Tight-binding model of spin-polarized tunnelling in (Ga,Mn)As-based structures

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Abstract

The Landauer-Büttiker formalism combined with the tight-binding transfer matrix method is used to describe the results of recent experiments: the high tunneling magnetoresistance (TMR) in (Ga,Mn)As-based trilayers and highly polarized spin injection in p-(Ga,Mn)As/n-GaAs Zener diode. For both TMR and Zener spin current polarization, the calculated values agree well with those observed experimentally. The role played in the spin dependent tunneling by carrier concentration and magnetic ion content is also studied.

Key words: spin polarization, tunneling magnetoresistance, Zener tunneling

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1. Introduction

Efficient spin injection is a fundamental prerequisite for construction of spintronic devices. On the other hand, the tunneling magnetoresistance (TMR) effect, examined in a pioneering work by Jullière [1], has found already many applications in, e.g., magnetic field sensors and magnetic random access memories, where the polycrystalline transition metals are usually employed as ferromagnetic layers. Both effects have been observed in (Ga,Mn)As-based structures. The first observation of a high (of about 75\%) TMR effect was reported for a trilayer structure (Ga,Mn)As/AlAs/(Ga,Mn)As [2]. Recently, TMR was observed in (Ga,Mn)As/GaAs/(Ga,Mn)As structures, [3,4] reaching about 300\% at low temperatures in devices, in which (Ga,Mn)As contained about 8\% of Mn [4]. Furthermore, peculiar behavior of TMR was observed in nanoconstrictions [5] as well as when the holes in (Ga,Mn)As were at the localization boundary [6]. Also, it has been demonstrated that highly spin polarized electron current, with polarization reaching 80\%, can be obtained from a p-(Ga,Mn)As/n-GaAs Zener diode [7].

2. Theoretical Model

To describe the spin dependent processes we employ the Landauer-Büttiker formalism for coherent tunneling. The transmission coefficients, needed in this approach, are determined in terms of the ex-
tended transfer-matrix method within the tight-binding framework that takes into account spin dependent terms. The tight-binding Hamiltonian matrix is composed of three parts: the left and right leads, and the middle region, where the incoming Bloch waves from the left lead are scattered into outgoing Bloch states of the right lead. By solving the Schrödinger equation for the tight-binding Hamiltonian, we determine the transfer coefficients $t_{k_{\perp,i} \rightarrow k_{\perp,j}}(E, k_{\parallel})$, which describe the probability of tunneling from the incoming state $k_{\perp,i}$ to the outgoing state $k_{\perp,j}$ for given electron energy $E$ and wave vector parallel to the surface $k_{\parallel}$ [8]. The tunneling current $j$ is given by,

$$ j = \frac{-e}{4\pi^2\hbar} \int_{BZ} d^2k_{\parallel} dE \sum_{k_{\perp,i},k_{\perp,j},v_{\perp,i},v_{\perp,j}>0} \left( f_L(E) - f_R(E) \right) |t_{k_{\perp,i} \rightarrow k_{\perp,j}}(E, k_{\parallel})|^2 \frac{v_{\perp,j}}{v_{\perp,i}} \frac{1}{\sqrt{v_{\perp,i}}}, \tag{1} $$

where $f_L$ and $f_R$ are the electron Fermi distributions in the left and right interface and $v_{\perp,i}$ are the group velocities of the corresponding Bloch states.

In order to construct the empirical tight-binding Hamiltonian matrix for the heterostructure we have to start from the description of the constituent materials. To describe the band structure of bulk GaAs we adopt the $sp^3d^5s^*$ tight-binding parametrization, with the spin-orbit coupling included, as proposed by Jancu et al. [9]. This model reproduces correctly the effective masses and the band structure of GaAs in the whole Brillouin zone, in agreement with the results obtained by empirically corrected pseudopotential method. The parametrization includes only the nearest neighbor (NN) interactions. For each anion and cation 20 orbitals are used - hence, with each GaAs layer (0.28 nm) of the structure the size of the tight-binding matrix increases by 40. The same set of orbitals is used to describe the (Ga,Mn)As layer. It should be pointed out that the $d$ orbitals used in our $sp^3d^5s^*$ parametrization are not related to the Mn ions incorporated into GaAs. The presence of Mn ions in (Ga,Mn)As is taken into account only by including the $sp$-$d$ exchange interactions within the virtual crystal and mean-field approximations. The values of the exchange constants are determined by the experimentally obtained spin splittings: $N_0\alpha = 0.2$ eV of the conduction band and $N_0\beta = -1.2$ eV of the valence band [10]. The other parameters of the model for the (Ga,Mn)As material are taken to be the same as for GaAs - this is well motivated because the valence-band structure of (Ga,Mn)As with small fraction of Mn was shown to be quite similar to that of GaAs [10]. We construct the tight binding matrix for the heterostructure taking for each double layer of the structure the description of the corresponding bulk material. The NN interactions between GaAs and (Ga,Mn)As are described by the same parameters as the interactions in bulk GaAs. Consequently, the valence band offset between (Ga,Mn)As and GaAs originates only form the spin splitting of the bands in (Ga,Mn)As.

The Fermi energy in the constituent materials is determined by summing up the occupied states over the entire Brillouin zone. The number of occupied states is determined by the assumed carrier concentration in the material. Our calculations of the dependence of Fermi energy on hole concentration are consistent with the corresponding results presented previously [11]. It should be noted that the Fermi energy in Ga$_{1-x}$Mn$_x$As depends crucially on the hole concentration, whereas very little on the Mn content $x$.

3. Results

3.1. Tunneling Magnetoresistance

In our calculations of the TMR effect we consider the structure containing three layers. The two half-infinite leads are build of the ferromagnetic p-type Ga$_{1-x}$Mn$_x$As. The middle scattering region is composed of the non-magnetic GaAs, which forms a barrier for the holes. We compare the tunneling currents in two configurations, i.e., with parallel (ferromagnetic – FM) and the antiparallel (anti-ferromagnetic – AFM) alignments of the magnetizations in the leads. We define the tunneling magnetoresistance as

$$ TMR = \frac{I_{FM} - I_{AFM}}{I_{AFM}}. $$
where $I_{FM}$ and $I_{AFM}$ are the currents in the FM and AFM configurations, respectively. In Fig. 1 (a) the obtained TMR values, for a given (8%) Mn content and a set of different hole concentrations in the FM layers, are plotted as a function of the applied bias. As shown, TMR depends strongly on the hole concentration. As TMR is primarily determined by spin polarization of the carriers at the Fermi level, the higher hole concentration the smaller is spin polarization at the Fermi level at given Mn spin polarization. For $p = 3.5 \times 10^{20} \text{cm}^{-3}$, which is the typical hole concentration in (Ga,Mn)As samples [12], the TMR of about 250% is obtained.

Because of self-compensation, the hole concentration depends rather weakly on $x$ — thus, we have calculated the TMR for different $x$ in the magnetic layers, while keeping the hole concentration constant, $p = 3.5 \times 10^{20} \text{cm}^{-3}$. The results of such computations are presented in Fig. 1(b).

As seen, our simple model reproduces fully the experimental data: for structures with 8% of Mn we obtain the TMR of the order of 250%, as observed recently by Chiba et al. [4]; for 4% of Mn the calculations lead to the TMR of the order of 60%, in perfect agreement with the observations of Tanaka and Higo [2] and Mattana et al. [3]. Therefore, our calculations seem to suggest that for obtaining a high TMR, large exchange splittings, i.e., high content of magnetic ions is needed. Unfortunately, the presented in Fig. 1 dependence suggests that the attempts to increase the hole concentration in (Ga,Mn)As, in order to obtain higher Curie temperature, may result in a reduced TMR value.

### 3.2. Zener Diode

As a second application of the developed formalism for spin-dependent tunneling, we consider the Zener diode in which high polarization of the spin current has been recently observed [7]. Alas, in approaches involving transfer matrix formalism, computational constraints hinder the simulations of the spin-dependent tunneling through the whole device used in the experiments in Ref. [7]. Therefore, we consider the simpler p-Ga$_{1-x}$Mn$_x$As/n-GaAs structure with relatively narrow depletion region consisting of 4 double-layers. Albeit simplified, such structure captures the essential physics concerning tunneling of electrons from the spin-polarized valence band of (Ga,Mn)As to the GaAs conduction band. Moreover, this approach can provide quantitative information on spin polarization of the current, even though it overestimates necessarily the tunneling current. Simulations which take into account a more realistic description of the depletion region are presented elsewhere [13].

In our computation, we assume that the magnetization vector is in 110 direction and we evaluate the spin current polarization in respect to this direction. We use Eq. (1) to compute separately the currents $j^\uparrow$ of spin up and $j^\downarrow$ of spin down electrons. The spin current polarization $P_j$ is defined as follows:

$$P_j = \frac{j^\uparrow - j^\downarrow}{j^\uparrow + j^\downarrow}.$$ 

We assume that the electron concentration is $n = 10^{19} \text{cm}^{-3}$ as indicated by the experimental results in Ref. [7]. The dependencies of $P_j$ on the hole concentration $p$ and Mn content $x$ are depicted in Fig. 2.

Similarly to TMR, the presented in Fig. 2 results show a strong decrease of the tunneling current spin polarization with the increase of hole concentration. The spin injection in the Zener diode, again like in TMR, depends crucially on the con-
Hole concentration - $p$ [cm$^{-3}$]

\begin{align*}
\text{P}_j \ (\text{a}) & \quad 0 \ 0.02 \ 0.04 \ 0.06 \ 0.08 \\
\text{Mn content - x} & \quad 0 \ 0.2 \ 0.4 \ 0.6 \ 0.8 \ 1 \\
\end{align*}

Fig. 2. Spin current polarization $P_j$ in p-Ga$_{1-x}$Mn$_x$As/n-GaAs as a function of: (a) hole concentration $p$ (for $x = 0.08$); (b) Mn content (for $p = 3.5 \times 10^{20}$ cm$^{-3}$). The bias applied to the structure is $V = 0.05$ V.

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