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Spin polarization and spin-dependent transmittance in II–VI diluted magnetic semiconductor heterostructure

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ABSTRACT

In this work, we carried out detailed investigation of a $Cd_{1-x}Mn_xTe/CdTe/Cd_{1-x}Mn_xTe$ diluted magnetic semiconductor based quantum well. Our theoretical results are based on an accurate self-consistent resolution of the one-dimension Schrödinger and Poisson's equations in the framework of the mean-field approximation for spin-up and spin-down orientations of carriers coupled via the sp–d exchange interaction. From the calculation of spin-dependent carrier densities for ferromagnetic and anti-ferromagnetic coupling, we evidence the spin-up and spin-down space separation for holes in quantum well for different values of band offsets. From deduced spin polarizations, we show that the CdTe region acts as a layer of spin rearrangement and spin reversal, respectively, in the ferromagnetic and anti-ferromagnetic coupling. The transmittance coefficients T_+ and T_- of injected spin-up and spin-down carriers are evaluated as a preliminary work to *assess* the spin-dependent currents in devices consisting of alternatively layers of non-magnetic and diluted magnetic semiconductors.

1. Introduction

Diluted magnetic semiconductors (DMSs) also known as semi-magnetic semiconductors, are a wide class of materials in which a fraction of the original semiconductor atoms are substituted by magnetic atoms. Combining magnetic ordering with properties of semiconductors, they are generally considered key ingredients of spin-related devices and lead to many striking new effects. Extensive experimental and theoretical investigations have been devoted to these compounds since they are natural materials-of-choice for spintronics and other spin-related ultra-fast magneto-optic applications like spin-light emitting diodes [1], magnetic tunnel junctions [2], spin-resonant tunneling diodes [3] or spin-field effect transistors [4]. They have shown many impressive effects such as the giant Faraday effect [5,6], formation of magnetic polarons [7,8] or magnetic field induced metal–insulator transitions [9]. The ternary nature of DMSs makes it possible to alter their material parameters, such as the band gap and/or the lattice constant by varying the composition, i.e., the content of magnetic atoms. This ability to fine-tune lattice parameters of the DMS crystals has allowed researchers to grow quantum wells (QWs) and superlattices in order to investigate new magnetic effects related to low dimensional phenomena [10,11]. Recently, several types of DMS quantum structures have been fabricated [12]. III–V ferromagnetic DMSs has attracted interests and enjoyed rapid progress [1,13]. However, in these DMS, the same impurity (Mn) carries the localized spins and acts as an acceptor, which puts strong limits on the realization of QWs and two dimensional systems [14,15]. On the contrary, II–VI semiconductors form, with II–IV–V_2 [16–18] ones, the unique systems where Mn is an isoelectronic magnetic impurity; so that carrier density can be controlled independently of magnetic ion concentration. In particular, modulation doping can be used to introduce a 2D electron or hole gas in a quantum well containing a diluted magnetic semiconductor. In addition to the bias-control of magnetic order, to change the carrier density one can also use illumination and even thermally-excited carriers to promote the magnetic order and enhance the magnetization [19–21]. Furthermore, in Mn:II–VI quantum dots, it may even be possible to reversibly control magnetization without any change in the carrier density [22]. Moreover, the lattice mismatch between II–VI semiconductor layers and magnetic layers is relatively small. Thus the epitaxial growth with high crystalline characteristics is possible. Consequently, the most extensively studied DMSs are II–VI semiconductors and transition metal alloys, particularly those containing manganese. Finally, the digital doping of the anti-ferromagnetic MnTe [23] layers with a Neel temperature of 310 K [24] and the paramagnetism of II–VI DMS [25] layers were reported. Even better, a single Mn-ion has been controllably added to II–VI quantum dots [26]. In recent years, there have also been intensive studies of DMSs containing other transition-metals, such as iron [27] and cobalt [28].

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For a systematic exploitation of the carrier spin orientation, e.g., in devices with polarization selective optical properties, it is necessary to understand the dynamics of the carrier spins. In our paper, we focus our attention on the $Cd_{1-x}Mn_xTe$ alloy, which has shown a ferromagnetic phase. Nevertheless, although the existence of a ferromagnetic phase in DMS is experimentally well established [29–31], the physical origin of this phenomenon is not yet well understood [13,32].

Zener [33] first proposed the model of ferromagnetism driven by the exchange interaction between carriers and localized spins. However, this model was later abandoned, both the itinerant character of the magnetic electrons and the quantum oscillations of the electron spin polarization around the localized spins were neglected. It is now established that these effects are critical issues for the theory of magnetic metals. The indirect Ruderman–Kittel–Kasuya–Yosida (RKKY) approach [34], which successfully explains the ferromagnetism observed in magnetic metals, can be applied to the case of magnetic semiconductors. In fact, since its discovery, the RKKY exchange interaction between localized magnetic impurities embedded in a host metal has played an important role in the theory of magnetism. We emphasize that in the case of semiconductors, however, the effect of the Friedel (quantum) oscillations averages to zero because the mean distance between the carriers is greater than that between the spins. In such a case, the Zener model becomes equivalent [35] to the approach developed by RKKY, in which the presence of the oscillations is taken explicitly into account.

In this work, we study the magnetic properties of heterostructures formed by Mn-based magnetic layers of thickness d_m separated by non-magnetic layers of thickness d_p in the framework of the mean-field approximation. To simplify the presentation of the methodology, although our conclusions are not restricted to any material, we assume that the DMS region is CdMnTe and the non-magnetic semiconductor region is CdTe. After the introduction in Section 1, we provide in Section 2, the formulation of the equations involved and briefly describe the calculation method. Numerical results are presented and discussed in Section 3 followed by conclusions in Section 4.

2. Computational method theory

We consider the $Cd_{1-x}Mn_xTe/CdTe/Cd_{1-x}Mn_xTe$ quantum heterostructure, where carrier spins interact with the localized magnetic moments of the Mn ions via the sp–d exchange interaction. Fig. 1 shows the potential profile of the multilayer heterostructure under consideration. In general way, the DMS systems are described by the following Hamiltonian:

$$H = H_h + J\sum_{I,i} S_I s_i \delta(r_i - R_I) + W\sum_{I,i} n_i \delta(r_i - R_I) \tag{1}$$

Let us analyze the three terms contributing to H. H_h is the part of Hamiltonian, which describes the itinerant carriers (holes). It is the sum of kinetic energy of holes treated in the framework of the envelope function approximation and the hole–hole interaction energy. The second term proportional to J is the anti-ferromagnetic exchange interaction S_I between the magnetic ion spin (Mn^{2+} ions) at the site R_I and the spins s_i of the itinerant carriers with r_i coordinate. The last term is an interaction between the carrier charge n_i and the potential arising from the magnetic dopants. The origin of W is the difference in electro-negativity between the Mn and the CdTe atoms. We note here that in CdMnTe based heterostructures, J is anti-ferromagnetic. Indeed, the hybridization coupling is anti-ferromagnetic and is more important than the ferromagnetic exchange due to the Coulomb interaction. As J is expressed in eV cm^3, we use the product JN_0, where $N_0 = 1/\Omega$, e.g. the number of the elementary cells of volume Ω (volume units), to describe the s–d and p–d coupling for a given material. In the case of CdMnTe, $JN_0 = \alpha N_0 = 0.22$ eV for conduction electrons and $JN_0 = \beta N_0 = -0.88$ eV for valence-band holes where $\alpha = \langle \psi_e | J | \psi_e \rangle$ and $\beta = \langle \psi_t | J | \psi_t \rangle$.

Eq. (1) is solved in the mean-field approximation where the local magnetic interaction of the spin carriers with the Mn spins is substituted by the interaction with an effective magnetic field of intensity $V_c = (S_I Jx)/a^3$ [36] where a^3 represents the unit cell volume of the host semiconductor. Furthermore, in the same model, the electro-negativity difference between the Mn and the CdTe atoms produces a potential discontinuity, $V_w = (Wx)/a^3$ between the Mn doped semiconductor and the undoped semiconductor. Since there is no reliable experimental information on the value of W, we consider it as a parameter in the range $0 \le W \le J$. We use the mean-field approximation by inserting the mean value of Mn spin in the z direction.

Within this approach, in our heterostructure, the holes are free to move in the (x,y) plane and the one-particle wave functions and eigenvalues have the following forms:

$$\Phi^{F(AF)}_{i,k,\pm} = \frac{\exp j(k_\perp r_\perp)}{\sqrt{S}} \varphi^{F(AF)}_{i,\pm}(z) \quad E^{F(AF)}_{i,k,\pm} = \frac{\hbar k_\perp^2}{2m_\perp} + \varepsilon^{F(AF)}_{i,\pm} \tag{2}$$

here S is the areal dimension of the sample, $r_\perp$ and $k_\perp$ are the position and the momentum of the carriers, respectively, in the plane perpendicular to the growth direction, i is a subband index, $m_\perp$ is the effective mass in the in-plane motion, perpendicular to the growth direction. $\varphi^{F(AF)}_{i,\pm}(z)$ and $\varepsilon^{F(AF)}_{i,\pm}$ are obtained from the one dimensional Schrodinger equation

$$H_h \varphi^{F(AF)}_{i,\pm}(z) = \frac{\hbar^2}{2m^*}\left(\frac{\partial^2}{\partial z^2} + V^{F(AF)}_{tot}(z)\right)\varphi^{F(AF)}_{i,\pm}(z) = \varepsilon^{F(AF)}_{i,\pm}\varphi^{F(AF)}_{i,\pm}(z) \tag{3}$$

where the indexes + and − refer to the carriers with spin-up and spin-down, respectively, F and AF stand for the solutions with ferromagnetic or anti-ferromagnetic coupling, respectively, between the DMS layers. m^* is the effective mass in the z direction, $V^{F(AF)}_{tot}(z)$ is the sum of the electrostatic potential $V^{F(AF)}_{elec}(z)$ and the effective potential $V^{F(AF)}_{\pm}(z)$ shown in Fig. 1 is obtained by the following form:

$$V^{F(AF)}_{\pm}(z) = \begin{cases} \mp V_c + V_w & \text{for} \quad 0 < z < d_m \\ 0 & \text{for} \quad d_m < z < d_m + d_p \\ \mp C_{F(AF)} V_c + V_w & \text{for} \quad d_m + d_p < z < 2d_m + d_p \\ \infty & \text{otherwise} \end{cases} \tag{4}$$

C_{F-AF} is + (−) in the F–AF coupling case.

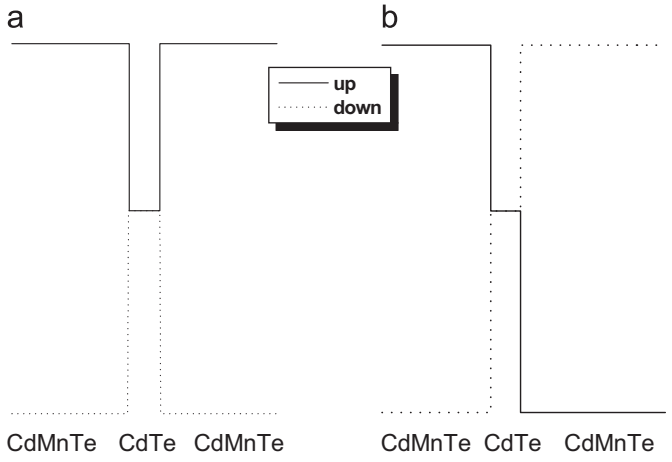

Fig. 1. Potential profiles for spin-up and spin-down in the ferromagnetic (F) and anti-ferromagnetic (AF) configurations, respectively, for a tri layers quantum well.