Spontaneous Magnetization in Diluted Magnetic Semiconductor Quantum Wells

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A diluted magnetic semiconductor (DMS) quantum well is an interesting system for exploring spintronic applications. We calculated the spontaneous magnetization (SM) in a 100-Å $\text{Ga}_{1-x}\text{Mn}_x\text{As}/\text{Al}_{0.35}\text{Ga}_{0.65}\text{As}$ quantum well. The Schrodinger equation was described by a 4×4 Luttinger Hamiltonian in the envelope function approximation with the exchange interaction between Mn ions and holes treated in the mean-field approximation. The Schrodinger-Poisson-DMS self-consistency was solved by using the finite element method. We studied how the SM depended on the hole concentration p , the temperature T , the effective Mn concentration x_{eff} , the antiferromagnetic temperature T_{AF} , and the exchange integral βN_o . For $T = 0$ K, $x_{\text{eff}} = 0.05$, $T_{\text{AF}} = 0.5$ K, and $\beta N_o = -1.2$ eV, the SM begins to appear at $p = 5 \times 10^{17} \text{ cm}^{-3}$ and saturates around $3 \times 10^{19} \text{ cm}^{-3}$. For $p = 10^{18} \text{ cm}^{-3}$, the SM disappears around 5 K.

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I. INTRODUCTION

Since successful Mn doping in III-V semiconductors such as InAs [1] and GaAs [2], there has been a considerable interest in diluted magnetic semiconductors (DMS) for both fundamental physics and spintronic applications [3–6]. Since the realization of GaAs/AlGaAs quantum wells (QW) in 1974 [7], the QW has been utilized in electronic and optoelectronic devices through bandgap engineering [8] and wavefunction engineering [9]. Thus, a combination of DMS and QW is an interesting subject to study [10, 11]. The QW structure also can be used to enhance the exchange interaction responsible for ferromagnetism in DMS by localizing holes around Mn ions.

In this paper we calculated the spontaneous magnetization (SM) in a 100-Å $\text{Ga}_{1-x}\text{Mn}_x\text{As}/\text{Al}_{0.35}\text{Ga}_{0.65}\text{As}$ QW. The Schrodinger equation was described by a 4×4 Luttinger Hamiltonian [12] in the envelope function approximation [13] with the exchange interaction between Mn ions and holes treated in the mean-field approximation. The Schrodinger-Poisson-DMS self-consistency was solved by using the finite element method [14]. We stud-

ied how the SM depended on the hole concentration p , the temperature T , the effective Mn concentration x_{eff} , the antiferromagnetic temperature T_{AF} , and the exchange integral βN_o .

II. THEORY

Holes in a quantum well are described in the envelope function approximation by [13]

$$[H_{\mathbf{k}\cdot\mathbf{p}}(z) + V_o(z) + V_{ch}(z) + V_{xc}(z) + H_{\text{DMS}}(z)]f(z) = Ef(z). \quad (1)$$

The $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian $H_{\mathbf{k}\cdot\mathbf{p}}$ used is the valence 4×4 Luttinger Hamiltonian modified to correctly account for the boundary condition at the heterointerface [15]. V_o is the band offset potential, and V_{ch} is the potential due to ionized acceptors and free holes governed by the Poisson equation:

$$\begin{aligned} \frac{d}{dz} \frac{1}{\epsilon(z)} \frac{dV_{ch}(z)}{dz} &= \rho_A + \rho_p \\ &= \rho_A + \int dE D(E(\mathbf{k}_{||})) |f_{\mathbf{k}_{||}}(z)|^2 \\ &\times \frac{1}{\exp((E - E_F)/k_B T) + 1}. \end{aligned} \quad (2)$$

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We assumed that the charge density ρ_A due to ionized acceptors was uniform in the well region, and the density of states $D(E)$ to calculate the hole charge density ρ_p was numerically calculated from the in-plane dispersion $E(\mathbf{k}_{||})$. E_F , k_B , and T are the Fermi energy, the Boltzmann constant, and the temperature, respectively. We adopted the exchange-correlation potential V_{xc} in the local density approximation from Gunnarsson and

Lundqvist [16].

The exchange interaction between Mn ions and holes was obtained by considering the thermodynamics of the magnetic polarons [17] in the virtual crystal approximation and the mean field approximation. The details of the derivation will be published elsewhere. The final 4×4 DMS Hamiltonian is

$$H_{DMS} = \begin{pmatrix} b_{DMS}/2 & 0 & 0 & 0 \\ 0 & b_{DMS}/6 & 0 & 0 \\ 0 & 0 & -b_{DMS}/6 & 0 \\ 0 & 0 & 0 & -b_{DMS}/2 \end{pmatrix}, \quad (3)$$

where

$$b_{DMS} = -\beta N_o x_{eff} S B_S(\xi), \quad (4)$$

with

$$\xi = \frac{S(\beta N_o)}{2N_o k_B (T + T_{AF})} (\rho_- - \rho_+). \quad (5)$$

In the above, βN_o is the exchange integral for holes, x_{eff} is the effective Mn concentration [18], $S = 5/2$ is the spin of the Mn^{++} ion, B_S is the Brillouin function, $N_o = 4/a^3$ is the concentration of cation sites in a zinc-blende crystal with lattice constant a , T_{AF} is the antiferromagnetic temperature, and ρ_+ and ρ_- are the spin-up and the spin-down hole concentrations, respectively.

Since V_{ch} in Eq. (2) depends on the envelope function $f(z)$, we need to calculate the Schrodinger equation and the Poisson equation self-consistently. Furthermore, since V_{xc} and V_{DMS} depends on f_+ , the spin-up projection of f , and on f_- , we need a Schrodinger-DMS self-consistent calculation. The Schrodinger equation and the Poisson equation were solved by using the finite element method [14], and the Schrodinger-Poisson-DMS self-consistent calculation was performed in a way similar to the Schrodinger-Poisson self-consistency in Ref. [19]. The Fermi energy E_F in Eq. (2) is determined from the charge neutrality condition,

$$\int dz (\rho_A(z) + \rho_p(z)) = 0. \quad (6)$$

In the numerical calculation, we varied E_F as an input and chose E_F to satisfy Eq. (6).

In our model, the magnetization due to Mn alignment is given by

$$M(z) = g_{Mn} \mu_B x_{eff} N_o S B_s(\xi), \quad (7)$$

where $g_{Mn} = 2$ is the g -factor of Mn^{++} and μ_B is the Bohr magneton. If x_{eff} and p are sufficiently large, there

is a spontaneous magnetization without an external magnetic field.

III. RESULTS AND DISCUSSION

The calculation was done for a 100-Å $\text{Ga}_{0.95}\text{Mn}_{0.05}\text{As}/\text{Al}_{0.35}\text{Ga}_{0.65}\text{As}$ QW as an example. The input band parameters for GaAs and AlAs are taken from Ref. [20] and the binary parameters are linearly interpolated. The stable form of MnAs is the NiAs structure, and few parameters are known for zinc-blende MnAs, except the lattice constant [1,21]. Therefore, we used the GaAs band parameters for the $\text{Ga}_{0.95}\text{Mn}_{0.05}\text{As}$ layer. In III-V semiconductors, the antiferromagnetic ordering between Mn ions is known to be small so that x_{eff} is approximately the same as the nominal Mn concentration, and T_{AF} is close to 0 K [5]. We used $x_{eff} = 0.05$ and $T_{AF} = 0.5$ K. The exchange integral βN_o is taken to be -1.2 eV [22]. We will discuss how SM depends on these parameters later in this section. The input material parameters are summarized in Table 1.

In III-V semiconductors, Mn acts as an acceptor and the hole concentration depends on the Mn concentration; $x_{eff} = 0.05$ corresponds to $p = 1.11 \times 10^{21} \text{ cm}^{-3}$ if all the acceptors are ionized. However, in this calculation, we used the hole concentration as an input parameter independent of x_{eff} .

In Fig. 1, we show the SM as for various hole concentrations. The SM grows with the hole concentration and saturates to $3.20 \times 10^{17} \text{ eV T}^{-1} \text{ cm}^{-3}$ at about $p \approx 3 \times 10^{19} \text{ cm}^{-3}$. For $p = 5 \times 10^{17} \text{ cm}^{-3}$ and $1 \times 10^{18} \text{ cm}^{-3}$, only the 1st spin-down heavy-hole (hh) subband is occupied, and the shape of the SM resembles the shape of the 1st hh wavefunction. At $3 \times 10^{18} \text{ cm}^{-3}$, the SM has two peaks, reflecting the occupation of the 2nd hh band, and becomes almost flat at $1 \times 10^{19} \text{ cm}^{-3}$, where

Table 1. Input material parameters.

parameter	Ga _{0.95} Mn _{0.05} As	Ga _{0.35} Al _{0.65} As
Luttinger parameters		
γ_1	6.98	5.8530
γ_2	2.06	1.6260
γ_3	2.93	2.4015
valence band edge (eV)	0.0	-0.1855
equilibrium lattice constant (Å)	5.65325	5.65325
βN_o (eV)	-1.2	-
T_{AF} (K)	0.5	-

Fig. 1. Spontaneous magnetization for various hole concentrations at 0 K.

more spin down subbands are occupied. The magnetization saturates at $3 \times 10^{19} \text{ cm}^{-3}$, and the sign of the SM changes, reflecting occupation of the spin-up subbands, as in Fig. 1(b). The sign changes become more frequent for higher concentrations, as can be seen in Fig. 5 for $1 \times 10^{21} \text{ cm}^{-3}$.

Since the shape of the SM changes, it is difficult to represent the SM by one number. We plot the absolute

Fig. 2. Absolute value of the spontaneous magnetization at the center of the well as a function of the hole concentration. The solid and the dotted lines are calculated with and without the exchange-correlation energy.

value of the spontaneous magnetization at the center of the well as a function of the hole concentration in Fig. 2. The critical hole concentration at which the SM begins to exist seems to be around $5 \times 10^{17} \text{ cm}^{-3}$, but around this value of p , the Schrodinger-Poisson-DMS self-consistent calculation becomes very unstable, so we could not find a convergent solution. The SM rises fast around the critical hole concentration and shows a saturating behavior at high hole concentration. In Fig. 2, the solid line includes the exchange-correlation term V_{xc} while the dotted line is without V_{xc} . Since V_{xc} pushes the upper hole band with more holes further upward, it makes the difference $\rho_- - \rho_+$ larger, yielding a larger SM in the unsaturated range of p [23].

In Fig. 3, we show the SM at $p = 10^{18} \text{ cm}^{-3}$ for various temperatures. The SM decreases rapidly with increasing temperature. Fig. 4 shows the temperature dependence of the SM value at the center of the well, where SM becomes a maximum. As the figure shows, the maximum SM shows a decaying behavior rather than an abrupt transition. The SM seems to decay out around 5 K.

Fig. 3. Spontaneous magnetization for various temperatures at $p = 10^{18} \text{ cm}^{-3}$.

Fig. 4. Spontaneous magnetization at the center of the well as a function of the temperature for $p = 10^{18} \text{ cm}^{-3}$.

In Fig. 5, we show the SM as a function of the temperature for $p = 10^{21} \text{ cm}^{-3}$. At this large hole concentration, the Schrodinger-Poisson-DMS self-consistency is difficult to control, and we found that a small numerical round-off could easily build up. The shape of SM is rather complicated, and it is difficult to represent it by a number, but again the overall magnitude decays as the temperature increases. The SM does not change much above 70 K, and it does not seem to vanish. This needs further investigation.

We varied other parameters, such as T_{AF} , βN_o , and x_{eff} . The effect of increasing T_{AF} for $p = 10^{18} \text{ cm}^{-3}$ is similar to that of increasing T . If we plot the SM as a function of $T + T_{AF}$, we obtain almost the same curves whether we vary T or T_{AF} . This shows that, at least for this concentration, the effect of T in Eq. (5) is dominant even though T also enters in Eq. (2). There is some scatter in the reported value of βN_o , and we tried $\beta N_o = -1.0 \text{ eV}$ [24] and -3.3 eV [3]. The SM grows with the absolute

Fig. 5. Spontaneous magnetization for various temperatures for $p = 10^{21} \text{ cm}^{-3}$.

Table 2. Variation of spontaneous magnetization with βN_o and x_{eff} .

βN_o (eV)	SM ($\text{eV T}^{-1} \text{cm}^{-3}$)	x_{eff}	SM ($\text{eV T}^{-1} \text{cm}^{-3}$)
-1.0	2.76877×10^{17}	0.03	1.72019×10^{17}
-1.2	2.91427×10^{17}	0.05	2.91427×10^{17}
-3.3	3.19931×10^{17}	0.07	4.19508×10^{17}

value of βN_o , as expected. We also varied x_{eff} and found that the SM increased with increasing x_{eff} . The results for various βN_o and x_{eff} are summarized in Table 2.

IV. CONCLUSIONS

We have calculated the spontaneous magnetization in a p -doped 100-Å $\text{Ga}_{1-x}\text{Mn}_x\text{As}/\text{Al}_{0.35}\text{Ga}_{0.65}\text{As}$ QW. The Schrodinger equation was described by a 4×4 Luttinger Hamiltonian in the envelope function approximation with the exchange interaction between Mn ions and holes treated in the mean-field approximation. The Schrodinger-Poisson-DMS self-consistency was solved by using the finite element method. We studied how the SM depended on the hole concentration p , the temperature T , the effective Mn concentration x_{eff} , the antiferromagnetic temperature T_{AF} , and the exchange integral βN_o . For typical parameters of $T = 0 \text{ K}$, $x_{eff} = 0.05$, $T_{AF} = 0.5 \text{ K}$, and $\beta N_o = -1.2 \text{ eV}$, as p increases, the shape of SM gets complicated due to multi-subband occupation. In terms of its magnitude, the SM begins to appear at $p = 5 \times 10^{17} \text{ cm}^{-3}$ and saturates around $3 \times 10^{19} \text{ cm}^{-3}$. The exchange-correlation term enhances the SM by increasing the majority spin further. For $p = 10^{18} \text{ cm}^{-3}$, the SM decreases with increasing temperature and vanishes around 5 K. For $p = 10^{21} \text{ cm}^{-3}$, the SM becomes minimal around 70 K. At least at $p = 10^{18} \text{ cm}^{-3}$, increasing T_{AF} has almost the same

effect as increasing T . The SM increases with increasing x_{eff} and βN_o , as expected.

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