Model of circular polarization dependence on Mn delta-layer position in LED heterostructures with InGaAs/GaAs quantum well

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Abstract

A simple model of circular polarization dependence on Mn delta-layer position in LED heterostructures with InGaAs/GaAs quantum well is proposed, being able to explain quite accurately recent fascinating experimental results [S.V. Zaitsev, et al., Physica E (2009), doi:10.1016/j.physe.2008.11.003]. The model emphasizes the role of position-dependent exchange interaction between injected holes and Mn spins which significantly affects the hole level splitting in a magnetic field, leading to strong variations of polarization dependence. The role of effective temperature corresponding to the injected hole energy and the broadening caused by the geometrical structure imperfections is also discussed.

Key words: polarization, Mn delta-layer, level population, wavefunction overlap, exchange coupling, effective temperature

PACS: 61.72-U, 78.60.Fi, 75.30.Hx

1. Introduction

In recent experiments [1, 2] an intriguing strong enhancement of polarization degree in LED heterostructures with InGaAs/GaAs quantum well and Mn delta-layer with varying position has been reported. Since the early 1980s the properties of circular polarized emission from semiconductor structures
doped with magnetic atoms attract a considerable attention, and nowadays it became even more important in the scope of nanostructure design and possible applications in nanophotonics, tunable spin transport and quantum information processing. Firstly, the dependence of circular polarization on the magnetic field has been studied both experimentally and theoretically in bulk GaAs samples doped by Mn acceptors [3, 4]. In these pioneering papers a simple and effective model of polarization dependence has been derived which later was successfully applied for the explanation of several recent experiments with bulk samples [5, 6]. Later, as the focus of research has moved to the low-dimensional nanostructures, the triangular quantum wells delta-doped with Mn inside the well have been fabricated and studied [7, 8, 9] as well as the structures with delta Mn layer neighboring to the rectangular quantum well where interesting and promising magnetic properties of Mn layer have been discovered [10]. Another important type of interaction that can affect the polarization and relaxation of spins in quantum wells is the spin-orbit interaction [11] which is not included in the present model due to the stronger influence of the Mn d-electrons compared to the a relatively weak spin-orbit effects in rectangular InGaAs quantum wells. In the present paper we derive a simple quantitative model describing the magnetic field dependencies of circular polarization in InGaAs/GaAs quantum wells on the position of Mn delta-layer reported recently. We focus on the role of wavefunction overlap and exchange interaction between holes and Mn atoms which modify the hole energy spectrum and produce a measurable effect of the polarization dependence. The model presented here is intended to clarify only the primary features of the dependencies of polarization curves on the Mn delta-layer position. Hence, the manuscript is focused on the polarization dependencies only and it does not touch the fundamental and applied problems of magnetic and material properties of Mn layer which are of great importance for condensed matter physics and its applications [7, 8, 10]. Our paper is organized as follows: in Section 2 we briefly describe the experimental results obtained in [1, 2] which were the starting point of our studies, in Section 3 we derive the model of polarization dependence, in Section 4 we discuss the results, and the conclusions are given in Section 5.

2. Experimental results obtained by other authors [1, 2]

Here we shall briefly describe the setup and results of the experiments which we are going to describe theoretically in the manuscript; for more
Figure 1: Schematic band diagram, wavefunction overlap and the circular polarized transitions in the experiments on Mn delta-doped InGaAs/GaAs QW [1, 2]. The holes were injected into the area of 10-nm-thick InGaAs/GaAs quantum well, and then the photo- and electroluminescence have been measured in the Faraday geometry with the magnetic field perpendicular to the QW plane (pointed by the horizontal arrow $B$). The downward arrows indicate the transitions from the electron to hole levels accompanied by the right- and left-polarized emission of photons.

Details, see the original papers [1, 2]. The schematic view of the band structure which emission properties have been studied in the experiments is presented in Fig. 1. The holes have been injected into the area of 10-nm-thick InGaAs/GaAs quantum well, and then the photo- and electroluminescence have been measured in the Faraday geometry with the magnetic field perpendicular to the QW plane (pointed by the horizontal arrow $B$). The downward arrows indicate the transitions from the electron to hole levels accompanied by the right- and left-polarized emission of photons. The Mn delta-layer position located on the distance $L$ from the interface is shown schematically in the left part of GaAs layer, and the overlap of Mn and hole wavefunctions is indicated in the artificially magnified scope just for the qualitative explanation of the geometrical layout.

The experimental results together with the theoretical calculations presented below are shown in Fig. 2. The experimental polarization dependencies (vertically dashed lines) are plotted by using the results of the original paper [1], and the results of our model are shown as solid lines. Various curves correspond to different values of distance $L$ from the Mn layer to the inter-
Figure 2: (Color online) Comparison of experimental [1, 2] observations (vertically dashed lines) and the presently derived model (solid lines). Various curves correspond to different values of distance $L$ from the Mn layer to the interface, and two close lowest curves correspond to the reference (undoped) and Be-doped (nonmagnetic) structure.

face, and two close lowest curves correspond to the reference (undoped) and Be-doped (nonmagnetic) structure. One can see that the model provides a good approximation to the experimental results except the low-field regime for $L = 2$ nm. These properties and their convergence to the measured results will be described in details below.

3. Model for calculations

We start the description of the polarization dependence on the applied magnetic field with the Hamiltonian of holes in QW which includes the orbital part $H_0$, the Zeeman part $H_Z = m_J g_h \mu_B B$, and the exchange part $H_{ex} = -A (J \cdot S)$ which arises due to the presence of Mn delta-layer in the close proximity to the QW:

$$H = H_0 + m_J g_h \mu_B B - A (J \cdot S)$$ (1)

where $\mu_B$ is the Bohr magneton, $m_J$ and $g_h$ are the hole angular quantum number and g-factor, respectively, $B$ is the magnetic field amplitude, and the exchange operator is described by the coupling parameter $A$ and the scalar
product of the hole spin operator $\mathbf{J}$ and the Mn d-electrons spin operator $\mathbf{S}$ [4]. The exchange coupling parameter $A = A(L)$ in our model is an ensemble-average quantity and its dependence on the delta-layer distance $L$ from the QW edge will be discussed in details below.

First, we describe briefly the origin of the strong dependence of polarization on the Mn delta-layer position. The Zeeman term corresponds to the energy $E_Z(B) = \pm \frac{3}{2} g_h \mu_B B$ for two lowest hole levels with $m_J = \pm 3/2$ where $g_h \approx 3$ for holes in the strained InGaAs/GaAs structure [12]. Even in strong magnetic fields up to $B = 10$ T the Zeeman term provides only about 2 meV in energy splitting. Below we shall see that in addition to the Zeeman term the exchange coupling (the last term in Eq.(1)) produces a considerable effect in the hole level splitting and, hence, in the polarization dependence. Indeed, it is known that the coupling constant $A$ in GaAs is of the order of 4 meV for the case of Mn atoms located in the same region with holes in bulk sample [4]. If the angular quantum number $m_J = \pm 3/2$ for holes and $m_d = \pm 5/2$ for the Mn d-electrons, than the contribution from the exchange term in (1) can reach as high as 15 meV which is almost an order of magnitude greater than the Zeeman energy alone. We believe that such considerable effect of exchange coupling can be an origin of strong enhancement of polarization degree and its sensitive dependence on the Mn delta-layer position. The precise value of the hole g-factor can not make a big difference here since it only enters the Zeeman term which, as we see, can be weaker than the exchange term. Our model shows that the value $g_h = 3$ is in the agreement with the experimental data from the reference (undoped) sample (lowest curve labeled as "Undoped" in Fig.2).

We now turn to the detailed description of the theoretical model. The energy shift caused by the exchange interaction can be described by the average spin $\bar{S}_d(B, T)$ of the Mn d-electrons which interact with hole spins $m_J = \pm 3/2$:

$$E_{ex}(B, T, L) = \pm \frac{3}{2} \bar{S}_d(B, T) A(L).$$

The arguments in Eq.(2) mean that the average spin of d-electrons in Mn depends both on the magnetic field and on the temperature $T$ which takes into account both thermal and structural level broadening. We do not touch here the problem of possible ferro- or antiferromagnetic properties of Mn delta-layers in semiconductor heterostructures [10] since we are interested in the averaged macroscopic properties of the delta-layer rather than in its
micro- or mesoscopic magnetic structure. Since the Mn concentration was 0.4 of the monolayer [1], its statistical energy distribution function can be taken of the Boltzman form. Hence, we model the ensemble averaged spin of Mn atoms subjected to magnetic field as [13]

$$\bar{S}_d(B, T) = \frac{1}{Z} \sum_{m_d} \exp \left(-\frac{m_d g_e \mu_B B}{T}\right)$$

(3)

where $Z$ is the statistical sum and the Mn d-electrons g-factor $g_e = 2$ [3, 4]. In Eq. (3) the Mn d-electron spin projections $m_d = -5/2, -3/2, \ldots, 3/2, 5/2$.

The next step is the calculation of the dependence of exchange coupling parameter $A(L)$ on the distance $L$ between the Mn delta-layer and the heterostructure interface. Let us start with a simple result for the exchange coupling constant for two spherical atoms with energies $E_{1,2}$ which depends on the inter-atomic spacing shift $L - L_0$ as [14]

$$A(L) \propto A(L_0) e^{- (\kappa_1 + \kappa_2) |L - L_0|}$$

(4)

where $\kappa_{1,2} = \sqrt{2m |E_{1,2}|/\hbar}$. We believe that this simple result can be applied also in our case as a starting point since both the holes and the Mn atoms are characterized by the well-defined spatial locations in the narrow QW and in the delta-layer, respectively. According to the experimental data [1], the maximum value of the coupling constant $A(L_0) = 4$ meV [1] when the delta-layer is located at $L = L_0 = 3$ nm (see Fig.2). By comparing the acceptor Bohr radius in GaAs which is of the order of 2 nm together with the fluctuations in the individual delta-layer atomic positions with respect to the InGaAs/GaAs interface, the estimated barrier penetration length of the hole wavefunction may reach up to 1.5 – 2.0 nm. Thus, one can conclude that in all cases for $L = 2, 3, 5, 10$ nm presented in Fig.2 the Mn atoms will affect the hole energy levels in the QW via the exchange interaction with typical length in (4) equal to $1/(\kappa_1 + \kappa_2) \approx 4$ nm.

Now the exchange energy (2) is determined and we can calculate the polarization degree $P(B, L)$ by applying the standard definition of $P = (I_+ - I_-)/(I_+ + I_-)$ where $I_\pm$ is the right- and left-polarized radiation intensity, respectively and by using the relations for $P$ arising from the comparison of the level population [3, 4], which leads to the following result of the well-known form:

$$P(B, L) = \tanh [x(B, L)]$$

(5)
where the argument

\[ x(B, L) = \frac{E_Z(B) + E_{ex}(B, T, L)}{T_{eff}} \]  \( \text{(6)} \)

depends not only on the reservoir temperature or the fluctuation field amplitude (whichever is greater) \( T \sim 7 \text{ K} \) \( [3, 4] \) but also on the effective temperature \( T_{eff} \) which may be different from \( T \). The meaning of the effective temperature here reflects the fact that the incoming injected holes participating in the recombination process are non-equilibrium hot holes, so they can not be described by the reservoir temperature \( T \). Of course, the detailed properties of such hot holes including their energy distribution deserve a separate investigation but for our purposes the primary relevant quantity is their average energy (or temperature). The value of \( T_{eff} \) can be estimated from the voltage drop since the holes gain the kinetic energy from this source and the resulting value can be tested by applying Eq.(5) to the reference undoped sample. Following this approach, we find that \( T_{eff} \approx 20 \text{ meV} \) which is in agreement with the real experimental setup where the total voltage drop of 1...2 V has been applied to the structure of 0.5 microns of total thickness.

4. Results and discussion

The calculated polarization dependence \( (5) \) corresponding to various positions of the Mn delta-layer is presented in Fig.2 together with the experimental results previously obtained by other authors \( [1, 2] \). Various curves correspond to different values of distance \( L \) from the Mn layer to the interface, and two close lowest curves correspond to the reference (undoped) and Be-doped (nonmagnetic) structure. One can see that the model derived here provides a satisfactory approximation of the experimental observations everywhere except the low-field regime for the closest position of the Mn layer at \( L = 2 \text{ nm} \) and the high-field area at \( L = 10 \text{ nm} \) which is discussed below. Indeed, the effects from the exchange interaction can lead to a substantial increase of the polarization degree which rises when the Mn delta-layer is located closer to the QW and its interaction with holes is increased. This dependence on \( L \) holds until the region of very close proximity \( L = 2 \text{ nm} \) is reached where the amplitude of the polarization degree drops and the theoretical calculations diverge from the experimental data in the region of low magnetic field. We believe that such discrepancy is coming from the increasing microscopic geometrical disorder in the position of Mn atoms as
long as the delta-layer is moved very close to the interface. This assumption is supported by the meaning of the temperature $T$ in Eq. (6) which takes into account not only the reservoir temperature but also the level broadening caused by the defects, impurities and the fluctuating field which role has been recognized in the earliest studies of this problem [3, 4]. Our calculations have shown that even at the reservoir temperature $T_0 = 2$ K the actual value of $T$ to reproduce the experimental data is close to 7 K which is in the agreement with level broadening of 0.6 meV even in high purity samples. It is known that a fluctuation of the QW width of just one or two atomic monolayers can lead to the broadening of the optically detected emission lines of the order of 15 meV [15]. In the experiments with Mn doped GaAs structures the amplitudes of the fluctuating field were of the order of 1 meV corresponding to $T \approx 11$ K. Hence, when the geometrical disorder is increased at $L = 2$ nm, some higher values of $T$ are expected, and we found that the actual level broadening here is satisfactory described by 4.5 meV corresponding to $T = 50$ K. We stress that this deviation from the previously obtained uniform set of parameters ($T = 7$ K, $T_{eff} = 20$ meV) is the only one which we allowed through the calculations and we believe that it can be adequately explained by the increase of the geometrical disorder caused by the very close proximity of the doping layer to the QW interface. The slight deviation between theory and experiment at high fields and $L = 10$ nm (see Fig. 2) can be explained by the coupling position dependence between Mn atoms and the holes which can decrease a little faster at high distances for the isolated Mn delta-layer and two-dimensional holes confined in the QW than the simple approximation (4) predicts.

5. Conclusions

We have derived a quantitative model of circular polarization dependence on Mn delta-layer position in LED heterostructures with InGaAs/GaAs quantum well which is able to explain quite accurately the experimental results. We have studied the role of position-dependent exchange interaction between injected holes and spins of Mn d-electrons which significantly affects the hole level splitting in a magnetic field, leading to strong variations of polarization dependence as a function of the delta-layer position. The injected hole energy and the level broadening caused by the geometrical structure disorder are also included in the model providing a satisfactory level of convergence between experimental observations and theoretical calculations.
Acknowledgements

The author is grateful to Yu.A. Danilov, V.D. Kulakovskii, S.V. Zaitsev and M.V. Dorokhin for useful discussions. The work has been supported by the RNP Program of Ministry of Education and Science RF, by the CRDF, and by the RFBR.

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