Spin Relaxation in Mn doped CdTe/ZnTe QDs

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Abstract. The spin relaxation times of the electron have been calculated for phonon assisted transitions between the Zeeman sublevels arising as a result of magnetic impurity doping and applied magnetic field in Mn doped CdTe/ZnTe quantum dots. Taking into account effective mass approximation with four band k.p perturbation theory and incorporating the sp-d exchange interaction, the energies of the split states have been obtained and analyzed with magnetic field and effective concentration. The spin relaxation times have been found to be considerably longer with higher dopant concentration in high magnetic fields at very low temperature.

1. Introduction
In the recent years, spin dynamics in semiconductor nanostructures has drawn considerable attention due to the enormous potential for spintronics devices.[1] Semiconductor quantum dots (QDs) doped with transition metal (TM) ions form a new class of materials called diluted magnetic semiconductors (DMS), which appear to be promising candidates for the spintronics devices because of their ability to control single spin carriers. The DMSs exhibit interesting magnetic, optical and magneto-optical properties such as large Faraday rotation, giant Zeeman splitting etc with many practical applications in spin transport, spin filtering, charge-controlled magnetism, etc [1, 2]. Such magneto-electronic phenomenon in the DMS QDs is attributed to the exchange interaction between the magnetic moments of the dopant TM ions and electron or hole spins of the host semiconductor [2, 3]. Moreover, quantum confinement effects in semiconductors significantly enhance the sp-d exchange interactions. This enhancement can be ascribed to the strong overlapping of the carrier wave functions in the TM ion doped QDs. As a consequence, the spin-splitting is enhanced manifold in DMS QDs in the presence of magnetic field.

In II-VI semiconductor QDs, the optical transitions between the electron and heavy hole bands are polarization sensitive. The spin-up and spin-down electrons in the conduction band can be created by exciting the QD with right and left circularly polarized light, respectively. The spin dephasing from the Zeeman sublevels generates circularly polarized light with distinct phase shifts. In this article, we have theoretically calculated the spin relaxation times in CdTe/ZnTe QDs doped with Mn. The spin flipping is considered to be longitudinal optical (LO) phonon mediated transition between the spin-split Zeeman states. The numerical analysis has been carried out for Mn doped CdTe/ZnTe QDs.

2. Theoretical Formulation
The DMS QDs are considered to experience parabolic axial confinement $V_z$ and a step like $V_{\text{II}}$ confinement along the growth axis such that the total confinement potential is given by $V_{\text{tot}}(\rho, z) = V_z + V_{\text{II}}$ where

$$V_z(\rho) = \frac{1}{2}m^*\omega_0^2\rho_1^2$$

(1)
and

\[ V_i^+(z_i) = \begin{cases} \Delta V_i', & |z_i| \geq w/2, \\ 0, & |z_i| < w/2, \end{cases} \] (2)

The superscript \(i\) represents electron (e) or hole (h). \(\rho_i\) and \(z_i\) are the cylindrical coordinates, \(m_i\) represents the effective masses, \(\omega_i\) corresponds to the oscillator frequencies and \(\Delta V_i'\) refers to the conduction \((i = e)\) and valence \((i = h)\) band offset. Also, \(w\) is the width of the potential well. Under the effective mass approximation, the electron and hole wave functions for the above mentioned confinement can be written as [4]

\[ \Psi_i^+(\rho_e, z_e, \phi) = \sum_{n_z} c_{n_z} \psi_{s, n_z}(\rho_e, \phi) f_n(z_e) u_s(\rho_e, z_e) \] (3a)

\[ \Psi_i^-(\rho_h, z_h, \phi) = \sum_{j_z} c_{j_z} \psi_{s, j_z}(\rho_h, \phi) f_j(z_h) u_j(\rho_h, z_h) \] (3b)

Here, \(c_{n_z}\) and \(c_{j_z}\) are the constants of normalization for the electron and hole, respectively with \(n\) and \(s\) being the principal and spin-quantum numbers, respectively. Also, \(j\) and 1 are the angular momentum quantum numbers for electron and hole, respectively and \(j_z = \pm 3/2, \pm 1/2\) corresponds to the hole spin. \(u_s(\rho_e, z_e)\) and \(u_j(\rho_h, z_h)\) are the Bloch functions for electron and hole, respectively. In eq. (3) \(f_n(z_e)\) is the wave function arising due to the step like confinement potential of the form [7]

\[ f_n(z_e) = \frac{\sqrt{2}}{L} \sin \left( \frac{n'\pi}{2} \left( z_e + \frac{L}{2} \right) \right); |z_e| \leq L/2 \] (4)

In eq. (4), \(q = (1, 2, \ldots, \ldots)\) represents the band index number arising due to the \(z\)-confinement. The envelope function due to parabolic confinement potential slowly varying over the nanodimensions of the QD is defined as

\[ \psi_{n_z}(\rho, \phi) = C_{n_z}(\rho) \frac{1}{\sqrt{\pi a_z^n}} H_{n_z}^{(1)}(\rho^{2} / a_z^2) \] (5)

where \(C_{n_z} = \frac{\pi^{n_z+1}}{\Gamma(n_z+1)} \left( \frac{1}{a_z} \right)^{n_z+1} \) is the normalization constant; \(a_z = \left( \frac{\hbar}{m_e^{*} w} \right)^{1/2}\) is the geometrical confinement length parameter that incorporates the effects of both geometrical and magnetic confinements which influence the electronic spectra. \(\lambda_z = (\hbar / m_e^{*} \omega_i)^{1/2}\) is the geometrical confinement length and \(a_z = (\hbar / eB)^{1/2}\) is the cyclotron radius. Also, \(H_{n_z}^{(1)}\) is the generalized Laguerre polynomial. The electron Hamiltonian in the TM impurity doped QD in presence of the magnetic field \(B\) (applied along the \(z\)-direction) is described by

\[ H_e = \frac{\hat{\mathbf{P}}^2}{2m_e^{*}} + V_e(\rho, \phi, z) + J_{\rho, z} \mathbf{S} \cdot \mathbf{\sigma} + \frac{1}{2} g_e^{*} \mu_B B \] (6)

where \(\mathbf{A}\) is the vector potential in the symmetric gauge, \(g_e^{*}\) and \(\mu_B\) are the effective g-factor for the electron and Bohr magneton, respectively. \(\mathbf{S}\) is the spin of the magnetic ion and \(\mathbf{\sigma}\) is the pauli spin corresponding to the spin of the conduction band electron. The second term in Eq. (6) represents the geometrical confinement potential; the third term describes the exchange interaction between the conduction band electron and the magnetic impurity ions while the last term gives the Zeeman splitting.

Taking into account four-band \(k\vec{p}\) approximation in the Luttinger Hamiltonian \(H^L\) for the hole states, the hole Hamiltonian \(H_h\) in the presence of magnetic field and confinement potential for a DMS QD can be written as

\[ H_h = H_L + V_h^+(\rho_h, z_h) + J_{\rho, z} \mathbf{S} \cdot \mathbf{\sigma} - \frac{\epsilon_B}{m_h} \mathbf{S} \cdot \mathbf{\sigma} \] (7)

where \(m_o\) being the rest mass of the electron. In Eq. (7), last term refers to the Zeeman splitting energy and the last term stands for the p-d exchange interaction between the carriers of p-subband and Mn2+ ions. This exchange interaction is expressed within the molecular field approximation for electron and hole as
\[ H_{ex} = J_{s-d} x_{d} N_{o} \alpha / 2 \quad \text{and} \quad J_{p-d} = x_{d} N_{o} \beta / 2 ; \quad N_{o} \] being the number of cations per unit volume and x is the effective concentration of TM ions contributing to the exchange interaction in the quantum dot [5]. \( \alpha \) and \( \beta \) are the exchange constants for s-d and p-d exchange interactions, respectively. \( \langle S_{x} (X) \rangle = \langle S_{y} B(X) \rangle \) is the thermodynamical average of the spin component along the magnetic field B where \( \hat{X} = S_{x} B / k_{B} (T + T_{s}) \). \( g_{ms} \) being the effective Lande g-factor for transition metal ions and S is the spin of the localized d-electrons of the TM ions and BS (X) is the Brillouin function describing overall paramagnetic behavior of the magnetization at temperature T [5]. S0 and T0 are the fitting parameters accounting for magnetism arising due to TM-TM ionic interaction.

The spin relaxation rate of the electron has been calculated from the Fermi Golden Rule, considering electron spin-phonon coupling and is given by

\[ \frac{1}{\tau_{s}} = W_{S} = \frac{8 \pi \mu_{e}^{2} \Delta \omega^{3}}{3 \hbar c_{l}^{3}} \left( \frac{1}{\varepsilon_{s}} - \frac{1}{\varepsilon_{e}} \right) \]

where \( c_{l} \) is the longitudinal sound velocity, \( \Delta \omega \) is the transition frequency between the Zeeman sublevels defined as \( \Delta \omega = E_{x}^{+} - E_{h}^{+} \). \( E_{x}^{+} \) and \( E_{h}^{+} \) are the electronic and heavy hole energies of the system, respectively. \( \varepsilon_{s} \) and \( \varepsilon_{e} \) are the high frequency and static dielectric constants. Also, \( \mu_{0} \) is the induced dipole moment for the transitions between the spin split states given by

\[ \mu_{0} = \frac{e p_{e}}{m_{e} \Delta \omega} \int \psi_{x}^{*} (\rho_{e}, \phi) f_{e} (z_{e}) \psi_{x} (\rho_{s}, \phi) d \tau \]

Here, \( p_{e} = \langle u_{e} (\rho_{e}, z_{e}) | \hat{p} | u_{e} (\rho_{s}, z_{h}) \rangle \) is the interband momentum matrix element.

3. Conclusions

In this section we have studied the effect of magnetic field and TM concentration on the transition frequency and the spin relaxation times between the spin-split Zeeman sublevels in Cd1-xMnxTe/ZnTe QD using the formulation developed in section 2. The material parameters used in the present numerical analysis are: \( m_{e} = 0.096 m_{0} \) [7], the conduction (valence) band offset \( \Delta V_{c} \left( \Delta V_{v} \right) \) is 0.85 eV (0.05 eV) [6]. Luttinger parameters under spherical approximation are taken as \( \gamma_{1} = 4.7, \gamma_{2} = 1.45 \) and \( \gamma_{3} = 1.9 \) [6] while the exchange constants \( N_{o} \alpha \left( N_{o} \beta \right) \) are 0.22 eV (-0.88 eV) [2].

![Figure 1. Transition frequency as a function of magnetic field at effective concentration (x = 0, 0.01, 0.02).](image-url)
Figure 1. Variation of spin relaxation time with effective Mn concentration at B = 1 T and 5 T for Mn-doped CdTe/ZnTe quantum dots at 1.5 K.

Lande g-factor for electron $g_e = 1.12$ [2] and for Manganese $g_{Mn} = 2.0$, spin quantum number of 3d electrons S = 5/2. The speed of sound of LO phonons $c_i = 3083$ m/s [7] and high frequency and static dielectric constants are $\varepsilon_\infty = 10.9$ and $\varepsilon_0 = 7.1$. [7]

We have considered very small DMS QDs in the strong confinement regime with both magnetic field and geometrical confinements influencing the optical properties of the QDs. The dimensions of the cylindrical QDs are taken to be of 1.25 nm radius and 1.5 nm height (under strong confinement limit). In Fig. 1, the transition frequency has been plotted as a function of magnetic field for undoped ($x = 0.0$) and Mn$^{2+}$ doped ($x = 0.01, 0.02$) CdTe/ZnTe. It is clear from this figure that the transition frequency increases with increasing magnetic field and dopant concentration. Since the Zeeman splitting enhances with increasing magnetic field and Mn concentration due to the presence of strong sp-d exchange interaction. Hence, the transition energy between the Zeeman sublevels also increases.

The spin relaxation time has been plotted with increasing Mn concentration. Longer spin relaxation time has been observed in Mn doped QDs as compared to undoped QDs. Also, it is evident from Fig. 2 that the spin relaxation time increases with increasing magnetic field. The effect of dopant concentration is also apparent from the figure. We have obtained 1.24 ns of spin relaxation time for a small concentration of 0.003 mol % at 1T field and 1.5 K temperature which is in agreement with Worschech et al. [3]

In conclusion, the incorporation of TM ions into the semiconductor QDs enhances the spin relaxation time of the electron for the transition between the Zeeman sublevels.

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5. References
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