Simulation of the tunnelling transport in ferromagnetic GaAs/ZnO heterojunctions

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Abstract. In this work we have implemented a numerical simulator and analytical model to study the dependence of the tunnelling current on the polarization ratio of the carrier spin for a degenerate and ferromagnetic heterojunction. We have applied these models to study the behaviour of a magnetically doped GaAs/ZnO PN junction and the current transport in a PN heterojunction where the polarization of the spin of the charge carriers is also a control variable.

1. Introduction
Spintronic devices based on diluted magnetic semiconductor (DMS) have been studied in the last years [1] due to the simultaneous control of both charge and spin of the carriers. Two of the most popular DMSs are (Ga,Mn)As and (Zn,Co)O, the first one because it is compatible with the current GaAs technology [2] and the second one because of its high Curie temperature [3]. Structures such as PN junctions [1] and resonant tunnelling devices [4] are being fabricated and studied. We develop analytical and numerical models that facilitate the study of magnetic tunnel junctions (MTJ) because of their potential applications as new magnetic sensors or magnetoresistive random access memory (MRAM). In this work we focus on the analysis of a theoretical GaAs/ZnO PN junction doped with magnetic impurities to study the dependence of the charge and spin transport on the spin polarisation of the charge carriers. The analytical model [5] is based on Kane’s theory [6] and the numerical simulator solves the drift-diffusion equations modified to consider the spin polarization. These two models allow us to predict the behaviour of the tunnel magnetoresistance (TMR) with the applied bias and temperature variation. In this paper we will show how we calculate the split bands in section 2, the tunnelling current in section 3 and the characteristics of the analytical model and how we implement the numerical model in sections 4 and 5, respectively. Finally we summarize our current results and the conclusions in section 6.

2. Spin splitting
Adding magnetic dopants to the semiconductors leads to the appereance of an exchange interaction between the carriers and the magnetic impurities. The effect on the energy band structure and transport properties can be studied using perturbation theory. It leads to a first order
correction in the band energies which means that the bands become spin split [7]. The new energy bands are:

\[ E_\sigma = E_0 + \frac{\Delta}{2} (\delta_{\sigma \uparrow} - \delta_{\sigma \downarrow}) \]  

where \( E_0 \) is the energy band when there is no spin polarisation, \( \sigma = \{\uparrow, \downarrow\} \) means spin up and down and \( \Delta = xJ_{exch}(S^z) \) is the energy splitting value, which depends on the magnetic impurity concentration \( x \), the strength of the exchange interaction \( J_{exch} \) and the average spin polarization which is obtained using the Brillouin function:

\[ x\langle S^z \rangle = xSB_S \left( \frac{g_1 \mu_B B_{eff}}{k_B T} \right) \]  

where \( S \) is the net spin that each magnetic impurity contributes \((S = 5/2 \text{ for Mn})\) and \( B_{eff} \) is the effective molecular magnetic field produced by the coupling between magnetic ions and charge carriers. Figure 1 shows the variation of the splitting energy with the temperature in Ga\(_{1-x}\)Mn\(_x\)As calculated using the previous model with a manganese concentration of \( x = 0.05 \) and a carrier concentration of \( p = 3 \cdot 10^{20} \text{ cm}^{-3} \). The Curie temperature is 110 K for this carrier concentration and above that temperature the ferromagnetic properties disappear.

\begin{figure}
\centering
\includegraphics[width=0.8\textwidth]{figure1.png}
\caption{Dependence of band splitting for (Ga,Mn)As on the temperature. The Curie temperature in this case, \( p = 3 \cdot 10^{20} \text{ cm}^{-3} \), is 110K. Above that temperature the ferromagnetism disappears.}
\end{figure}

\begin{figure}
\centering
\includegraphics[width=0.8\textwidth]{figure2.png}
\caption{Schematic representation of the spin split bands in a ferromagnetic PN junction. Two different configurations, one for (a) antiparallel and another for (b) parallel magnetisations between both sides of the junction.}
\end{figure}

3. Tunnelling current

Due to the high carrier concentration required in DMS to ensure ferromagnetic behaviour near or above room temperature, these are highly degenerate semiconductors. Therefore, the carrier transport at low bias will be dominated by tunnelling processes. The probability that an electron tunnels through the depletion region from the conduction band to the valence band is calculated using the WKB approximation:

\[ \Gamma_{c\rightarrow v} = \exp \left( -2 \int^{x_0} \frac{\kappa_c(x, \epsilon) \cdot \kappa_v(x, \epsilon)}{\sqrt{\kappa_c^2(x, \epsilon) + \kappa_v^2(x, \epsilon)}} dx \right), \]  

where \( \kappa_c \) and \( \kappa_v \) are the wavenumber vectors, which contain information about the effective mass and the energy of the carriers that take part in the tunnel process, and \( u \) and \( l \) are the classical turning points in the potential barrier.
Figure 2 shows a schematic representation of the two possible configurations in a MTJ for the tunnelling current depending on the relative magnetization between the P and N sides. The one shown in figure 2(a) has a low resistance because the majority spin for holes and electrons are recombining. We call this antiparallel configuration ($I_a$). However, in figure 2(b) the MTJ is more resistive and we call it parallel configuration ($I_p$). The TMR is evaluated as the relative difference of the tunnelling current in both cases, $TMR = |I_p - I_a|/(I_p + I_a)$.

The transport equations in the numerical simulator

where $\eta$ is the carrier concentration, $n$, $I$ is the electric field, $E_{Fn}$ and $E_{Fp}$ are the Fermi pseudo-levels for electrons and holes, $\epsilon$ is the carrier energy and $A_{cv}$ is the effective Richardson constant.

4. Analytical model

The analytical model solves an abrupt junction using the depletion region approximation. The energy band diagram is calculated considering a triangular barrier plus the discontinuity of the Fermi statistic to obtain the occupancy of the overlapped states, $F_c(E)$, and the tunnelling coefficient $\Gamma_{c-v}$:

$$I_t \propto \sum_{\sigma, \sigma'} \int_{E_{min}}^{E_{max}} [F_c(E) - F_v(E)] \Gamma_{c-v}(E, E_C^\sigma, E_V^\sigma) N_c(E, E_C^\sigma) N_v(E, E_V^\sigma) dE$$

4.1 Transport equations in the numerical simulator

The numerical simulator solves the Poisson equation and the continuity equations consistently with the spin split bands calculated in each point of the device. The drift-diffusion equations ($\nabla J_n = -q \mu_n (R_{c-v} + R_{c-v})$ and $\nabla J_p = q \mu_p (R_{c-v} + R_{c-v})$) are modified to consider the degenerate case using a correction factor $\xi(\eta) = \frac{F_{1/2}(\eta)}{F_{-1/2}(\eta)}$ to take account of the degeneration level:

$$J_n = \mu_n n \nabla E_C + n \nabla E_C$$

5. Results

We use the following parameters: $E_g = 1.4$ eV, $\chi = 4.07$ eV, $\epsilon_r = 13.2$, $m_n^* = 0.06m_0$ and $m_p^* = 0.5m_0$ for GaAs and $E_g = 3.4$ eV, $\chi = 4.20$ eV, $\epsilon_r = 8.6$, $m_n^* = 0.24m_0$ and $m_p^* = 0.59m_0$ suitable for ZnO [9]. The doping levels are $10^{20}$ cm$^{-3}$ in the N-side and $3 \cdot 10^{20}$ cm$^{-3}$ in the P-side. The calculations were done considering a 70% of spin polarization and the temperature was set to 77 K.
Figures 3(a) and 3(b) show the energy band diagram obtained from the analytical model and the numerical simulator, respectively. In figure 3(b) it is possible to see how the splitting disappears as the carrier concentration drops in the depletion region. The analytical model does not show this because the splitting is constant.

Figures 3(c) and 3(d) show the tunnelling current and TMR from the analytical model and the numerical simulator, respectively. The red solid line is the tunnelling current in a non ferromagnetic diode and the blue dashed line and the green dot-dashed line are the tunnelling current for the parallel and antiparallel configurations. The I–V characteristic shows that in the region where the diode is showing negative resistance, in biases between 0.2 V and 0.4 V, the TMR reaches the highest values. Half way in the negative resistance region, bias ∼ 0.3 V, the analytical model shows a higher value of the TMR, ∼ 50%, than in the drift-diffusion model, ∼ 40%. This can be explained by the constant splitting in the analytical model that reduces the tunneling-barrier width with respect to the numerical model, giving larger values of the parallel tunnelling current. The TMR for larger biases can not be considered because other components of the current (defect assisted or thermal current) have to be taken into account. The values of the TMR are in the same range as experimental values in resonant MTJs [4].

The analytical model is giving more optimistic results for the TMR than the numerical model. However, the numerical model allows a more precise description of the tunnelling current and its dependence on the spin splitting that leads to more realistic results.

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