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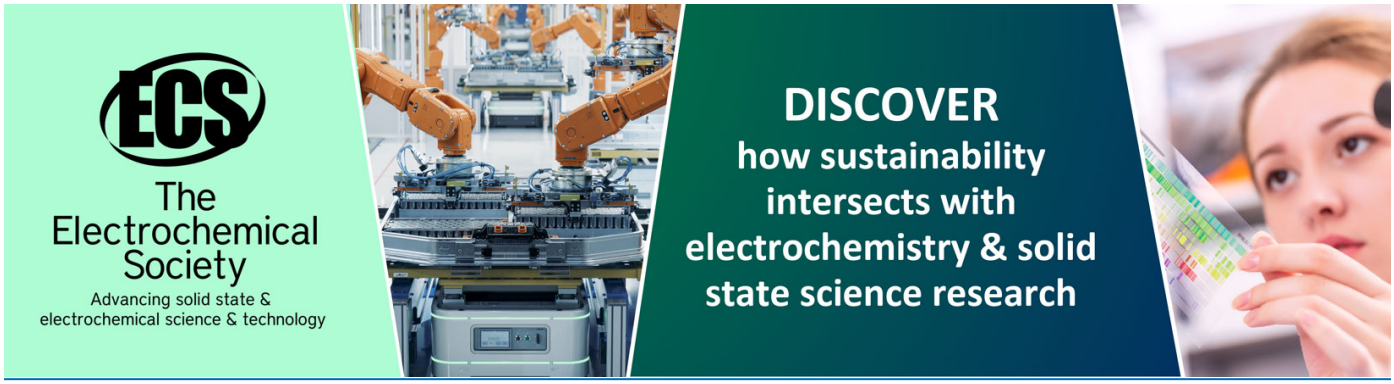

Journal of Physics: Conference Series **245** (2010) 012036 doi:10.1088/1742-6596/245/1/012036

Effect of magnetic field on optical anisotropy of CdZnSe quantum dots

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Abstract. The effect of magnetic field on the electronic structure and optical anisotropy of $Zn_{1-x}Cd_xSe/ZnSe$ quantum dots (QDs) has been analyzed for varying geometrical confinement related to the in-plane asymmetry. The disk-shaped QD is modeled by anisotropic parabolic potential with the magnetic field considered in Faraday geometry. The multiple band Hamiltonian in presence of magnetic field has been numerically diagonalized using appropriate basis functions and coordinate transformations for fast convergence. The eigenvalues and eigenvectors thus obtained are utilized for obtaining the dipole matrix elements. Hence, the photoluminescence spectra and the degree of linear polarization have been studied for the anisotropic QDs. The polarization degree is found to increase with magnetic field and anisotropy parameter.

1. Introduction

Spintronic devices offer a possibility to inject, modulate and detect spin of charge carriers In the new area of spintronics aimed at quantum computing and quantum communication, self-assembled semiconductor quantum dots (QDs) are a promising systems for spin-based quantum computers. Quantum computation applications based on spins of electons or holes as quantum bits require the preparation of the system in definite spin state and the ability to readout the spin of the output state. These tasks can be achieved through resonant excitation of excitons or trions using polarized optical pulse and analysis of the polarized photoluminescence (PL) spectrum of the output radiation [1].

The precise information about the the spin polarization of the system can be obtained from the study of optical anisotropy of the PL spectra of QDs which depend on the geometrical symmetry of the QDs. Magnetic field plays an important role in a spin based application by lifting the spin degeneracy and controlling the separation between the states of opposite spins.

The objective of this work is to analyze the effect of magnetic field on the electronic structure and optical anisotropy of $Zn_{1-x}Cd_xSe/ZnSe$ QDs for varying geometrical confinement related to the in-plane asymmetry. The disk-shaped QD is modeled by anisotropic parabolic potential with the magnetic field considered in Faraday geometry. The multiple band Hamiltonian in presence of magnetic field can be solved by constructing the Hamiltonian matrix in the Hilbert space of Hermite Gaussian functions for QDs with significant in-plane anisotropy [2, 3]. However, in order to achieve faster convergence, we have worked with the canonical transformations suggested by Madhav and Chakraborty [4] for conduction band electrons in anisotropic quantum dots, and

generalized to the case of multiple valence band structure. The Hamiltonian calculated in the transformed coordinates has been diagonalized numerically. The eigenvalues and eigenvectors thus obtained are utilized for obtaining the dipole matrix elements. Hence, the degree of linear polarization (P_L) have been studied for the anisotropic QDs. The polarization degree is found to increase with magnetic field and anisotropy parameter A.

2. Theoretical formulations

The anisotropic $Zn_{1-x}Cd_xSe/ZnSe$ QD is modeled using a quantum well confinement potential, $V_z(z)$ along the z-axis (growth direction) and a parabolic confinement $V_{xy}(x, y)$ along the x- and y-axes, respectively. Further, we consider magnetic field applied in the Faraday configuration, i.e. along z-axis. The potential energy functions $V_z(z)$ and $V_{xy}(x, y)$, are determined by various physical parameters including the extent of interdiffusion of the barrier ions in the QD, valence band offsets, hydrostatic and biaxial strain, size and the shape anisotropy of the QD. The variation of the composition x of the QD material modifies the energy band gap as $E_g(\mathrm{x}) = E_{g\mathrm{CdSe}} + (E_{g\mathrm{ZnSe}} - E_{g\mathrm{CdSe}} - b)\mathrm{x} + b\mathrm{x}^2$ where b is the bowing parameter [5]. The other parameters for $Zn_{1-x}Cd_xSe$ are obtained from a linear interpolation of the ZnSe and the CdSe parameters.

The electronic structure of the QD can be obtained by solving the Luttinger Hamiltonian including the strain effects [6, 7]. Due to the s-type symmetry of the conduction band, the strain simply leads to the shifting of the conduction band edge caused by the hydrostatic deformation potential. The effect of strain on the valence band is more complicated due to the p-type symmetry. The hydrostatic strain shifts the heavy-hole (hh) and light-hole (lh) bands by the same amount, so that, in the strained QD structure the valence band shifts towards higher energy as compared to the unstrained case. In addition to this, in our system $Zn_{1-x}Cd_xSe/ZnSe$, the biaxial strain component has the effect of increasing the energy splitting between the two valence subbands [8]. We have considered the magnetic field in the Faraday geometry and adopted Coulomb gauge whereby the vector potential is given by $\mathbf{A} = (-By/2, Bx/2, 0)$. The in-plane confinement V_{xy} is defined by the anisotropic parabolic potential $V_{xy}(x, y) = (\alpha_x x^2 + \alpha_y y^2)/2$. Here, $\alpha_{x,y}$ is dependent on the confinement energies along x and y axes. The Hamiltonian for z variable can be solved in terms of usual quantum well wavefunctions. For the in-plane confinement potential V_{xy} the standard solution would be the Hermite-Gaussian functions as in the case of Harmonic oscillator. Further, the $Zn_{1-x}Cd_xSe/ZnSe$ QDs tend to show a high degree of in-plane anisotropy. This effect is quantified in our model as the anisotropy parameter A which is defined through the difference in the harmonic oscillator frequencies along x and y directions resulting in the expression $A = (\omega_x - \omega_y)/(\omega_x + \omega_y)$ [3]. Thus, an isotropic QD is denoted by $A = 0$ whereas $A = \pm 1$ would mean a very high degree of in-plane anisotropy approaching the case of a quantum wire. Here, $\omega_{x,y} = \sqrt{(\alpha_{x,y}/m_j)}, m_j$ being the mass of electron, hh or lh depending on the j^{th} band under consideration.

With the inclusion of magnetic field there is coupling of the terms in x and y coordinates in the Hamiltonian, thus complicating the solution. The equations can be uncoupled through the canonical transformation of the Hamiltonian [4] so that the diagonal terms reduce to a system of uncoupled Harmonic oscillators. The off-diagonal terms which are coupled in all four variables of the transformed coordinate system can be calculated algebraically. The Hamiltonian is diagonalized numerically using the product of harmonic oscillator wavefunctions in the transformed coordinates for the basis. The off-diagonal terms in this basis lead to a reasonably fast convergence as they just provide a correction factor due to mixing of valence subbands. This transformation introduces an approximation due to presence of two hole species, however, from the numerical estimates the error was found to be less than 2%.

The energy eigenvalues and wavefunctions obtained after the numerical diagonalization of

the Hamiltonian are used for the analysis of various optical properties of the QDs. The intensity for a particular transition can be obtained from the square of the absolute value of the corresponding dipole matrix element, $\left|\langle\psi^c_{n_c}|\mathbf{e}.\mathbf{p}|\psi^v_{n_v}\rangle\right|^2$ where $\mathbf{e}$ gives the direction of linear polarization of radiation, $\mathbf{p}$ is the momentum operator, and $\psi^c_{n_c}$ ($\psi^v_{n_v}$) is the conduction (valence) band state under consideration [3]. The degree of linear polarization is obtained using the relation $P_L = (I_{max} - I_{min})/(I_{max} + I_{min})$ where, I_{max} and I_{min} are the maximum and minimum intensities obtained by varying the polarization angle of the electric field vector $\mathbf{e}$.

3. Results and discussion

In this section, we study the effect of magnetic field on the energy eigenvalues and the degree of linear polarization in a $Zn_{1-x}Cd_xSe$/ZnSe QD using the formulation developed in Section 2. The material parameters used in the present numerical analysis are given in Table 1. We have considered the QDs to have Cd content of 40% which yields results in close conformity with the experimental observations [10, 11]. The dimension of the QD is taken to be 3.5 nm along the growth axis. The characteristic lateral size of the QD is estimated through the relation $r_0 = \sqrt{(\hbar/m\omega_0)}$ and gives an order of 8 nm for QD diameter at the typical value of $\hbar\omega_0 = 5$ meV. The effect of z-confinement has been calculated through a finite quantum well model with confinement potential determined by the band offsets and strain effects. The band offsets for x=0.4 calculated through linear interpolation from the pure ZnSe and CdSe parameters are found to be 387 meV and 108 meV for the conduction band and valence band, respectively. In case of valence band, the biaxial compressive strain shifts the energy of hh subband by 40 meV closer to the conduction band thus increasing the confinement potential for hh to 148 meV. The effect is just the opposite for the lh subband, thus decreasing the well potential by about 96 meV so that the lh remains weakly confined. Using the above values for the band offsets and the confinement potential along z-direction, the hole energy eigenvalues and eigenfunctions

Table 1. Material parameters for CdSe, ZnSe [5, 9] and $Zn_{0.6}Cd_{0.4}Se$ (linearly interpolated from data of CdSe and ZnSe).

	CdSe	ZnSe	$Zn_{0.6}Cd_{0.4}Se$
$E_g(eV)$	1.765	2.821	2.326
γ_1	2.1	3.77	3.10
γ_2	0.55	1.24	0.96
γ_3	0.55	1.67	1.22
m_c	0.13	0.16	0.15
C_{11}(GPa)	66.7	82.6	76.2
C_{12}(GPa)	46.3	49.8	48.4
$D_c(eV)$	-2.44	-2.83	-2.68
$D_{v1}(eV)$	-1.22	-1.41	-1.34
$D_{v2}(eV)$	-0.8	-1.2	-1.04
a_L (Å)	6.077	5.668	5.831

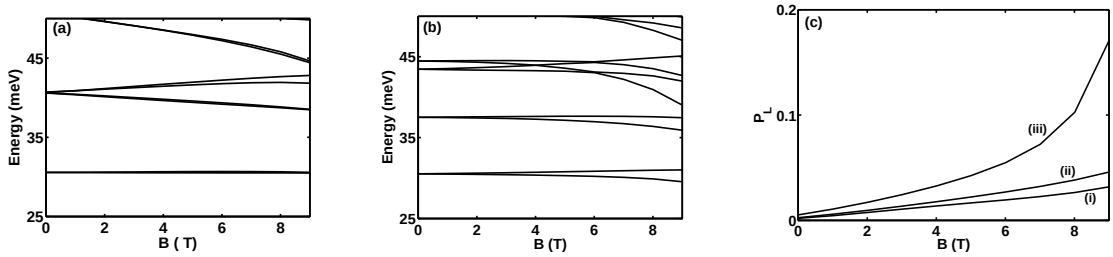

Figure 1. Plots (a) and (b) show the variation of hole energy eigenvalues of $Zn_{0.6}Cd_{0.4}Se$ QD with magnetic field for $A = 0.0$ and 0.3, respectively. Plot (c) shows the Variation of P_L with magnetic field for $Zn_{0.6}Cd_{0.4}Se$ QD at (i) A =0.1, (ii) A =0.3, and (iii) A =0.5.

are calculated. Fig.1 (a) and (b) show the variation of energy eigenvalues with respect to the magnetic field for the isotropic ($A = 0.0$) and anisotropic QDs ($A = 0.3$), respectively. The zero of the energy is taken to be the valence band edge for strained CdZnSe without confinement effects. In case of isotropic QDs, the mixing of hole states results in an extremely small splitting of lowest pair of states and the first excited states. On the other hand, in the anisotropic QDs there is an enhancement in splitting energy with red-shifting of the states [12]. This anomalous red-shifting of the lowest states has been experimentally observed by Miura et al [13].

We have also plotted the degree of linear polarization, P_L of the lowest state as a function of magnetic field for different values of A (Fig. 1(c)). We find that it increases with the magnetic field which is a clear signature of hh and lh mixing[3]. It can be seen that the P_L enhances as A is changed from 0.1 to 0.3 and 0.5 which can be attributed to the fact that the anisotropy increases the valence subband mixing effects leading to enhanced degree of linear polarization.

4. Conclusions

We have studied the effect of magnetic field on the electronic structure and optical properties of strained $Zn_{1-x}Cd_xSe$ QDs. Zeeman splitting of energy levels is seen which enhances with increase in magnetic field. This splitting is found to be more for anisotropic QDs. The degree of linear polarization is also seen to increase with magnetic field and is higher for the anisotropic QDs. These features are explained in terms of valence subband mixing which gets accentuated by the magnetic field.

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