Field-effect magnetization reversal in ferromagnetic semiconductor quantum wells

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We predict that a bias-voltage-assisted magnetization reversal process will occur in Mn-doped II-VI semiconductor quantum wells or heterojunctions with carrier-induced ferromagnetism. The effect is due to strong exchange-coupling-induced subband mixing that leads to electrically tunable hysteresis loops. Our model calculations are based on the mean-field theory of carrier-induced ferromagnetism in Mn-doped quantum wells and on a semiphenomenological description of the host II-VI semiconductor valence bands.

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The strong dependence of transport properties in metallic multilayers on magnetic configuration has inspired a new field of research,[1] spintronics, in which the electron spin degree of freedom is exploited. Semiconductors that become ferromagnetic when doped with magnetic elements—for example, GaAs doped with Mn—are of special interest in this field in part because of their compatibility with conventional semiconductor technology and because of the large range of possibilities for the control of device functionality. Ferromagnetism has already been observed in such systems at relatively high temperatures ($T_c > 100$ K),[2] and strategies for obtaining T_c's larger than room temperature are of a great current interest in this scientific community.[3–5]

Our interest here is in the magnetic properties of modulation-doped quantum wells containing Mn local moments. We expect[6,7] these systems to be unusual ferromagnets because of the reduced dimensionality of the itinerant hole system and the possibility of using confinement effects and doping profiles to manipulate their magnetic properties. For example, the ferromagnetic critical temperature can be tuned by an external electric field,[6] as demonstrated in recent studies of (In,Mn)As field effect transistors.[8] In this paper we study their hysteresis properties which will be, we predict, extremely sensitive to external bias voltages. The interplay between local moment–itinerant hole exchange coupling, Zeeman coupling of the localized moments to external magnetic field, and the coupling of an external electric field to the orbital degrees of freedom of itinerant holes makes it possible to vary the coercive field by over an order of magnitude with rather modest external electric fields. As a consequence, we predict that the magnetization orientation in quantum wells can be manipulated electrically without changing the magnetic field. Our calculations also suggest that capacitance measurements can be used to probe the magnetic state of biased ferromagnetic semiconductor quantum wells.

The system we consider is a (Cd,Mn)Te quantum well grown in the $\langle 001 \rangle$ crystal direction. Unlike III-V host materials, where Mn acts as an acceptor, the Mn concentration and the itinerant hole density can be varied independently in II-VI hosts. The quantum size effects discussed here are more pronounced when only one or two subbands are occupied, a condition that can easily be achieved with sizable Mn concentrations in II-VI diluted magnetic semiconductor (DMS) quantum wells.

The Hamiltonian of a DMS system is written using an envelope function description of valence band electrons and a spin representation of their kinetic-exchange interaction[9] with d electrons[10] on the Mn^{2+} ions:

$$\mathcal{H} = \mathcal{H}_m + \mathcal{H}_b + J_{pd} \sum_{i,I} \vec{S}_I \cdot \vec{s}_i \delta(\vec{r}_i - \vec{R}_I), \tag{1}$$

where i labels a valence band hole and I labels a magnetic ion. In Eq. (1), $\mathcal{H}_m$ describes the coupling of magnetic ions with total spin quantum number $S = 5/2$ to an external field, $\vec{S}_I$ is a localized spin, $\vec{s}_i$ is a hole spin, and $\mathcal{H}_b$ is a four-band envelope-function Hamiltonian[11] for the valence bands. The four-band Kohn-Luttinger model describes only the total angular momentum $j = 3/2$ bands and is adequate at low hole densities when spin-orbit coupling is large. The degeneracy between heavy-hole ($|j_z| = 3/2$) and light-hole ($|j_z| = 1/2$) bands at the Γ point in the bulk is lifted by size quantization effects in a quasi-two-dimensional system. The resulting heavy-light gap is larger than the Fermi energy, in the relevant range of hole densities, allowing only the two heavy-hole bands to be occupied. The heavy holes have their spin aligned along the $\hat{z}$ axis ($\langle 001 \rangle$ crystal direction) so that the band electron spin matrix elements get smaller when the magnetization tilts away from the growth direction. This leads, as discussed below, to very strong magnetic anisotropy with easy axes along and opposite to the growth direction. This anisotropy is reduced in magnitude but is still large when mixing between heavy- and light-hole bands is fully accounted for, as we show below. The exchange interaction between valence band holes and localized moments is believed to be antiferromagnetic,[9] i.e., $J_{pd} > 0$. For (Cd,Mn)Te, $J_{pd} \approx 0.06$ eV nm^3.

Our mean-field theory is derived in the spin-density-functional framework and leads to a set of physically transparent coupled equations.[12] The effective magnetic field seen by localized magnetic ions is the sum of the external magnetic field and the kinetic exchange coupling mean-field contribution from spin-polarized carriers:

$$\vec{H}_{eff}(\vec{R}_I)=\vec{H}_{ext}+J_{pd}\langle\vec{s}(\vec{R}_I)\rangle/g\mu_B, \tag{2}$$

where $\vec{H}_{ext}$ is the external magnetic field, $\langle\vec{s}(\vec{R}_I)\rangle$ is the carrier spin density at Mn sites, and $g=2$ is the g factor of the local moments. The mean polarization of a magnetic ion is given by[13]

$$\langle\vec{S}\rangle(\vec{R}_I)=-SB_S[Sg\mu_B H_{eff}(\vec{R}_I)/k_BT]g\mu_B\hat{H}_{eff}(\vec{R}_I), \tag{3}$$

where $B_S(x)$ is the Brillouin function and $\hat{H}_{eff}(\vec{R}_I)$ is the unit vector along the direction of the effective magnetic field defined in Eq. (2). The itinerant-hole spin density is determined by solving the Schrödinger equation for holes which experience chemical quantum confinement and electrostatic external potentials, a local-spin-density-approximation exchange-correlation potential, and a spin-dependent kinetic-exchange potential $h(z)$. The field $h(z)$ is nonzero only in the ferromagnetic state. We assume that the magnetic ions are randomly distributed and dense on a scale set by the free carrier Fermi wave vector and that any desired density profile $N_{Mn}(z)$ can be achieved during growth. This allows us to take a continuum limit where

$$h(z)=J_{pd}N_{Mn}(z)\langle S\rangle(z). \tag{4}$$

Results presented in the following paragraphs are based on a self-consistent solution of Eqs. (2)–(4) in the zero-temperature limit. This approach does not account for disorder associated with randomness in the Mn spin locations, which could have some importance in general or for direct interactions between Mn spins on neighboring lattice sites.[14] There is, however, a large body of literature, mostly concerning the magnetic field dependence of optical properties of paramagnetic DMS systems, that supports the reliability of these approximations for qualitative predictions.

The magnetization reversal properties of these quantum well ferromagnets are quite unusual as we now establish. We first discuss the dependence of the ground-state energy on uniform magnetization orientation. As explained above we expect that quantum confinement and valence-band spin-orbit coupling should conspire to yield a large anisotropy energy. In Fig. 1 we plot the change in the total band energy per particle $E_b(\theta)$ as a function of angle θ of the magnetization measured from the growth direction for several two-dimensional (2D) densities p_{2D}. We assumed a (Cd,Mn)Te/(Cd,Zn)Te quantum well of the width $w=10$ nm with valence-band offset of 150 meV and uniformly distributed Mn ions of density $N_{Mn}=6\times10^{20}$ cm^{-3}. The energy increase at nonzero angles, i.e., the growth direction easy-axis anisotropy, is consistent with experiment[15] and with the expectations based on $\langle001\rangle$ growth quantum confinement effects explained above. If there were no heavy-light subband mixing at any orientation, the magnetic condensation energy would vanish for $\theta=\pi/2$ (the operators s_x and s_y vanish in the heavy-hole subspace) and the anisotropy energy per electron would equal $JSN_{Mn}/2\sim45$ meV, much larger than the values obtained in Fig. 1. This limit is reached, however, only when quantum well subband splittings are much larger than JSN_{Mn} and we are not close to this limit. Nevertheless,

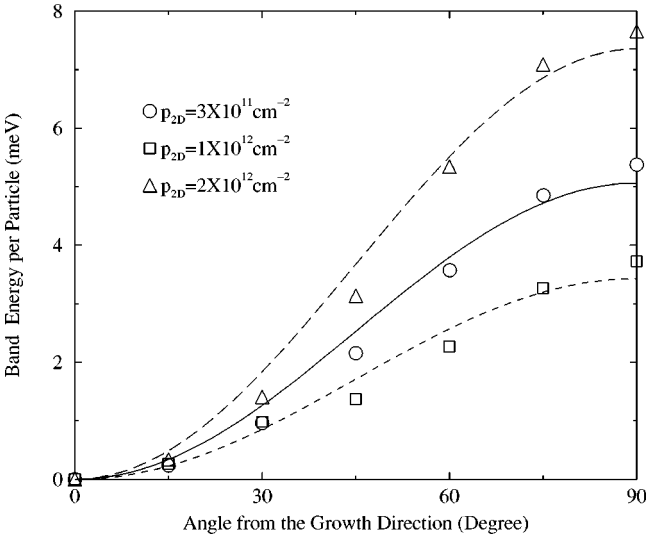

FIG. 1. Band anisotropy energy calculated from the self-consistent Hartree approximation using the four-band Luttinger model as a function of magnetization direction from the growth direction. The anisotropy energy is defined as the energy difference compared to the growth direction orientation. At the lowest density only one subband is occupied while two subbands are occupied at the two higher densities. The curves fit the numerical data in a uniaxial form.

the magnitude of the anisotropy energy we obtain is still several times larger than in bulk ferromagnetic semiconductors.[16] It is interesting to note that the anisotropy energy per electron in these ferromagnets is nearly three orders of magnitude larger than in cubic transition metal ferromagnets.[17]

For magnetization along the easy axis, with given carrier densities of order of 10^{11} cm^{-2}, heavy-light mixing is very weak and the numerical calculations for a four-band model and a single spin-split band model with effective mass $m_{\|}=0.25m_0$ and out-of-plane mass $m_z=0.55m_0$ do not reveal any difference. In this (Cd,Mn)Te/(Cd,Zn)Te quantum well, the spin splitting is about 3 times larger than the splitting between the two lowest majority-spin subbands. This enormous exchange gap between majority- and minority-spin states is the origin of the peculiar magnetic reversal properties in biased DMS quantum wells that we now discuss. Consider the effect of a field in the positive $\hat{z}$ direction on the state where all spins are polarized in the negative $\hat{z}$ direction. Because of the antiferromagnetic p-d coupling, spin-up holes are the majority carriers at zero external magnetic field. At the 2D hole densities of interest here, only the lowest spin-up subband is occupied and all spin-down subbands are empty; i.e., the itinerant system is fully polarized. When the magnetic field is applied, direct Zeeman coupling to a local moment competes with the local mean-field kinetic-exchange coupling which is proportional to the itinerant-hole spin density. Since the carrier density is smaller at the edges of the quantum well than at the center, spin reversal starts from the well edges. This, in turn, creates an exchange barrier for the majority spins which effectively narrows the quantum well in which they reside. At the same time an

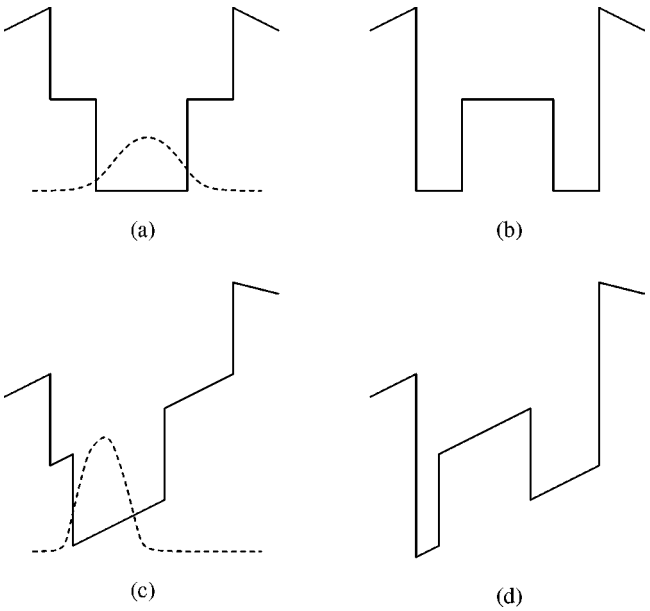

FIG. 2. Schematic diagram of potentials in a DMS QW with external magnetic field, $0<|H_{ext}|<|H_r|$, which is oriented in opposition to the local spin moment. H_r, the reversal field, is close to the field at which the lowest minority-spin level crosses the majority-spin energy level. (a) and (b) show majority- and minority-spin potentials without a bias potential, while (c) and (d) show majority- and minority-spin potentials with a bias potential applied. The dashed lines indicate the envelope wave functions.

effective double-well potential develops for the minority spins as illustrated in Fig. 2. Note that because of the strong kinetic-exchange potential, the symmetric and antisymmetric minority-spin states in the unbiased double-well remain nearly degenerate throughout the whole metastable part of the hysteretic magnetization curve.

As the external magnetic field increases, the minority-spin energy levels are lowered and the majority-spin energy levels are raised. When the lowest down-spin energy level reaches the Fermi energy, holes start to occupy the down-spin states. Our self-consistent calculations show that once this occurs, the magnetization reversal is rapidly completed and only the uniform down-spin state is stable.

This unusual process in which magnetization reversal and quantum confinement effects are linked suggests that the hysteresis curve can be modified by applying an external electric field, as shown in Fig. 2. We can parametrize the electric field between the front gate and the quantum well, fixing the field at the back side of the well, by the total two-dimensional carrier density. We have calculated local moment magnetization loops for several carrier densities where $p_{2D}=3\times10^{11}$ cm^{-2} corresponds to the balanced quantum well. The results are plotted in Fig. 3. Two effects contribute to the change of the hysteresis loop with applied electric field. First, the hole-density profile is compressed and moves toward one edge of the well, permitting an abrupt localized moment reversal throughout the depleted region of the quantum well. Second, the increase (decrease) of the 2D hole density enhances (suppresses) the kinetic-exchange coupling.

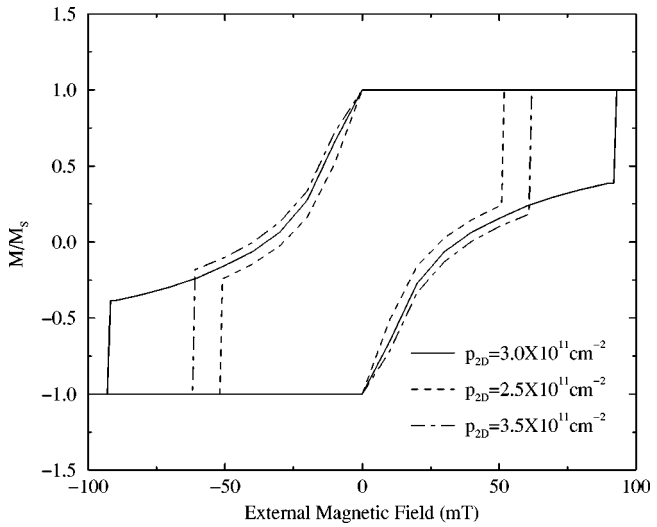

FIG. 3. Local moment hysteresis loops in a quasi-2D DMS system with different carrier densities. Results are made with a single spin-split band model including exchange-correlation potentials.

The hysteresis loops shown in Fig. 3 imply that, at a fixed magnetic field, the magnetization can be changed by applying an electric field. This possibility of narrowing or broadening hysteresis loops electrically is an attractive feature of ferromagnetic semiconductor quantum well systems. It is somewhat reminiscent of recent interest in current-driven magnetization reversal[18] in metallic ferromagnets and could be extremely useful if other obstacles (most obviously the low ferromagnetic transition temperatures) to the use of these systems in nonvolatile memory devices can be overcome.

The interplay between quantum confinement and magnetization reversal in ferromagnetic semiconductor quantum wells is reflected in unusual magnetocapacitance effects. The inverse capacitance can be written as

$$C^{-1}=C_b^{-1}+C_c^{-1}, \tag{5}$$

where C_b^{-1} is the inverse geometric capacitance and C_c^{-1} is the inverse 2D-channel capacitance. The geometric capacitance depends only on the distance from the quantum well to the gate and on the barrier dielectric constant ϵ, and does not reflect the electronic structure of the 2D hole gas. The inverse channel capacitance

$$C_c^{-1}=\frac{d\phi_c}{dp_{2D}}=\frac{d}{dp_{2D}}\left(\frac{\overline{z}}{\epsilon}p_{2D}+\frac{E_F}{e^2}\right) \tag{6}$$

is the sum of the electrostatic term related to the density-dependent center of mass of the quasi-2D hole system and a thermodynamic term originating from the concentration dependent Fermi energy. This separation is physically sensible and convenient and can be made precise by the arbitrary choice of a reference position outside the quantum well; only the total capacitance is measurable. Figure 4 demonstrates the similarity of electric and magnetic responses to the electric bias field, indicating that the magnetic state of this quasi-2D system can be detected electrically. These curves are calculated by starting in the partially magnetized state at

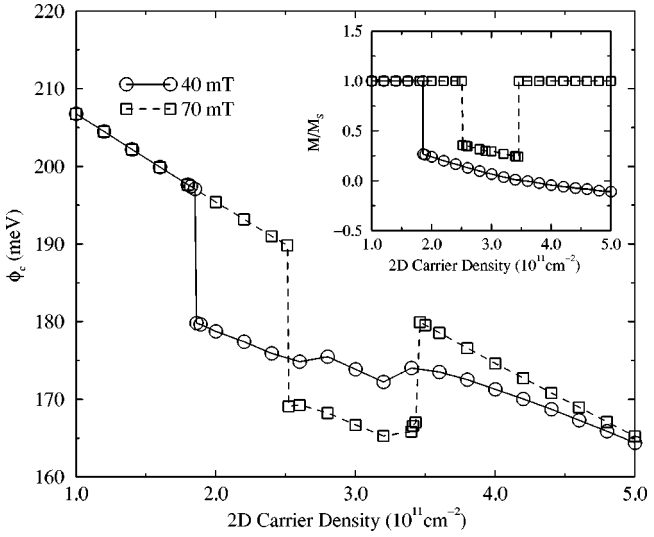

FIG. 4. Difference between the electric potential at a reference point outside the quantum well and the chemical potential of the two-dimensional electron system as a function of carrier density. Inset: local moment magnetization as a function of carrier density.

the balanced density, $p_{2D}=3\times10^{11}$ cm^{-2}; as explained previously the metastable state persists to the largest reversal fields for balanced quantum wells. When the density is varied, metastability is lost and the magnetization reversal is completed. The discontinuity in magnetization is accompanied by a discontinuity in the electrochemical potential difference between channel and gate that appears as a singularity in the capacitance.

In closing we remark that this unusual magnetization reversal process can be operative only if the system is always stable against coherent magnetization reorientation. We do not expect that this stability will hold for wider quantum wells, but believe that it does for the geometry considered here, as we now argue. Accounting for the coupling to an external field along the easy axis to the Mn spins, the total energy per electron as a function of the coherent spin orientation θ is

$$E(\theta)=E_b(\theta)-\cos(\theta)g\mu_B SH_{ext}N_{Mn}\zeta(H_{ext})w/p_{2D}, \tag{7}$$

where $\zeta(H_{ext})=(N^{\uparrow}_{Mn}-N^{\downarrow}_{Mn})/(N^{\uparrow}_{Mn}+N^{\downarrow}_{Mn})$ is the spatially averaged local moment polarization. Our band anisotropy energy results, summarized in Fig. 1, are accurately described by a uniaxial form, $E_b(\theta)=K\sin^2(\theta)$ with $K=5$ meV per electron for $p_{2D}=3\times10^{11}$ cm^{-2}. If K were constant and the $\zeta(H_{ext})$ were equal to 1, the coherent rotation field would be $H_c=2K/(g\mu_B SN_{Mn}w/p_{2D})\sim17$ mT. However, ζ is reduced in the spatially inhomogeneous state and K will be increased by the effectively narrower quantum well in which the majority spin electrons are confined. These two effects will combine to make the unusual reversal process discussed in this paper an operative one for quantum wells narrower than ~10 nm.

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