Valence-band states in diluted magnetic-semiconductor quantum wires

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We present a theoretical study of the valence-band states in diluted magnetic semiconductor quantum wire structures. As a consequence of confinement in two directions, the hole states in a quantum wire are known to be mixtures of heavy- and light-hole components. Due to a strong *p-d* exchange interaction in diluted magnetic semiconductors, the relative contribution of these components is strongly affected by an external magnetic field **B**, a feature that is absent in nonmagnetic quantum wires. This leads, in turn, to a strong magnetic-field dependence of the probabilities of various optical dipole transitions in diluted magnetic semiconductor quantum wires. Numerical calculations performed for the case of $Cd_{1-x}Mn_xTe/Cd_{1-x-y}Mn_xMg_yTe$ T-shaped quantum wires demonstrate the possibility to efficiently control the polarization characteristics of light emitted from such structrures by means of an external magnetic field **B**.

INTRODUCTION

The properties of many physical quantities in low-dimensional semiconductor structures such as quantum wells (QW's), quantum wires (QWR's), and quantum dots, behave differently from their counterparts in bulk material. In many cases, the values of these quantities can be varied by controlling the degree of the electronic confinement. Use of diluted magnetic semiconductors (DMS's) in such quantum structures adds yet another possibility of independent control of several important parameters simply by applying an external magnetic field **B**. This possibility originates in a strong carrier-magnetic ion exchange interaction which leads, e.g., to the effect of giant spin splitting of energy bands in DMS's (see, e.g., Ref. 1). The applied magnetic field **B** induces a magnetization **M** of the magnetic ion subsystem, which gives rise to the exchange field $\mathbf{G}_{e(h)} \sim \mathbf{M}$ acting on the electron (hole) spin in proportion to the exchange integrals α (β). The resulting spin-dependent energy shifts of the band edges can easily be comparable in value to the band-offset energies U_e and U_h for electrons and holes in typical heterostructures. This fact gives rise to a series of interesting physical phenomena in DMS-containing quantum heterostructures (see Refs. 2–5).

Any meaningful, quantitative analysis of the interband optical phenomena in low-dimensional structures (and quantum wires in particular) requires a detailed account of the hole eigenenergies and eigenstates, which in zinc-blende semiconductors are quite complicated. In this paper we focus on this problem in the special case of diluted magnetic semiconductors. We show that the giant spin splitting introduces additional peculiarities to an already intricate problem of hole eigenstates.

The valence-band states in QWR's have been studied theoretically earlier (see Ref. 6). In the case of semiconductor QW's, the Luttinger Hamiltonian describing the holes in a zinc-blende environment is diagonal for holes, with a vanishing in-plane wave vector. This means that the projection of the total angular momentum on the growth direction, J_z, is a good quantum number, and that the hole states in a two-dimensional (2D) QW can be represented by either purely heavy-hole (HH) or light-hole (LH) states, with $J_z = \pm 3/2$ and $J_z = \pm 1/2$, respectively. The ground state of a hole in an unstrained QW is the HH state. The situation is very different in the case of quasi-1D QWR structures. First, due to the confinement in two directions, the Luttinger Hamiltonian is nondiagonal even for vanishing wave vectors along the wire direction, and the total angular momentum projection J_z thus ceases to be a good quantum number. The hole eigenstates in QWR's then become mixtures of heavy- and light-hole components. Moreover, as shown in Ref. 6, the ground-hole state in a QWR consists mostly of the light-hole contribution, in contrast to the case of quasi-2D QW structures. The relative contribution of the heavy and light holes to the total wave function depends in this case on the barrier height as well as the dimensions of the wire.

In this context, the use of diluted magnetic semiconductors to make QWR structures gives us a unique possibility of effectively controlling the relation between the heavy- and the light-hole contributions to the valence-band states simply by changing the magnetic field **B**. This in turn allows us to influence the polarization of light emitted (or absorbed) in various interband optical transitions. The paper is organized as follows. We introduce the notation and the basic theoretical ingredients of our calculation in the next section. Then we apply our calculations for the specific case of T-shaped DMS QWR's. We note parenthetically that such wires have already been fabricated.[7]

FORMULATION OF THE PROBLEM

The main difference between calculations for DMS-based and nonmagnetic structures arises from the presence of the carrier-magnetic ion (sp-d) exchange interaction. The corresponding Hamiltonian for the electron and the hole envelope functions in crystals with the zinc-blende structure can be written in the form of a contact interaction[1,8]

$$\hat{H}_{s-d} = \alpha \sum_j \delta(\mathbf{r} - \mathbf{R}_j)\mathbf{S}_j\mathbf{S}_e\,,$$

$$\hat{H}_{p-d} = \frac{1}{3}\beta \sum_j \delta(\mathbf{r} - \mathbf{R}_j)\mathbf{S}_j\mathbf{J}_h\,, \qquad (1)$$

where $\mathbf{S}_e$ is the electron spin operator ($S_e = 1/2$) and $\mathbf{J}_h$ is the hole total angular momentum ($J_h = 3/2$) operator, α and β

are the exchange integrals, and the sum is over all cation lattice sites occupied by the magnetic ions having spins S_j.

An external magnetic field induces a magnetization in the sample with the total moment $\langle \Sigma_j \mathbf{S}_j \rangle$. The exchange interaction given by Eq. (1) in the mean-field approximation can be written in terms of Zeeman-like Hamiltonians $\hat{H}_e^{\rm ex}$ and $\hat{H}_h^{\rm ex}$:[1]

$$\hat{H}_e^{\rm ex} = \mathbf{G}_e \mathbf{S}_e ; \quad \hat{H}_h^{\rm ex} = \frac{1}{3} \mathbf{G}_h \mathbf{J}_h , \tag{2}$$

where

$$\mathbf{G}_e = N_0 \alpha x \langle \mathbf{S}_j \rangle \quad \text{and} \quad \mathbf{G}_h = N_0 \beta x \langle \mathbf{S}_j \rangle \tag{3}$$

are effective exchange fields, and x is the molar fraction of magnetic ions. To describe the average value of the component of the localized spins along the applied magnetic-field direction $\langle S_j^Z \rangle$, a modified Brillouin function with two phenomenological parameters $S_0 = S_0(x)$ and $T_0 = T_0(x)$ is commonly used:[9]

$$\langle S_j^Z \rangle = S_0 B_S \left(\frac{g \mu_B B S}{k_B (T + T_0)} \right). \tag{4}$$

Here g and S are, respectively, the g factor and magnitude of the spin of the magnetic ions, and μ_B is the Bohr magneton. The remaining two components of average spin vanish in the materials in question $\langle S_j^X \rangle = \langle S_j^Y \rangle = 0$.

According to this notation, the Hamiltonian describing the hole states in DMS QWR's takes the form

$$\hat{H}_h = \hat{H}_L + \frac{1}{3} \mathbf{G}_h \mathbf{S}_h + V(x,y), \tag{5}$$

where $V(x,y)$ is the confining potential in the x-y plane due to the presence of the barriers, and $\hat{H}_L$ is the Luttinger Hamiltonian.[10] The form of the Luttinger Hamiltonian depends on the crystallographic direction of the axis of quantization, and will be given explicitly in the next section. In typical experimental conditions the exchange-induced splitting is much larger than the intrinsic Zeeman effect and the direct Landau quantization (up to 100 times). One can thus, to a good approximation, neglect the two latter contributions to the Hamiltonian.

T-SHAPED QUANTUM WIRES

We perform our calculations specifically for $Cd_{0.97}Mn_{0.03}Te/Cd_{0.72}Mg_{0.25}Mn_{0.03}Te$ T-shaped QWR's, since such structures have already been obtained and have been preliminarily studied experimentally.[7] Thus the potential $V(x,y)$ in Eq. (5) describes now the T-shaped confining potential (see Fig. 1). The shaded regions in the figure correspond to $Cd_{0.72}Mg_{0.25}Mn_{0.03}Te$ barriers, while $Cd_{0.97}Mn_{0.03}Te$ QW's are unshaded. The wire structure consists of two intersecting QW's with [00-1] and [-110] orientations, corresponding in our notation to X and Y directions, respectively. The Z axis is taken along the wire direction, i.e., is perpendicular to the plane of the figure, and extends along the [110] crystallographic direction.

For such choice of axes the Luttinger Hamiltonian takes the form[11]

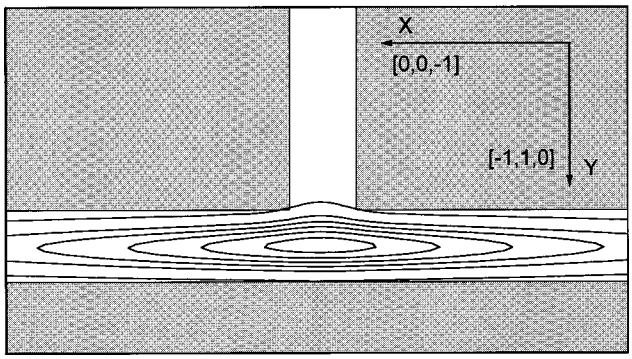

FIG. 1. Potential profile of a 40-Å-wide $Cd_{0.97}Mn_{0.03}Te/Cd_{0.72}Mg_{0.25}Mn_{0.03}Te$ T-shaped quantum wire structure. Gray regions correspond to barriers, and well regions are unshaded. Arrows indicate crystallographic directions. The line contours show the shape of $|\Psi(x,y)|^2$ (see text), indicating that the holes are only weakly localized at the intersection region.

$$\hat{H}_L = \frac{\hbar^2}{2m_0} \begin{array}{c} \begin{matrix} \left|\frac{3}{2},\frac{3}{2}\right\rangle & \left|\frac{3}{2},\frac{1}{2}\right\rangle & \left|\frac{3}{2},-\frac{1}{2}\right\rangle & \left|\frac{3}{2},-\frac{3}{2}\right\rangle \end{matrix} \\ \begin{pmatrix} P+Q & -S & R & O \\ -S^* & P-Q & 0 & R \\ R^* & 0 & P-Q & S \\ 0 & R^* & S^* & P+Q \end{pmatrix} \end{array} \tag{6}$$

with

$$P \pm Q = \left(\gamma_1 \mp \frac{3\gamma_3 + \gamma_2}{2} \right) k_z^2 + (\gamma_1 \pm \gamma_2) k_x^2 + \left(\gamma_1 \pm \frac{3\gamma_3 - \gamma_2}{2} \right) k_y^2,$$

$$R = \frac{\sqrt{3}}{2} [(\gamma_2 - \gamma_3) k_z^2 - 2\gamma_2 k_x^2 + (\gamma_2 + \gamma_3) k_y^2 + i 4 \gamma_3 k_x k_y],$$

$$S = 2\sqrt{3} (\gamma_3 k_x k_z - i \gamma_2 k_y k_z),$$

where $\gamma_1, \gamma_2, \gamma_3$ are the Luttinger parameters, m_0 is the free electron mass, and $k_i = -i(\partial/\partial q_i)$ $(q_i = x,y,z)$.

In this work we restrict our consideration to the case of the magnetic field applied along the wire, $\mathbf{B} \| Z$. In this case, the exchange Hamiltonian $\hat{H}_h^{\rm ex}$ becomes diagonal in the basis of $|\pm 3/2\rangle, |\pm 1/2\rangle$:

$$\hat{H}_h^{\rm ex} = \frac{1}{3} G_h^z J_z , \tag{7}$$

where J_z represents the matrix of operator of the z projection of total angular momentum $J = 3/2$. Therefore, for a vanishing hole wave vector along the wire direction ($k_z = 0$) the 4×4 matrix of the hole Hamiltonian (5) splits into two 2×2 matrices for $(+3/2, -1/2)$ and $(-3/2, +1/2)$ subspaces. In dimensionless variables, where the length unit $d = 1$ Å and the energy unit $E_0 = \hbar^2/2m_0 d^2$, the Hamiltonian for the $(+3/2, -1/2)$ subsystem takes the form

$$\hat{H}_h=\begin{pmatrix} -(\gamma_1+\gamma_2)\frac{\partial^2}{\partial x^2}-\left(\gamma_1+\frac{3\gamma_3}{2}\right)\frac{\partial^2}{\partial y^2}+\frac{G_h^z}{2} & \sqrt{3}\left(\gamma_2\frac{\partial^2}{\partial x^2}-\frac{\gamma_3+\gamma_2}{2}\frac{\partial^2}{\partial y^2}-2i\gamma_3\frac{\partial^2}{\partial x\,\partial y}\right) \\ \sqrt{3}\left(\gamma_2\frac{\partial^2}{\partial x^2}-\frac{\gamma_3+\gamma_2}{2}\frac{\partial^2}{\partial y^2}+2i\gamma_3\frac{\partial^2}{\partial x\,\partial y}\right) & -(\gamma_1-\gamma_2)\frac{\partial^2}{\partial x^2}-\left(\gamma_1-\frac{3\gamma_3}{2}\right)\frac{\gamma^2}{\partial y^2}-\frac{G_h^z}{6} \end{pmatrix}+V(x,y). \tag{8}$$

The Hamiltonian for the $(-3/2, +1/2)$ subsystem can be obtained from Eq. (8) by taking its conjugate and changing the sign of the exchange field G_h^z. It is seen that the exchange field G_h^z appears in the diagonal matrix elements in Eq. (8) multiplied by two different coefficients. We can thus expect that there will be a strong magnetic-field dependence of the degree of mixing of the heavy- and light-hole states in such QWR structures.

The Hamiltonian (8) commutes with the symmetry operator $\hat{P}$, which corresponds to a superposition of a reflection in the $x=0$ plane and the conjugation operation: $\hat{P}\Psi(x,y)=\Psi^*(-x,y)$. Eigenvalues of this operator are $p=\pm 1$. The hole wave function must therefore satisfy the following condition:

$$\Psi^*(-x,y)=\pm\Psi(x,y). \tag{9}$$

We expand our two-component hole wave function in the basis of the solutions of the Schrödinger equation for two-dimensional, infinitely deep QW's (L_x and L_y are well widths in the X and Y directions, respectively). In agreement with Eq. (9), we have used as the basis functions in the X direction only the functions with definite parity (sine or cosine) for real part of Ψ, and with opposite parity for its imaginary part. For the ground states of the holes this expansion takes the form

$$\Psi=\begin{pmatrix}\Psi_h\\ \Psi_l\end{pmatrix}=\frac{2}{\sqrt{L_xL_y}}\sum_{n,m}\left[\begin{pmatrix}a_{nm}^h\\ a_{nm}^l\end{pmatrix}\cos\left(\frac{\pi nx}{L_x}\right)\delta_{-1,(-1)^n}+i\begin{pmatrix}b_{nm}^h\\ b_{nm}^l\end{pmatrix}\sin\left(\frac{\pi nx}{L_x}\right)\delta_{1,(-1)^n}\right]\left[\cos\left(\frac{\pi my}{L_y}\right)\delta_{-1,(-1)^m}+\sin\left(\frac{\pi my}{L_y}\right)\delta_{1,(-1)^m}\right], \tag{10}$$

where indices h and l correspond to heavy- and light-hole components.

Matrix elements of the Hamiltonian (8) can be calculated analytically using the expansion given by Eq. (10), resulting in a $(2*N*M)\times(2*N*M)$ symmetric square matrix, N and M denoting the numbers of the basis functions in the X and Y directions, respectively. Performing numerical diagonalization of the resulting matrix, one can then obtain the hole energies and the coefficients $a_{nm}^{h(l)}, b_{nm}^{h(l)}$. Note that in the case of a T-shaped potential profile, when the confinement region is not well defined, one should be careful to choose L_x, L_y large enough to avoid any influence of these parameters on the final result of the calculation. This applies especially to the hole states in T-shaped QWR structures, which are only very weakly localized at the intersection region (see Fig. 1).

In Fig. 2 we plot the magnetic-field dependence of the relative contributions of the light-hole and the heavy-hole components, $\langle\Psi_l|\Psi_l\rangle=\Sigma_{n,m}(a_{n,m}^l)^2+(b_{n,m}^l)^2$ and $\langle\Psi_h|\Psi_h\rangle=\Sigma_{n,m}(a_{n,m}^h)^2+(b_{n,m}^h)^2$, to the ground-state wave function for a 40-Å-wide (solid lines) and a 65-Å-wide (dashed lines) $Cd_{0.97}Mn_{0.03}Te/Cd_{0.72}Mg_{0.25}Mn_{0.03}Te$ T-shaped QWR. Positive values of magnetic field correspond to the $(+3/2, -1/2)$ hole subsystem, and negative values of the field to the $(-3/2, +1/2)$ subsystem. We see immediately that the character of the hole ground state can be very strongly varied by an applied magnetic field.

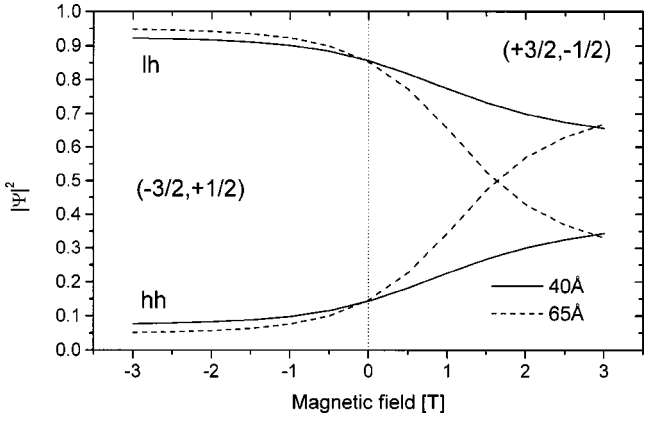

FIG. 2. Magnetic-field dependence of the relative contributions of the heavy-hole and the light-hole components to the wave function of the hole ground state for a 40-Å-wide (solid line) and a 65-Å-wide (dashed line) $Cd_{0.97}Mn_{0.03}Te/Cd_{0.72}Mg_{0.25}Mn_{0.03}Te$ T-shaped QWR. Positive and negative values of the magnetic field correspond to $(+3/2, -1/2)$ and $(-3/2, +1/2)$ hole subsystems, respectively.

One of the possible manifestations of this effect can be a magnetic-field dependence of the polarization of interband optical transitions in DMS QWR's. Since the heavy-hole states are optically inactive in the light polarization $\varepsilon\|Z$, we may expect a decrease of the intensity of optical transition in this polarization with an increasing heavy-hole contribution to the hole ground state.

In order to calculate quantitatively the matrix elements describing the dipole-allowed optical transitions, one needs to include in the considerations also the excitonic effects. However, the polarization characteristics of the optical transitions depend mainly on the relative contribution of the heavy- and the light-hole components to the hole ground state. So, neglecting the excitonic effects and writing down the expressions for the intensities of optical transitions in the $\pi(\varepsilon\|Z\|\mathbf{B})$ and the $\sigma(\varepsilon\|X\perp\mathbf{B})$ polarizations, we have:

$$I_\pi \propto \frac{4}{6}\langle \Psi_e|\Psi_l\rangle^2 = \frac{4}{6}\left[\sum_{n,m} a^l_{n,m} a^e_{n,m}\right]^2,$$

$$I_\sigma \propto \left[\frac{1}{\sqrt{2}}\langle \Psi_e|\Psi_h\rangle - \frac{1}{\sqrt{6}}\langle \Psi_e|\Psi_l\rangle\right]^2$$

$$= \left[\frac{1}{\sqrt{2}}\sum_{n,m} a^h_{n,m} a^e_{n,m} - \frac{1}{\sqrt{6}}\sum_{n,m} a^l_{n,m} a^e_{n,m}\right]^2, \qquad (11)$$

where Ψ_e is the wave function of the conduction electron ground state, and $a^e_{n,m}$ are the coefficients of its expansion in the basis of the solutions of the Schrödinger equation for a two-dimensional, infinitely deep QW, analogous to the expression for the holes given by Eq. (10). Since the expansion involves in the case of electrons only functions even in the X direction, only terms with $a^{h(l)}_{n,m}$ appear in the sums in Eq. (11).

In Fig. 3 we present the results of calculations of the magnetic-field dependence of the polarization of optical transitions, $P=(I_\pi - I_\sigma)/(I_\pi + I_\sigma)$, for 40-Å-wide (solid line) and 65-Å-wide (dashed line) $Cd_{0.97}Mn_{0.03}Te/Cd_{0.72}Mg_{0.25}Mn_{0.03}Te$ T-shaped QWR's. As expected, when the contribution of the heavy-hole component to the ground-state hole wave function increases, the probability of the optical transitions in the π polarization decreases (see Fig. 2). This clearly leads to a strong magnetic-field dependence of the polarization of optical transitions occurring in QWR's made of DMS, a feature not encountered in such structures fabricated of nonmagnetic materials.

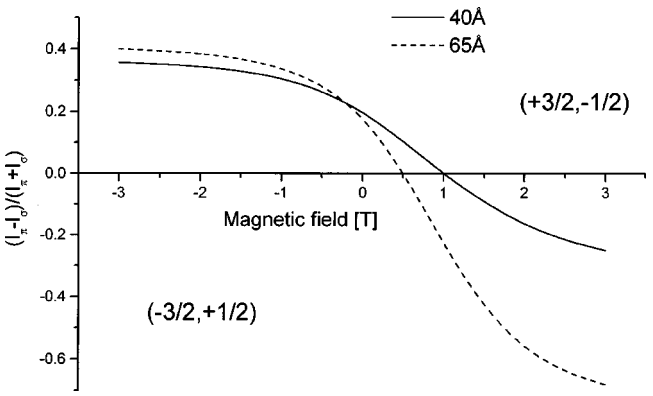

FIG. 3. Magnetic-field dependence of the polarization of optical transitions between the electron and hole ground states for a 40-Å-wide (solid line) and a 65-Å-wide (dashed line) $Cd_{0.97}Mn_{0.03}Te/Cd_{0.72}Mg_{0.25}Mn_{0.03}Te$ T-shaped QWR. Positive and negative values of magnetic field correspond to the $(+3/2, -1/2)$ and $(-3/2, +1/2)$ hole subsystems, respectively.

CONCLUSIONS

We have shown that in the case of QWR's made of diluted magnetic semiconductors it is possible to control the relative contribution of the light- and the heavy-hole components to the total wave function of the holes by changing an external magnetic field **B**. This is in contrast to the case of nonmagnetic quantum wire structures, where the character of the hole states is determined only by the structure parameters, such as the well width and the barrier height. Numerical calculations performed for the case of T-shaped DMS QWR's demonstrate a strong magnetic-field dependence of the polarization of optical transitions in such structures due to field-induced changes of the character of the hole ground state. It is expected that similar effects should also occur in the case of DMS-based quantum dots.

ACKNOWLEDGMENT

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