Stark Effect in CdTe/$Cd_{1-x}Mn_x$Te Strained Double Quantum Wells

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Received on 31 March, 2003

We report a detailed analysis of how the existence of interface roughness can change exciton localization in CdTe/$Cd_{1-x}Mn_x$Te strained double quantum wells (DQW's) taking into account magnetic and electric field effects. We consider that the potential, effective mass, and the intrinsic magnetization are dependent on the profile of the Mn molar fraction at the interfacial region. Results obtained with CdTe/$Cd_{0.68}Mn_{0.32}$Te DQW's show that the energy band tailoring generated by the strain and the Zeeman effect is responsible by a displacement of the exciton energy peaks and that small changes in the interface width (10 Å) can be responsible for a 30 meV exciton energy broadening.

1 Introduction

Excitons in semiconductors double quantum wells (DQW's) have been the subject of several experimental and theoretical investigations, finding applications in optical modulators and tunable and free-electron lasers [1, 2]. Confinement of excitons in DQW's increases their binding energy and the spatial separation of electrons and holes increases the exciton lifetime, which has been used for fundamental studies of the Bose Einstein condensation of excitons [3].

Diluted magnetic semicondutor (DMS) heterostructures like CdTe/$Cd_{1-x}Mn_x$Te are of particular interest due to the unique magneto-optical properties generated by their strong exchange interaction between the spin of the band states and the spin of the localized paramagnetic Mn^{+2} ions [4]. When a magnetic field is applied to these heterostructures, the alignment of the carriers leads to a spin splitting which is much larger then the Zeeman one ($\approx$ 100 times the usual value of $g = 0.5$), inducing the so-called giant Zeeman effect of the band edges [5]. In these systems, the strain due to the lattice mismatch, as well as the external applied magnetic field, can be considered as additional parameters for tailoring the electronic properties of semiconductors devices.

Continuing advances in modern crystal-growth techniques are leading to improvement in the quality of quantum wells devices, but the interfacial fluctuations still exists. The existing works in literature on the study of gradual interfaces in CdTe/$Cd_{1-x}Mn_x$Te quantum wells show that occurs a broadening of the exciton energy spectrum due to the existence of well width fluctuations [4, 5].

The purpose of this work is to describe how the existence of smooth interface modifies the exciton localization in CdTe/$Cd_{1-x}Mn_x$Te DQW's taking into account strain and electric field effects. Three kinds of interface profiles (governed by growth conditions of the QW) are analyzed: error function (related to diffusion); exponential (segregation); and the abrupt picture. The tailoring of the conduction and valence bands generated by the existence of strain is responsible for a strong shift of the exciton energy peaks.

2 Magnetization Effects

When an external magnetic field acts on a DMS such as CdTe/$Cd_{1-x}Mn_x$Te, it produces a giant Zeeman splitting of both the conduction and valence bands. This splitting is proportional to the average magnetization of the Mn spin in the semimagnetic semiconductor [4, 5], which is given by

$$M_{Bulk}\left(x,B,T\right)=x\overline{S}\left(x\right)B_{5/2}\left\{\frac{g\mu_B B}{\left[T+T_0\left(x\right)\right]}\right\}, \quad (1)$$

where $B_{5/2}$ is the modified Brillouin function: $B_j\left(y\right)=J\coth\left(Jy\right)-\coth\left(y/2j\right)/2j$; $J=(2j+1)/2j$; $\overline{S}\left(x\right)=5/2\left[0,265\exp\left(-43,34x\right)+0,735\exp\left(-6,19x\right)\right]$ and the temperature $T_0\left(x\right)=(35,37x)/(1+2,752x)$.

In the presence of a magnetic field B applied along the growth axis, the respective Zeeman splitting of the conduction and valence bands are given by

$$\begin{aligned} V_e^{Mag}\left(z\right) &= \pm\frac{1}{2}N_0\alpha M\left[\chi(z),z,B,T\right], \\ V_{lh,hh}^{Mag}\left(z\right) &= \pm\frac{1}{2}N_0\beta M\left[\chi(z),z,B,T\right], \end{aligned} \quad (2)$$

where $M[\chi(z),z,B,T]$ is the heterostructure magnetization, which is dependent on the Mn molar fraction $\chi(z)$. The sign of the magnetic potential is related to the total spin quantum states $m_z = s_e + j_h = \pm 1$, which characterizes the spin Zeeman splitting. We follow the same procedure as described in Ref. [4] considering that $M\left[\chi(z), z, B, T\right] \approx M_{bulk}\left[\chi(z), z, B, T\right]$.

3 Strain Contribution

The strain related splitting is proportional to its magnitude. It is described in terms of the deformation potentials. For strain along [001], the energy of the conduction and valence bands taking into account strain and spin orbit effects is given by [6]:

$$\begin{aligned} E_c &= E_v^0 + E_g + P_c, \\ E_{hh} &= E_v^0 - P_\varepsilon - Q_\varepsilon, \\ E_{lh} &= E_v^0 - P_\varepsilon + \frac{Q_\varepsilon}{2} - \frac{\Delta_0}{2} + \frac{1}{2}\sqrt{S(\Delta_0, Q_\varepsilon)}, \\ E_{so} &= E_v^0 - P_\varepsilon + \frac{Q_\varepsilon}{2} - \frac{\Delta_0}{2} - \frac{1}{2}\sqrt{S(\Delta_0, Q_\varepsilon)}. \end{aligned}$$

In the above equations, $E_v^0 = E_{v,av}^0 + \Delta_0/3$, $S(\Delta_0, Q_\varepsilon) = (\Delta_0^2 + 2\Delta_0 Q_\varepsilon + 9Q_\varepsilon^2)$, and Δ_0 is the spin-orbit splitting; $P_c = a_c\left(\varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz}\right)$, $P_\varepsilon = -a_v\left(\varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz}\right)$, $Q_\varepsilon = -b\left(\varepsilon_{xx} - \varepsilon_{zz}\right)$, where b is the shear deformation potential, a_c and a_v are the hydrostatic deformation potential for the conduction and valence bands, respectively; $\varepsilon_{xx}^i = \varepsilon_{yy}^i = [(a_\parallel - a_i)/a_i]$, $\varepsilon_{zz}^i = -2(C_{12}/C_{11})\varepsilon_{xx}^i$ are the components of the strain tensor, where $a_\parallel$ is the lattice constant in the plane, a_i is the equilibrium lattice constant, and C_{ij} is the elastic coefficient of the material [6].

The conduction and valence band offsets are:

$$\begin{aligned} \Delta V_e^{Strain} &= E_c^{Cd_{1-x}Mn_xTe} - E_c^{CdTe}, \\ \Delta V_\beta^{Strain} &= E_\beta^{CdTe} - E_\beta^{Cd_{1-x}Mn_xTe}, \end{aligned} \tag{3}$$

with β = hh, lh, and so.

4 Graded Interfaces

The exciton Hamiltonian and the total exciton wave function, within the effective mass approximation, can be expressed as $H = H_e\left(z_e\right) + H_z\left(z_h\right) + H_{exc}\left(r, z_e, z_h\right)$ and $\Psi\left(r, z_e, z_h\right) = \psi_e\left(z_e\right)\psi_h\left(z_h\right)\phi_{e-h}\left(r, \varphi\right)$, respectivelly. Using this assumption, the Schrödinger equation for the perpendicular motion is

$$\begin{aligned} \Big\{ -\frac{\hbar}{2}\frac{\partial}{\partial z_i}\left[\frac{1}{m_i\left(z_i\right)}\frac{\partial}{\partial z_i}\right] + V_i\left(z_i\right) \\ + V_i^{Mag}\left(z_i\right) - E_i \Big\}\psi_i\left(z_i\right) = 0, \end{aligned} \tag{4}$$

where $V_i\left(z\right)$ $\left[m_i(z_i)\right]$ describes the carrier confinement (effective mass) in the quantum well, and $V_i^{Mag}\left(z_i\right)$ is related with the Mn magnetization contribution, see Eq. (2).

The model of Freire *et al.* [7] is used to describe the interface region, where is assumed that the potential, effective mass, and the intrinsic magnetization are dependent on the profile of the Mn molar fraction $\chi(z)$ at the interfacial region. The effective potential and carrier effective mass are expressed in function of $\chi(z)$ by the following expressions:

$$m_i\left(z_i\right) = \mu_1 + \mu_2\chi\left(z_i\right), \tag{5}$$

$$V_i\left(z_i\right) = Q_i\left[1.587\chi\left(z_i\right)\right], \tag{6}$$

where Q_i is the band offset [7]. Three kinds of interface profiles (governed by growth conditions of the QW) are analyzed: error function (related to diffusion); exponential (segregation); and the abrupt picture [4, 5, 7].

The Schrödinger-like equation for the radial motion can be written, in cylindrical coordinates, as

$$\begin{aligned} \Big\{ -\frac{\hbar^2}{2\mu_\pm}\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2}{\partial\varphi^2}\right] \\ + V(r) + E_b\Big\}\phi_{e-h}(r, \varphi) = 0, \end{aligned} \tag{7}$$

where E_b is the exciton binding energy; $E_{exc}=E_{gap}+E_e+E_h-E_b$ is the total exciton energy; $V(r)$ is defined as an effective in-plane Coulomb potential, which is expressed as

$$V(r) = -\frac{e^2}{\varepsilon}\int dz_e \int dz_h \frac{|\psi_e(z_e)|^2|\psi_h(z_h)|^2}{[r^2 + (z_e - z_h)^2]^1/2}. \tag{8}$$

The eigenvalues of the perpendicular wave equation, Eq. (4), and the exciton binding energy, Eq. (7), are calculated through a discretization technique [7].

5 Results

We have calculated the binding and total exciton energy of $CdTe/Cd_{0.68}Mn_{0.32}Te$ strained DQW's taking into account electric and magnetic field effects. We have taken the CdTe and MnTe parameters from Ref. [7]. The $Cd_{0.68}Mn_{0.32}Te$ parameters are obtained from those of CdTe and MnTe through linear interpolation.

The exciton energy dependence with the interfaces thicknesses is shown in Fig. 1 for the exponencial like (curves) and for the error function like interfacial profile (symbols), in the σ^- orientation. Notice that there are almost no changes in the exciton energy by considering the exponencial or the error function profile in the interfaces. This is not true for the abrupt interface picture, where we can see a large displacement of the excitonic energy when considering interfaces thicknesses of only 10 Å, which can be of the order of 30 meV (34 meV) when considering magnetic fields of $B = 8$ T ($B = 0$ T).

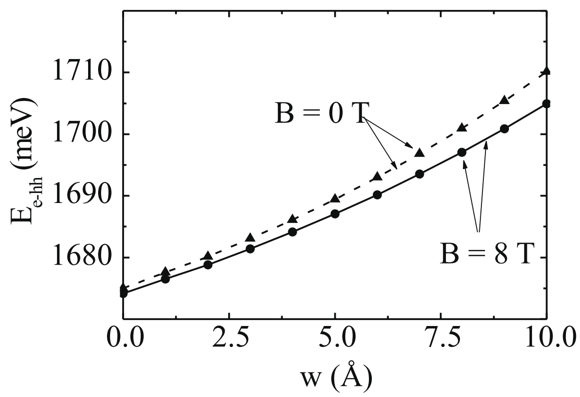

Figure 1. Ground state exciton energy as a function of the interfaces thicknesses, for a 50 Å (40 Å) well width (barrier width), for the exponencial like interfacial profile (curves) and for the error function profile (symbols).

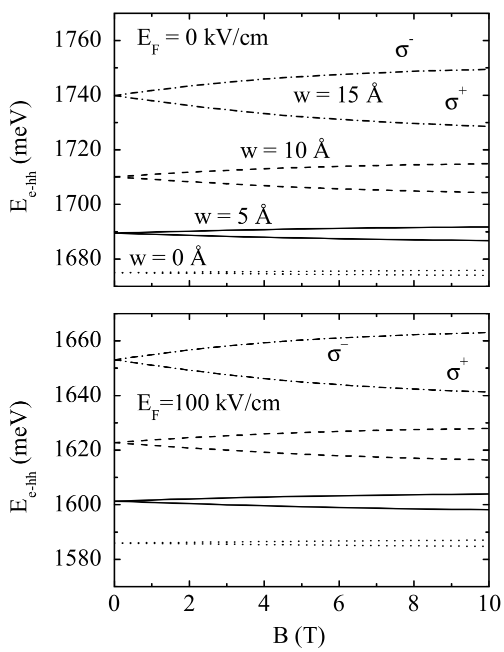

Figure 2. Ground state energy of the e-hh exciton as a function of the applied magnetic field, for a 50 Å (40 Å) well width (barrier width).

The Zeeman effect due to the applied electric and magnetic field in the exciton energy is shown in Fig. 2 as a function of the magnetic field intensity, for several values of the interface thickness w. The giant Zeeman splitting increases with the increasing of the interface thickness, e.g., it increases from 2 meV (2meV) for the abrupt well up to 10 meV (22 meV) for a 15 Å interface thickness, when considering an electric field of $E_F = 0$ kV/cm ($E_F = 100$ kV/cm) and a magnetic field of 8 T.

In conclusion, we believe that the results presented in this paper have shown the necessity of considering realistic DQW's (existence of interfacial fluctuations) for a better description of the excitonic energy peaks in CdTe/$Cd_{1-x}Mn_x$Te strained double quantum wells (DQW's). Our paper is expected to stimulate further developments in experimental work.

Acknowledgments

This work was supported by CAPES and by CNPq/NanoSemiMat grant N. 550.015/01-9.

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