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Magneto-optical analysis of anisotropic CdZnSe quantum dots

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ABSTRACT

The effect of magnetic field and geometrical anisotropy on electronic and optical properties of self-assembled CdZnSe quantum dots is theoretically investigated. The Luttinger Hamiltonian formulation has been used in a transformed coordinate system for obtaining the energy eigenvalues and wavefunctions for the holes. The variation of energy eigenvalues with the magnetic field has been studied for anisotropic quantum dots. The degree of linear polarization is also calculated and is found to increase with magnetic field which is explained in terms of anisotropy induced valence subband mixing.

1. Introduction

Self-assembled semiconductor quantum dots (QDs) are gaining importance due to a wide variety of applications in optoelectronic devices [1] and their promise as future candidates for quantum computation [2]. Quantum computation applications based on spins of electrons 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 [3].

The spin state of a QD is determined to a large extent by exchange and spin–orbit interactions which depend strongly on the symmetry of the QD confining potential [4–6]. The precise information about the spin polarization of the system can be obtained from the study of optical anisotropy of the PL spectra of 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. In addition, it enhances the confinement of the carriers in the QDs. High magnetic fields provide powerful means to study the electronic structure of QDs. Magneto-optical studies of a variety of QD systems have revealed a wealth of information regarding the discrete character of energy spectrum, Zeeman splittings, spin–flip transitions, and spin-relaxation times which exhibit a strong dependence on the interplay of QD size, geometrical anisotropy and externally applied fields [7–16].

The theoretical analysis of the effect of magnetic field for laterally isotropic quantum dots has been carried out widely [17–20]; however, a systematic study for anisotropic QDs is important as the Stranski–Krastanov QDs often display elliptic shape in the plane perpendicular to the growth axis which in turn significantly enhances the spin–orbit coupling [21,22].

The objective of this paper is to develop a theoretical approach to analyze the effect of magnetic field on the electronic structure and optical anisotropy of $Zn_{1-x}Cd_xSe/ZnSe$ QDs with different geometric profiles due to the in-plane asymmetry. The disk-shaped QD is modeled by anisotropic parabolic potential with the magnetic field considered in Faraday geometry. The confinement potential for electrons (holes) in a QD is decided by the conduction (valence) band offset between the barrier and the QD material, which is significantly modified due to the strain effects. Strain alters the bandgap, the splitting between heavy and light holes, the hole masses and the density of states [23,24]. The strain effects along with the valence subband mixing are incorporated through Bir Pikus Hamiltonian [25,26].

Furthermore, the existing TEM data indicate that there can be a considerable interdiffusion in this system, and in many cases the dots actually consist of CdZnSe alloy rather than CdSe which needs to be included for a thorough understanding of the experimentally observed QD features [10,27]. The diffusion of Zn in the Cd islands has been considered with a typical value of Cd content chosen to be 40% [27,28].

The multiple band Hamiltonian in presence of magnetic field can be solved by constructing the Hamiltonian matrix in the

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Hilbert space of generalized Laguerre polynomials for cylindrically symmetric QDs [19] or Hermite Gaussian functions for QDs with significant in-plane anisotropy [29]. However, due to slow convergence for the basis used in Ref. [29] for anisotropic QDs, we have worked with the canonical transformations suggested by Madhav and Chakraborty [30] 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 faster convergence obtained with the transformed coordinates facilitates more detailed analysis with moderate computational resources. The eigenvalues and eigenvectors thus obtained are utilized for obtaining the dipole matrix elements. Hence, the degree of linear polarization has been studied for the anisotropic QDs. It is found to increase with magnetic field and anisotropy parameter. The results have been explained in terms of the spin–orbit coupling effects. The details of the Hamiltonian formulation and the techniques used for diagonalization are discussed in Section 2. The results of the numerical computations are analyzed in Section 3.

2. Theoretical formulations

The disc shaped anisotropic $Zn_{1-x}Cd_xSe/ZnSe$ quantum dot as shown in Fig. 1 is modeled using a quantum well confinement potential, $V_z(z)$ along the z-axis (which is taken to be the growth direction) and a parabolic confinement $V_{xy}(x,y)$ in the plane perpendicular to the growth axis (x–y plane).

The in-plane confinement V_{xy} is defined by the anisotropic parabolic potential

$$V_{xy}(x,y) = \tfrac{1}{2}\alpha_x x^2 + \tfrac{1}{2}\alpha_y y^2. \tag{1}$$

The parameters $\alpha_{x,y}$ depend upon the strength and anisotropy of in-plane confinement, and are determined by various factors including the extent of interdiffusion of the barrier ions in the quantum dot, valence band offsets, hydrostatic and biaxial strain, size and shape anisotropy of the QD.

The variation of the composition x of the QD material modifies the energy band gap as [31] $E_g(x) = E_{gCdSe} + (E_{gZnSe} - E_{gCdSe} - b)x + bx^2$ where b is the bowing parameter. The other parameters for $Zn_{1-x}Cd_xSe$ are obtained from a linear interpolation of the ZnSe and the CdSe parameters: $p(Zn_{1-x}Cd_xSe) = (1-x)p(ZnSe) + xp(CdSe)$, where p indicates the various physical parameters used in our calculations.

The interplay of quantum confinement and strain leads to significant modification of the electron and hole energy levels in $Zn_{1-x}Cd_xSe/ZnSe$ QDs. The quantum confinement potential is determined by the band offset between $Zn_{1-x}Cd_xSe$ QD and ZnSe barrier. The band offset for the conduction band is much larger than that for the valence band. Thus, when strain effects are included in the formalism, there is a change in confinement energies for both the conduction and valence bands. 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 and resulting doubly degenerate heavy and light hole subbands. The hydrostatic deformation shifts the heavy and light hole 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 [32,33]. The shifts of the conduction band, heavy hole (hh) and light hole (lh) band edges due to the hydrostatic and biaxial deformation of the strained $Zn_{1-x}Cd_xSe/ZnSe$ QD are given by

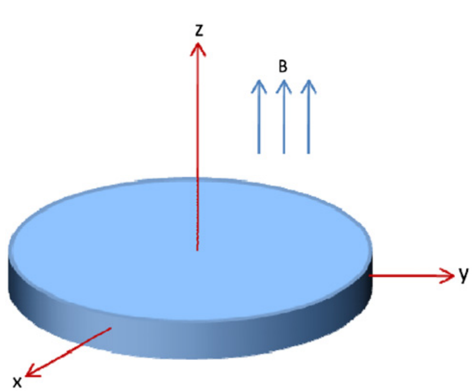

Fig. 1. The quantum dot geometry (color online).

$$\delta E_c = 2D_c\left[\frac{C_{11}-C_{12}}{C_{11}}\right]\varepsilon, \tag{2a}$$

$$\delta E_{hh} = \left[-2D_{v1}\frac{C_{11}-C_{12}}{C_{11}} + D_{v2}\frac{C_{11}+2C_{12}}{C_{11}}\right]\varepsilon, \tag{2b}$$

$$\delta E_{lh} = \left[-2D_{v1}\frac{C_{11}-C_{12}}{C_{11}} - D_{v2}\frac{C_{11}+2C_{12}}{C_{11}}\right]\varepsilon, \tag{2c}$$

where D_c and D_{v1} are the hydrostatic deformation potentials for the conduction and valence band, respectively, D_{v2} is the biaxial deformation potential, C_{11} and C_{12} are the elastic stiffness constants and ε is the elastic strain defined as

$$\varepsilon = \frac{a_L(Zn_{1-x}Cd_xSe) - a_L(ZnSe)}{a_L(ZnSe)}, \tag{3}$$

where a_L is the lattice parameter. Here, we have assumed that the CdZnSe QD grows pseudomorphically on the ZnSe barrier material. The total hydrostatic deformation potential is shared between the conduction and the valence band with D_c being twice as large as D_{v1} [24].

The electronic structure of the quantum dot can be obtained by solving the Luttinger Hamiltonian given by [19,34]

$$H = \begin{bmatrix} H_{hh}+3\beta & S & R & 0 \\ S^{\dagger} & H_{lh}-\beta & 0 & -R \\ R^{\dagger} & 0 & H_{lh}+\beta & S \\ 0 & -R^{\dagger} & S^{\dagger} & H_{hh}-3\beta \end{bmatrix}. \tag{4}$$

The individual matrix elements are given by

$$H_{hh} = \frac{1}{2m_0}\left[(\gamma_1-2\gamma_2)P_z^2 + (\gamma_1+\gamma_2)(P_x^2+P_y^2)\right] + V_z(z) + V_{xy}(x,y) + \delta E_{hh}, \tag{5a}$$

$$H_{lh} = \frac{1}{2m_0}\left[(\gamma_1+2\gamma_2)P_z^2 + (\gamma_1-\gamma_2)(P_x^2+P_y^2)\right] + V_z(z) + V_{xy}(x,y) + \delta E_{lh}, \tag{5b}$$

$$R = \frac{\sqrt{3}}{m_0}\gamma_3 P_z(P_x - iP_y), \tag{5c}$$

and

$$S = \frac{\sqrt{3}}{2m_0}(\gamma_2(P_x^2-P_y^2) - 2i\gamma_3 P_x P_y), \tag{5d}$$

where $\beta = \kappa\mu_B B$, γ_1, γ_2 and γ_3 are the Luttinger parameters, κ is the hole g-factor, μ_B is the Bohr magneton and m_0 is free electron mass [32]. Here, we have considered the externally applied magnetic field in Faraday geometry and adopted Coulomb gauge