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Magnetic Phase Structure Study of Modulation-Doped III-V Dilute Magnetic Semiconductor Quantum Wells with Broken Spin Symmetry

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We present a self-consistent magnetic phase structure in modulation-doped dilute magnetic III-V semiconductor quantum wells (DMS QW). The temperature and the magnetic-field effects on the effective g-factor in the DMS QW are estimated, and a hysteretic behavior in the carrier-induced magnetism is demonstrated. possible ferromagnetic-paramagnetic phase transition is analyzed in terms of various material parameters of the quantum wells.

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tionIntroduction

A modulation-doped dilute magnetic semiconductor (DMS) quantum well (QW) is a two-dimensional electron gas (2DEG) in which the degree of spin symmetry is controllable by applying a homogeneous external magnetic field $\boldsymbol{B}$. By spatial modulation of the doping profile and the magnetic impurity concentration, DMS quantum structures can lead to a spin-polarized many-particle system and can exhibit a variety of unique properties which are absent in conventional non-magnetic structures [1–3]. A spin-polarized quantum well (SPQW) is a spin-symmetry-broken quasi-two dimensional system consisting of n_σ electrons of majority spin σ ($\downarrow$) and $n_{\bar{\sigma}}$ electorns of minority spin $\bar{\sigma}$ ($\uparrow$) per unit area embedded in a uniform positively charged background. The SPQW is described in terms of two spin-subband ladders with eigenvalues $\varepsilon_{i\sigma}(\boldsymbol{k})$ and eigenfunctions $|i\boldsymbol{k}\sigma >= e^{i\boldsymbol{k}\cdot\boldsymbol{r}}|i\sigma >$, where i and σ stand for the subband and spin indices, respectively, and $\boldsymbol{k}$ is the wavevector parallel to the layer. $|i\sigma >= \psi_i^\sigma(z)\chi_\sigma$ is the product of an envelope function $\psi_i^\sigma(z)$ and a spin eigenfunction χ_σ. An additional degree of freedom associated with the exchange coupling of itinerant carriers and magnetic impurities in the DMS has renewed interests in both basic and applied research [4]. The spin polarization ζ is defined by $\zeta = (n_\sigma - n_{\bar{\sigma}})/n_{2D}$, where $n_{2D} = n_\sigma + n_{\bar{\sigma}}$ is the 2D free-carrier concentration. The ζ of the DMS QW structure can be tuned from paramagnetic $\zeta = 0$ to fully polarized ferromagnetic $\zeta = 1$ by varing the strength of the applied magnetic field without any dramatic effect on the orbital motion of the electrons. [5]

In this work, we investigate the magnetic phase structures of modulation-doped III-V DMS QWs with emphasis on the control of the magnetic structure of the system in terms of various QW parameters. A hysteretic behavior in the carrier-induced magnetism is demonstrated in the DMS QW, and the magnetization M is shown to depend strongly on the concentration of substituted Mn^{2+} ions, the free carrier density n_{2D}, and the geometric and doping-profile parameters of the quantum well.

I. THEORETICAL MODEL

We consider a symmetrically modulation-doped QW of AlGaAS/$Ga_{1-x}Mn_xAs$/AlGaAs grown in the z direction and analyze the electronic structures based on a self-consistent one-band model of spin-polarized DMS QWs [5]. The effects of exchange and correlation of free carriers are included by employing a spin-dependent exchange-correlation potential $v_{xc}^\sigma(z;\zeta)$ [6]. The free-carrier Hartree potential v_H and the electrostatic potential v_s (which includes contributions from the QW band offset V_0, the modulation-doped ionized impurities of concentration N_a in nonmagnetic barriers, and magnetic ions of concentration $N_{\rm Mn}$ substituted in the well) are determined self-consistently by solving the Schrödinger equation, together with the Poisson equation, for $v_H(z) + v_s(z)$. The kinetic exchange interaction $J_{pd}(\boldsymbol{r} - \boldsymbol{R})$ of free carriers at $\boldsymbol{r}$ with d electrons on the localized Mn^{2+} ions of spin $S = 5/2$ at $\boldsymbol{R}$ is included in the mean-field approximation [7,8] to write $H_{\rm x} = \sigma_z < S_z > x \sum_{\boldsymbol{R}_i} J^{sp-d}(\boldsymbol{r} - \boldsymbol{R}_i)$, where x is the fractional occupancy of cation sites by magnetic ions and $\boldsymbol{R}_i$ denotes the coordinate of the cation sublattice. Here the summation extends over all cation sites. Hence, the spin-dependent part of the energy of a free carrier can

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be written as [5]

$$V_B^\sigma = \sigma_z[g^*\mu_B B - N_0\eta x < S_z >] = g_{eff}\mu_B B\sigma_z, \quad (1)$$

where N_0 and g_{eff} are the number of cation sites per unit volume and the effective g-factor of the carriers in the DMS QW structure, respectively. If the free-carrier wave function is used, the second term in V_B^σ describes the exchange interaction between the free carriers of spin $\boldsymbol{\sigma}$ and Mn^{2+} ions of spin $\boldsymbol{S}$ with $\eta = \frac{1}{\Omega} < \phi|J_{pd}|\phi >$ being the expectation value of the exchange coupling integral J_{pd} over a unit cell Ω. We confine our consideration to a magnetic QW of width L under an in-plane magnetic field B applied in the y direction parallel to the interface [9].

The spin-split subband wave function $\psi_i^\sigma(z)$ is determined by

$$\left[-\frac{\hbar^2}{2m^*}\frac{d^2}{dz^2} + \frac{m^*\omega_c^2}{2}(z-z_0)^2 + v_{s.c.}^\sigma(z)\right]\psi_i^\sigma(z) = E_{ik_x}^\sigma \psi_i^\sigma(z). \quad (2)$$

Here, $\omega_c = \frac{eB}{m^*}$, $z_0 = -k_x l_B^2$ with $l_B = \sqrt{\frac{\hbar}{eB}}$, $v_{s.c.}^\sigma(z) = v_H(z) + v_s(z) + V_B^\sigma + v_{xc}^\sigma(z;\zeta)$, and σ $(=\downarrow, \uparrow)$ is the z-component of the spin. The temperature effect is included by employing the spin-dependent Fermi distribution function in obtaining $v_{s.c.}^\sigma(z)$; $n_i^\sigma(z) = f(E_{ik_x}^\sigma, T)|\psi_i^\sigma(z)|^2$. We note that a parabolic magnetic confinement induced by the in-plane magnetic field, *i.e.*, the second term in Eq. (2), makes the solutions $\{E_{ik_x}^\sigma; \psi_i^\sigma(z)\}$ k_x-dependent, in general. However, in the weak-field region ($l_B >> L$), one can neglect the effect of the additional magnetic confinement and ignore the nonparabolic k_x dependence of the solution. The thermal average $< S_z >$ taken over all Mn^{2+} ions is given by

$$< S_z > = -\frac{5}{2}B_{5/2}(\xi), \quad (3)$$

where $B_{5/2}(\xi)$ is the standard Brillouin function and $\xi = \left(g_{\rm Mn}\mu_B SB + J_{pd}S\frac{n_{2D}\zeta}{2L}\right)/k_BT$ with $S = 5/2$. The second term in ξ denotes the contribution of the kinetic exchange coupling to the spontaneous magnetization of the DMS QW in the absence of an external magnetic field B [7]. We solve Eq.(2) to obtain the self-consistent subband structure $\{E_{ik_x}^\sigma, \psi_i^\sigma(z)\}$ by minimizing the total free-carrier energy E [5]:

$$E = \sum_{ik_x\sigma} n_{ik_x}^\sigma[\hat{E}_{ik_x}^\sigma + \frac{1}{2}(\mu - E_{ik_x}^\sigma)]. \quad (4)$$

In Eq. (4), $\hat{E}_{ik_x}^\sigma$ is given by

$$\hat{E}_{ik_x}^\sigma = E_{ik_x}^\sigma - \frac{1}{2} < v_H(z) >, \quad (5)$$

which is needed in order to avoid double counting of the Hartree interaction energy in evaluating the total energy E. In the rest of this work, we limit ourselves to the weak-field region ($l_B >> L$).

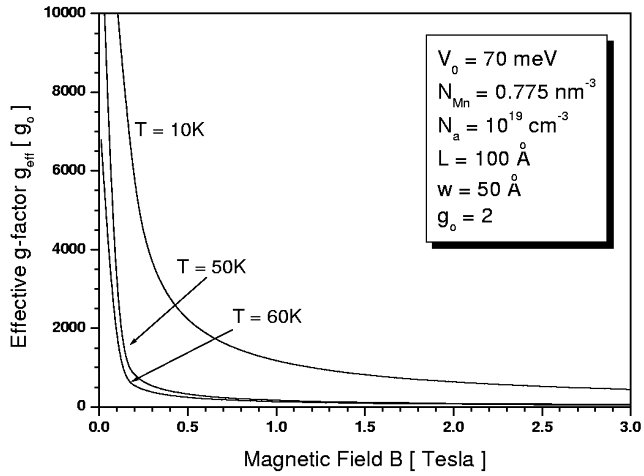

Fig. 1. Magnetic field dependence of the effective g-factor, g_{eff}, of dilute magnetic semiconductor quantum wells for various temperatures.

II. RESULTS AND DISCUSSION

In Fig. 1, the magnetic field and the temperature dependences of the effective g-factor, g_{eff}, defined in Eq. (1) are displayed in units of the free-carrier effective g factor, g^*, in the absence of magnetic ions. In the numerical calculations, $x = 0.035$, $m^* = 0.5m_e$, and the coupling strength $J_{pd} = 0.15$eV nm^3 for p-type $Ga_{1-x}Mn_xAs$ were used. We examined the subband structure $\{n_\sigma; E_{ik_x}^\sigma\}$ and analyzed the magnetic phase structure of the system in terms of the magnetic field and temperature. As the magnetic field increases, the quantum well depth of spin-down (majority-spin) electrons becomes deeper through the exchange interaction with Mn^{2+} ions (V_H^σ) and finally saturates to a constant value. As the temperature increases, the concentration of majority-spin electrons, $n_{i\downarrow}$, decreases, but that of minority-spin electrons, $n_{i\uparrow}$, increases until the system becomes paramagnetic. As one increases the degree of spin polarization ζ, the spin-split subband separation increases, and the free-carrier areal density, n_{2D}, in the quantum well increases steadily at high temperatures, but increases more rapidly at low temperatures. The spontaneous spin polarization depends strongly on the temperature T, the free-carrier density n_{2D}, and the geometric and doping profile parameters, such as the well depth V_0, the width L, N_a, and $N_{\rm Mn}$, of the QW.

The magnetic phase structure of the DMS QW is shown in Fig. 2 as a function of the temperature and the magnetic field. Even in the absence of an external field, the system becomes fully polarized in the ferromagnetic phase ($\zeta = 1$) below about 30K for the DMS QW with the parameters used in the figure. In the figure, w is the width of the spacer layer of the symmetric QW structure [5]. In our calculation, the exchange-correlation of free carriers is observed to enhance the ferromagnetic tendency. The threshold temperature T_{th} below which

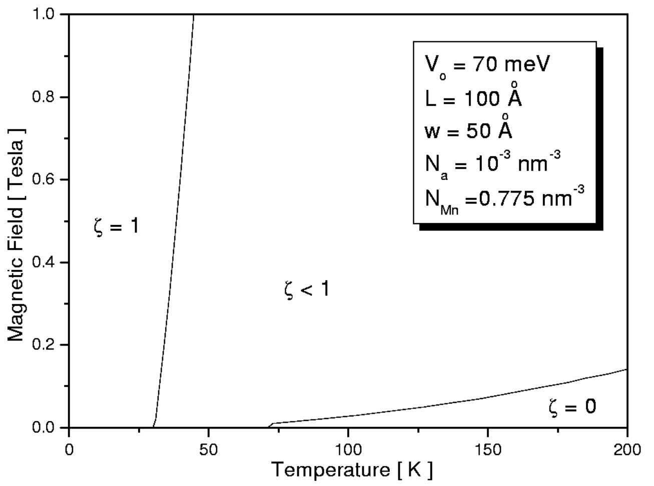

Fig. 2. Magnetic phase diagram of the modulation-doped DMS QW in terms of the temperature and the external magnetic field.

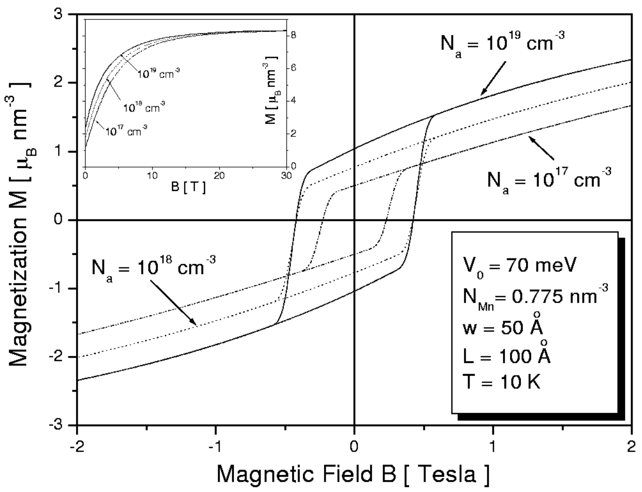

Fig. 3. Magnetic field dependence of the magnetization of the DMS QW for various impurity-doping concentrations N_a. The inset shows the *paramagnetic* behavior of M beyond a threshold magnetic field, B_{th}, before it saturates.

the system becomes fully polarized in the ferromagnetic phase ($\zeta = 1$) even in the absence of an external field increases as the doping concentration N_a in the nonmagnetic barriers increases.

We also calculated the magnetization M of the system at finite temperature as a function of the magnetic field B [10]. Figure 3 shows the magnetic-field dependence of the magnetization. Our result shows the hysteretic behavior of M by virtue of the exchange coupling of a Mn^{2+} ion and an itinerant carrier [11]. The remnant values of M_{rem} increase as the carrier concentration n_{2D} increases, and M shows a *paramagnetic* behavior beyond the threshold magnetic field B_{th} until it saturates toward the value $M_s = N_{Mn} g_{Mn} \mu_B S$, the dominating contribution of the localized spins. (See the inset.) The magnitude of B_{th} depends strongly on n_{2D}, $N_{\rm Mn}$, and the p-doping concentration N_a in the nonmagnetic barriers of the DMS quantum structure.

III. SUMMARY

We observe that the tendency to ferromagnetic ordering is increased as the strength of the confinement potential is increased and that the magnetization of the system is strongly dependent on the concentration of substituted Mn^{2+} ions, the free-carrier density n_{2D}, and the geometric and doping profile parameters of the QW. Our result shows a hysteretic behavior for the magnetization in the DMS QW by virtue of the coupling between a Mn^{2+} ion and an itinerant carrier. The threshold temperature, below which the system becomes spontaneously fully polarized in the ferromagnetic phase ($\zeta = 1$), increases as one increases the magnetic impurity concentration $N_{\rm Mn}$ in the well and the p-doping concentration N_a in nonmagnetic barriers.

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