Hole spin polarization in GaAlAs:Mn structures

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A self-consistent calculation of the electronic properties of GaAlAs:Mn magnetic semiconductor quantum well structures is performed including the Hartree term and the sp-d exchange interaction with the Mn magnetic moments. The spin polarization density is obtained for several structure configurations. Available experimental results are compared with theory.

During the last years spin-polarized transport became a matter of major interest, giving rise to a field usually called magnetoelectronics, or spintronics. Much effort has been made in studying and producing the so-called spin-valve, where a spin-polarized current is generated.

A promising system in that area is the recently grown A magnetic moment of Mn in the alloy is a strong analytica RKKY calculations for the spin polarization in several confined structures, and clarified the role of the confined states in the multilayer interaction. Recently, improvements on the standard RKKY mechanism were introduced by Byoung Hak Lee et al. to treat the ferromagnetism of GaMnAs quantum wells. In the present work we consider a Ga_{1-x}Mn_xAs layer in its metallic phase, grown inside a GaAs/AlAs quantum well structure. We obtain the spin-polarized electronic structure for holes, taking into account their interaction with the magnetic impurities. The Hamiltonian we consider is:

\[ H = H_0 + U_H + U_{mag}, \]  

\[ U_{mag}(\vec{r}) = -\frac{I}{N_i} \sum_{i=1}^{N_i} \vec{s}(\vec{r}) \cdot \vec{S}(\vec{R}_i) \delta(\vec{r} - \vec{R}_i). \]  

The \( H_0 \) term in the rhs of Eq. (1) contains the kinetic energy and the confining potential, \( U_c(z) \), due to the band edges mismatch at the semiconductor interfaces. Coulomb interactions between carriers are considered through the Hartree term \( U_H(\vec{r}) \). The hole system is supposed to be homogeneous in the \( xy \) plane, so \( U_H(\vec{r}) = U_H(z) \). In the present approach we treat the magnetic interaction as being due to a uniform magnetization in the DMS. If a net magnetization exists, it will polarize the hole gas. This problem is solved self-consistently by a secular matrix equation in the reciprocal space. The method would be exact were not for cutting the matrix size. For each spin, we define the wavefunction Fourier Transform (FT):

\[ \psi_\sigma(\vec{r}) = \int d^3q \exp(i\vec{q} \cdot \vec{r}) \psi_\sigma(\vec{q}). \]  

The hole eigenstates will be obtained by discretizing the integrals appearing in

\[ \int d^3r \psi_\sigma^*(\vec{r})(H - E)\psi_\sigma(\vec{r}) = 0. \]  

When integrating the magnetic term in the Hamiltonian over \( r \), we assumed the magnetic impurities to be uniformly distributed in the Ga_{1-x}Mn_xAs DMS layer, all of
them having the same magnetization, namely the thermal average magnetization $<\bar{M}>$. This treatment includes not only the ferromagnetic phase but also phases where a partial magnetization is observed, the “canted-spin” phases. Therefore,

$$-I \int dq^2 \exp[i(q - q')^2] \sum_{i=1}^{N_i} \delta(q_i - q_i') \delta(q_i - \vec{R}_i) \approx$$

$$-\frac{1}{2} \sqrt{\bar{I}} \frac{v_F}{\epsilon_0} \int dq^2 \exp[i(q - q')^2] \delta(q_i - q_i'),$$

(5)

where $\bar{I}$ is the impurity density and $\sigma = \pm 1$ for spin parallel (upper sign) or anti-parallel (lower sign) to the magnetization. $F_{DMS}$ is the integral performed on the $z$-coordinate along the DMS layer:

$$F_{DMS}(q) = \frac{1}{2\pi} \int_{DMS} dz \exp[iq.z].$$

(6)

In Eq. 6 we have defined $\bar{I} = \frac{1}{\epsilon_0}$, where $\epsilon_0$ is the volume of the Mn$^{2+}$ ion, which is the $f_{ec}$ lattice’s primitive cell volume, $a^3/4$. It is worthwhile to mention that, in experimental works, $\bar{I}$ is usually represented by $N_0\beta$. Here we used $N_0\beta = -1.2eV$. After performing the FT of the Hartree term plus the confining potential,

$$U_{el}(q) = \frac{1}{2\pi} \int dz \exp[iq.z][U_H(z) + U_{el}(z)],$$

(7)

the eigenvalues and eigenfunctions at the bottom of the 2-D subbands may be obtained by solving the secular matrix for each spin-polarization:

$$\det \left\{ \left[ \frac{\hbar^2 q^2}{2m^*} - E \right] \delta(q_i - q_i') + U_{el}(q_i - q_i') \right\} = 0.$$  

(8)

For applications, favorable spin configurations may be designed by growing a proper structure. In particular, the possibility of having a ferromagnetic order in the DMS heterostructures is important for spin tunneling and resonant spin tunneling in nanostructures. We have calculated the electronic structure, and the spin polarization, in three GaAlAs/GaAs:Mn quantum wells. We started with an AlAs/GaAs QW in the middle of which a DMS barrier (Ga$_{0.65}$Al$_{0.35}$), which is grown in its ferromagnetic metallic phase. In that case, we have, actually, two QW of widths $L$ separated by an internal barrier of 168.3 meV with thickness $d$, and barriers of 529 meV at the lateral boundaries. In a second structure, we assume that the DMS is just a Ga$_{1-x}$Mn$_x$As layer of thickness $d$, no internal barrier being structurally imposed. Finally, in a last structure, we explore the case of a single DMS QW: a Ga$_{1-x}$Mn$_x$As layer of thickness $2L + d$ is surrounded by thick layers of AlAs. It is well known that in ferromagnetic metallic Ga$_{1-x}$Mn$_x$As layers (in our calculation we assumed $x = 0.05$) the density of free carriers (holes) is just a fraction of the density of the magnetic ions. Throughout the present calculation we made the hole density $p = 1 \times 10^{20} cm^{-3}, T=0K$, and $<M> = \frac{5}{2}$. Due to the high carrier density, the Hartree term cannot be neglected, and several subbands happen to be occupied.

The results for the energy of the bound states are shown in Table 1 for samples #1 and #2. In the case of the first sample we observe a dip at the middle of the structure, as a consequence of the existence of the central barrier. A much less pronounced dip is observed in the sample #1’s spin polarization density, shown in Fig. 1. By integrating the spin density we obtain that 6% of the spins are polarized.

| state | sample 1 | sample 2 | sample 3 |
|-------|----------|----------|----------|
| spin 1 | -0.51819 | -0.54815 | -0.59511 |
| spin 2 | -0.51308 | -0.51799 | -0.58266 |
| spin 3 | -0.51244 | -0.51233 | -0.56052 |
| spin 4 | -0.51199 | -0.51167 | -0.52939 |
| spin 5 | -0.47744 | -0.49945 | -0.48941 |
| spin 6 | -0.46498 | -0.47861 | -0.44520 |
| spin 7 | -0.45885 | -0.46045 | -0.44070 |
| spin 8 | -0.45722 | -0.45806 | -0.43300 |
| spin 9 | -0.40581 | -0.42870 | -0.41125 |
| spin 10 | -0.38491 | -0.40766 | -0.38341 |
| spin 11 | -0.36957 | -0.37390 | -0.38069 |
| spin 12 | -0.36612 | -0.36903 | -0.34152 |
| spin 13 | -0.30218 | -0.32280 | -0.31775 |
| spin 14 | -0.27688 | -0.30397 | -0.29390 |
| spin 15 | -0.24647 | -0.25385 | -0.24409 |
| spin 16 | -0.24076 | -0.24624 | -0.23809 |
| spin 17 | -0.16722 | -0.18438 | -0.17455 |
| spin 18 | -0.14316 | -0.16859 | -0.16311 |
| spin 19 | -0.09378 | -0.10369 | -0.10420 |
| spin 20 | -0.08594 | -0.09386 | -0.07647 |
| spin 21 | -0.01095 | -0.02272 | -0.03001 |
| spin 22 | -0.01170 | -0.01170 | -0.04030 |

$E_F = -0.49846$
FIG. 1. Charge density as a function of the distance to the center of the well. Sample #1: two GaAs quantum wells of 50Å separated by a 10Å barrier of Ga$_{0.60}$Al$_{0.35}$Mn$_{0.05}$. Sample #2: a 10Å Ga$_{0.95}$Mn$_{0.05}$As instead of the middle barrier.

FIG. 2. Spin polarization density as a function of the distance to the center of the well, for samples #1 and #2.

The elimination of the central barrier in sample #2 increases the probability of finding the holes in the middle of the structure, now attracted by the unbalanced negative charges. The dip disappears giving rise to a pronounced peak in both the charge density and the spin polarization density. Another important difference is the Friedel-like oscillation in the polarization, being anti-parallel in the middle of the well, and parallel near the interfaces. The total polarization reaches 40%.

A radical change occurs when the DMS occupies the entire well, as shown in Fig. 3. The number of carriers per unit area is much greater than in the previous cases, and many subbands are occupied. The charge density shows an oscillation inside the well, as a consequence of the higher subbands occupation. The oscillations that occur in the spin polarization density follow those in the charge density. In the case where charges and magnetic moments cohabit inside a finite width determined by the quantum confinement, we obtain that the oscillations are not enough to invert the polarization in any region. We plotted the sum of the bare confining potential plus the self-consistent Hartree term in the inset of Fig. 3. An effective central barrier appears at the middle of the well, together with two valleys at the interfaces which increases the lateral barriers from 529 meV to about 600 meV. In sample #3 the magnetic interaction between holes and the ferromagnetic layer contributes to the confining potential with an increase of 150 meV for spin anti-parallel, and a decrease of the same amount for spin parallel. Therefore, there is no rigid shift of the eigenenergies as in a 3-D system. The total polarization is 82%.

FIG. 3. Sample #3: Charge density and spin density distributions in a single quantum well of 110Å Ga$_{0.95}$Mn$_{0.05}$As. Inset: bare confining potential plus self-consistent Hartree term.

The spin-polarized electronic structure in diluted magnetic semiconductors, as obtained here, points to the possibility of a self-consistent calculation of the magnetization in multilayered structures, as in Refs. 13 and 14, taking into account a spin-polarized RKKY mechanism. Recently Chiba et al. 17 investigated a GaMnAs trilayer structure and observed a ferromagnetic, although weak, interaction between two ferromagnetic layers. The present result is also important for determining properties like spin diffusion and spin filtering in cases where spin-coherence lifetimes are large. For instance, the spin motion for carriers polarized parallel and anti-parallel to the equilibrium polarization in otherwise non-magnetic GaAs samples has been predicted 20 to show a difference of an order of magnitude between the two speeds, with electrons and holes behaving in opposite way. This fact points to the importance of taking a properly calculated
electronic structure in obtaining the spin-polarized transport in magnetic GaMnAs structures. On the other hand, a spin filtering mechanism has been previewed in the ZnSe/ZnMnSe/ZnSe structure with an external applied magnetic field. The present results on the electronic structure of GaMnAs shows the possibility of filtering spins without needing an external field in the range of temperatures of ferromagnetic phases.

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