Spin-polarized charge densities in (In,Ga,Mn)As-based Diluted Magnetic Semiconductor ternary and quaternary alloy heterostructures

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Spin-polarized charge densities in (In,Ga,Mn)As-based Diluted Magnetic Semiconductor ternary and quaternary alloy heterostructures

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Abstract. In this work we present the electronic band structures, and the spin-polarized charge concentrations of selected AlAs/(InGaAs/$Ga_{1-x}Mn_x$ As) × n/AlAs and AlAs/ (GaAs/$InGa_{1-x}$ Mn_x As) × n/AlAs systems. The exchange-correlation, the split-off strain and the polarization effects are taken into account in a six-band Luttinger-Kohn (LK) model, solved self-consistently with the Poisson equation. Even for a small In content, the strain effects are shown to be important in order to maximize the heavy hole charge distribution, facilitating the spin polarization separation. From the results one can determine a set of parameters that maximize the presence of polarized charge distributions in the non-magnetic layers, enhancing the mobility of the carriers in the system.

INTRODUCTION

Diluted magnetic semiconductors (DMS) are promising materials for novel semiconductor based âĂIJspintronicâĂİ devices. III-V-based DMS, such as (In,Mn)As and (Ga,Mn)As, and their heterostructures have been, by now, extensively studied [1] showing paramagnetic-to-ferromagnetic phase transitions with high Curie temperatures (TC), of 50 K and 160 K, respectively. Quaternary DMS (In,Ga,Mn)As have many potential advantages that cannot be realized by their ternary counterparts. For instance, the band gap energy, the easy magnetization axis, and the band structure can be controlled by changing the In content of (In,Ga,Mn)As. Recently, it has been reported that in such system, the use of post-growth annealing techniques in strained structures can raise the TC above 100 K [2].

During the last years the LK model has been adapted to quantum wells and superlattices (SL), as described in Refs. [3, 4]. We adopt that approach, using a super-cell model. This means that we consider an unit cell consisting of the active region plus a thick insulator layer. The number of DMS layers in the unit cell can be varied at will. We assume, then, an infinite SL in the [001] direction. The multiband effective-mass equation (EME) is represented with respect to plane waves with wavevectors $K = (2\pi/a)l$ (l an integer and a the SL period) equal to the reciprocal SL vectors. The rows and columns of the 6×6 LK Hamiltonian relate to the Bloch-type eigenfunctions $|j,m_j,\vec{k}>$ of the Γ_8 heavy-hole bands, and the Γ_7 spin-orbit-hole band; $\vec{k}$ denotes a vector of the first Brillouin zone. Expanding the EME with respect to plane waves $< z \mid K >$ means representing this equation in terms of the Bloch functions $< \mathbf{x} \mid j,m_j,\vec{k}+K\mathbf{e}_z >$. For a Bloch function $< z \mid E,\vec{k} >$ of the SL corresponding to energy E and wavevector $\vec{k}$, the EME takes the form:

$$\sum_{j',m'_j,K'} < j,m_j,\vec{k},K \mid T+H_S+V_{het}+V_C+V_{xc}+V_{mag} \mid j',m'_j,\vec{k},K' > \times < j',m'_j,\vec{k},K' \mid E,\vec{k} > = E(\vec{k}) < j,m_j,\vec{k},K \mid E,\vec{k} >, \quad (1)$$

where T is the unperturbed kinetic energy term generalized for a heterostructure, H_S is the strain energy term originating from the lattice mismatch, V_{het} is the square potential due to the difference between energy gaps, V_{xc} is the exchange-correlation potential, and V_C is the sum of the Hartree potential with the ionized acceptor potential. Finally, V_{mag} is given by Eq.(2), for each material. The Luttinger parameters and the other terms appearing in the secular equation are to be taken for each epitaxial layer of the SL. For instance, in the case of the magnetic

interaction we have:

$$< j,m,\vec{k},K|V_{mag}|j',m',\vec{k}',K' >= \\ < \vec{k},K|\tilde{V}_{mag}^{jm;j'm'}g(K'-K)|\vec{k}',K' >, \quad (2)$$

where the integral

$$g(K'-K) = \frac{1}{d}\int_0^d e^{-iKz}g(z)e^{iK'z} \quad (3)$$

is performed in a DMS layer of width d, where the magnetic term stands as

$$\tilde{V}_{mag} = -\tfrac{x}{6}N_0\beta \times \\ \begin{pmatrix} 3M_z & 0 & i\sqrt{3}M_- & 0 & \sqrt{6}M_- & 0 \\ 0 & -3M_z & 0 & -i\sqrt{3}M_+ & 0 & -\sqrt{6}M_+ \\ -i\sqrt{3}M_+ & 0 & M_z & 2iM_- & 2\sqrt{2}iM_z & -\sqrt{2}M_- \\ 0 & i\sqrt{3}M_- & -2iM_+ & -M_z & \sqrt{2}M_+ & -2\sqrt{2}iM_z \\ \sqrt{6}M_+ & 0 & -2\sqrt{2}iM_z & \sqrt{2}M_- & -M_z & iM_- \\ 0 & -\sqrt{6}M_- & -\sqrt{2}M_+ & 2\sqrt{2}iM_z & -iM_+ & M_z \end{pmatrix} \quad (4)$$

.

The self-consistent potentials and the charge densities are obtained by solving the multiband EME equation and the Poisson equation:

$$< j,m_j,\vec{k},K \mid V_C \mid j',m_j',\vec{k},K' >= \\ \frac{4\pi e^2}{\kappa}\frac{1}{|K-K'|^2} < K \mid \rho^+ + \rho^- \mid K' > \quad \delta_{j,j'}\delta_{m_j,m_j'}, \quad (5)$$

where κ is the dielectric constant of the host, and ρ^+ and ρ^- are the density of charge of holes and acceptors, respectively, expressed in plane-wave representation.

RESULTS

We performed calculations on systems consisting of three $In_{0.3}Ga_{0.7}As$ wells of width d1 = 20 Å enclosed into four GaAs layers of width d2 = 20 Å. This complete set is separated of an AlAs barrier by other GaAs layers of width s=50 Å. In fig 1 we present spin charge density calculations for two different systems: in the left side we incorporate Mn into the well, and in the right side into the barrier. The left hand part of the figure shows that incorporating manganese into the DMS well increases spin polarization, but in the other hand all polarized charges are inside the well layers. In the right part we can see, that incorporating Mn into a DMS barrier enhances the polarization in the non-magnetic layer, leading to a system where we have spin polarized carriers with higher mobilities.

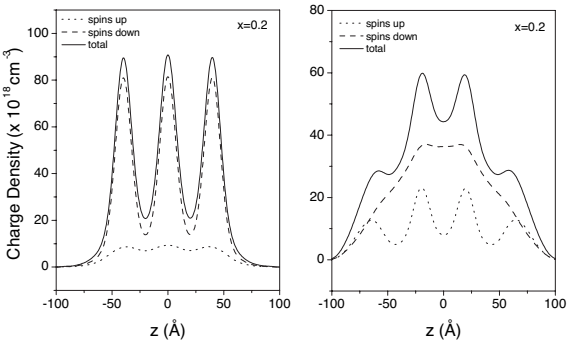

FIGURE 1. Density charge distribution of parallel and anti-parallel spin holes for three wells (InGaAs) and four barriers (GaAs). In the left side, Mn concentration in the well is x=0.2, in the right side, Mn concentration in the barrier is x=0.2. The well width is $d_1 = 20$ Å and barrier width is $d_2 = 20$ Å. the separation of the barriers/wells system to the enclosing AlAs layers is $s = 60$ Å.

CONCLUSIONS

In summary, we have investigated the spin charge distribution of strained $In_{0.3}Ga_{0.7-x}Mn_xAs/GaAs$ and $In_{0.3}Ga_{0.7}As/Ga_{1-x}Mn_xAs$ multilayers by using a super-cell model in the framework of the Luttinger-Kohn **k**.**p** approximation. By this study we find that incorporating Mn in the barrier would maximize spin charge distribution in the non-magnetic layer, increasing the carriers mobility.

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