathbf{C}$. The corresponding theory is developed in [4, 5]. Now we apply the above approach to description of some experimental results available in the literature.

The GSS of excitonic reflectivity spectra in the Faraday configuration ($\mathbf{B} \| \mathbf{C}$) in $Cd_{1-x}Mn_xTe/CdTe/Cd_{1-x}Mn_xTe$ quantum structures with $L_w = 88$ Å (QW width), $x_0 = 0.22$ and $L_w = 30$ Å, $x_0 = 0.18$ are reported in [6]. In Fig.4, we compare the experimental data (symbols) with the results of our calculations (lines) using Eqs. (10) – (12). Only one fitting parameter $\Delta L_{\rm if} = 7.2$ Å for the first structure and $\Delta L_{\rm if} = 3.4$ Å for the second allows us to obtain a fairly good agreement with the experiment.

In Fig.5, we compare the results of our calculations of exciton spin splitting in 75 Å wide $Cd_{0.95}Mn_{0.05}Te/CdTe/Cd_{0.95}Mn_{0.05}Te$ QW in the Voight configuration with experimental data on reflectivity spectra from [7]. Positions of excitonic lines as a function of the magnetic field $\mathbf{B} \perp \mathbf{C}$ are plotted by symbols. Lines represent the results of our calculations using the model of interface δ-potential with the parameter $\Delta L_{\rm if} = 2.5$ Å. One can see that our approach describes both heavy and light hole Zeeman splittings quite well.

Conclusions

A further development of the model of interface δ-potential has been performed for DMS quantum structures. The magnetic field dependence of the intensity $A_{\rm if}$ of δ-potential for various temperatures, barrier heights, and interface widths has been calculated for $CdTe/Cd_{1-x}Mn_xTe$-interface. It have been verified that this dependence can be approximated with reasonable accuracy by a modified Brillouin function with two fitting parameters $S_{\rm if}$ and $T_{\rm if}$ in con-

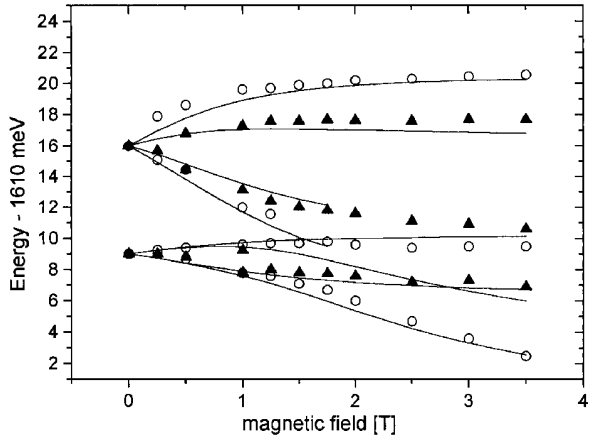

Fig.5. Exciton energies in σ (circles) and π (triangles) polarizations in the magnetic field $\mathbf{B} \perp \mathbf{C}$. The $Cd_{0.95}Mn_{0.05}Te/CdTe/Cd_{0.95}Mn_{0.05}Te$ QW has a width of 75 Å [7]. Lines are the results of calculations using Eqs. (10)–(12) with $\Delta L_{if} = 2.5$ Å

formity with assumptions of [4, 5]. The useful analytic approximations for the magnetic field dependence of the interface intensity A_{if} have been proposed. We have also shown that the effect of paramagnetic enhancement in DMS quantum structures can be satisfactorily described in a simple way with only one free parameter – interface width ΔL_{if}. It is evident that the approach developed in the present work can be applied to other DMS quantum structures and physical phenomena in DMS QWs: tunneling effects [8], superlattices [9], magnetic polaron effects [10], etc. Sometimes, the criteria of validity of the developed approach are broken down or are not evident. Nevertheless, we believe that the considered model can also be applied in these situations if one treats it as a simple phenomenological description of the paramagnetic enhancement effect in the DMS quantum structures.

This work was partially supported by the INTAS 1999-15 and Ukrainian FRF #2.4/638 grants.

1. *Ryabchenko S.M., Abramishvili V.G., Komarov A.V. et al.* //Acta phys. pol. A **94**, 165 (1998).
2. *Kyrychenko F.V., Ryabchenko S.M., Semenov Yu.G. et al.* (in print, Physica E).
3. *Gaj J.A., Grieshaber W., Boden-Deshayes C. et al.* //Phys. Rev. B**50**, 5512 (1994).
4. *Semenov Yu.G.* //Acta phys. pol. A **94**, 526 (1998).
5. *Siviniant J., Kyrychenko F.V., Semenov Yu.G. et al.* //Phys. Rev. B, **59**, 10276 (1999).
6. *Kuhn-Heinrich B., Popp M., Ossau W. et al.* //Semicond. Sci. and Technol. **8**, 1239 (1993).
7. *Peyla P., Wasiela A., d'Aubigne Y. M. et al.* //Phys. Rev. B **47**, 3783 (1993).
8. *Lee S., Dobrowolska M., Furdyna J.K. et al.* //Ibid. **54**, 16939 (1996); *Lawrence I., Haacke S., Marriette H. et al.* //Phys. Rev. Lett. **73**, 2131 (1994).
9. *N. Dai, H. Luo, F.C. Zhang et al.* //Ibid, **67**, 3824 (1991).
10. *Yakovlev D.R., Kavokin K.V.* //Comments on Cond. Matter Phys. **18**, 51, (1996); *Yakovlev D.R., Mackh G., Kuhn-Heinrich B. et a*l. //Phys. Rev. B **52**, 12033, (1995).

Reccived 10.05.2000