Spin Dependent Tunneling in FM|semiconductor|FM structures

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Abstract

Here we show that ordinary band structure codes can be used to understand the mechanisms of coherent spin-injection at interfaces between ferromagnets and semiconductors. This approach allows the screening of different material combinations for properties useful for obtaining high tunneling magnetoresistance (TMR). We used the Vienna Ab-initio Simulation Code (VASP) to calculate the wave function character of each band in periodic epitaxial Fe(100)|GaAs(100) and Fe(100)|ZnSe(100) structures. It is shown that Fe wave functions of different symmetry near Fermi energy decay differently in the GaAs and ZnSe.
Recently there has been much interest in spin-dependent tunneling between ferromagnetic (FM) electrodes separated by insulator (I) or semiconductor (S). This interest arises both from a desire to better understand spin-dependent transport and because of possible technological applications. It has been observed experimentally that the tunneling current through a FM[I]FM sandwich may depend on the relative alignment of the moments of the ferromagnetic electrodes on opposite sides of the barrier [1, 2, 3, 4, 5, 6].

Large magnetoresistance was predicted in recent calculations for certain epitaxial tunneling systems [7, 8, 9, 10, 11]. These predictions were based on a spin filtering effect that may arise from the symmetry of the wave functions. At the Fermi energies of bcc Fe, bcc Co and CoFeB, there is a difference in the symmetries of wave functions between the majority and minority spin channels. Specifically there is a $\Delta_1$ Bloch state for the majority, but not for the minority. For some insulating and semiconducting materials, states with this $\Delta_1$ symmetry will decay much more slowly than states with different symmetries. Recently these predictions have been largely confirmed [12, 13, 14, 15].

In this paper we consider the symmetric structures Fe(100)|GaAs(100)|Fe(100) and Fe(100)|ZnSe(100)|Fe(100). Because the lattice constant of bcc Fe is approximately half that of zinc blend GaAs ($2a_{Fe}/a_{GaAs} = 1.014$) and ZnSe ($2a_{Fe}/a_{ZnSe} = 1.011$), they fit very well epitaxially. Here we report investigations of the potential for spin-dependent transport by exploring the effect of wave function symmetry on the decay of Bloch states within the barrier. In systems with two-dimensional periodicity, the wave function symmetry is conserved as the electron traverses the interface. We observe that wave functions with different symmetries will decay at different rates within the barrier. These symmetries can be determined from the angular momentum composition of the Bloch states.

The interfacial structure is critical to understanding tunneling, especially, spin-dependent tunneling. For the case of bcc Fe(100)|MgO(100)|Fe(100) and similar systems, it was important to find ways of preventing the incorporation of oxygen into the interfacial Fe layer [8, 13]. Here we have studied three different epitaxial interfaces in order to search for the most stable interface of Fe(100)|GaAs(100) and Fe(100)|ZnSe(100) [16]. The structures are presented in Fig. 1 with following details:

Model A: Atomically abrupt interface of bcc Fe and zinc-blende GaAs;
Model B: Partially intermixed i.e., one Fe atom filling the vacancy site in GaAs lattice;
Model C: Fully intermixed i.e., two Fe atoms filling the vacancy sites in GaAs lattice.
For each model we attempted first to consider a supercell consisting of 12 Fe atoms (6 layers for Model A and 5 layers for Models B and C) and 9 atomic layers of GaAs. It turned out, however, to be impossible to construct all models with equal numbers of each type of atom while maintaining the same symmetry at both interfaces. To overcome this problem, we constructed Models A and C with 14 Fe atoms and 9 atomic layers of GaAs with symmetric interfaces. In the case of Model B, the interfacial symmetry requirement cannot be fulfilled with 14 Fe atoms. Therefore we approached this problem by calculating the energy for this configuration in two different ways. Assuming that the effect of the interface will be less in the middle of Fe layer, we have calculated the bulk Fe energy taking the interlayer distance at the middle of Fe layer. The energy of one layer of Fe from this calculation added to the energy of Model B (12 Fe atoms) gives the energy of 14 Fe atoms with symmetric interface. In the second case, the energy of Model B with 16 Fe atoms was calculated and subtracted from the energy of 12 Fe atoms giving thus the energy of 2 Fe layers. Taking half of this energy gives the energy of 1 Fe layer (2 Fe atoms per cell per layer), which was added to the energy of 12 Fe layers Model B ending up with the energy of 14 Fe atoms Model B. Finally, by comparison of all three models we found that the Model
A is the most stable, which is consistent with previous work [16]. We performed similar calculations for Fe|ZnSe structure and found again that Model A is more stable than other models.

As a next step, we evaluated the $s$, $p$ and $d$ site projected wave function character of bands with different symmetries near the Fermi energy for the relaxed structure corresponding to Model A with 14 Fe atoms. The calculations were performed using a plane wave based code (VASP) [17]. In Fig. 2 and Fig. 3 we present layer resolved wave function probability density, $\psi^*\psi$ for the majority spin state with $\Delta_1$, $\Delta_{2'}$ and double degenerate $\Delta_5$ symmetry for Fe|GaAs and Fe|ZnSe structures, respectively. One can see that the slowest decay rate is for states with $\Delta_1$ symmetry. States with $\Delta_5$ and $\Delta_{2'}$ symmetry decay much more rapidly. It is clear that there is a huge difference in the way wave functions that live primarily on the Fe decay into the GaAs and ZnSe. To clarify the nature of such decay rates, we plotted the dependence of the squared quasi momentum $k^2$ as a function of energy for Bloch states traveling in the (100) direction for GaAs and ZnSe. They are shown in Fig. 4 and Fig. 5, respectively. In the vicinity of the gap $k^2$ can be represented by

$$\frac{1}{k^2(E)} = \frac{\hbar^2}{2m^*_v(E - E_v)} + \frac{\hbar^2}{2m^*_c(E - E_c)}$$

(1)

where $E_v$ and $E_c$ are the top of the valence band and the bottom of the conduction band,

FIG. 2: Absolute square of $\Delta_1$ (squares), $\Delta_{2'}$ (circles) and $\Delta_5$ (triangles) wave functions in a Fe|GaAs supercell. The dashed lines without data points indicate the expected decay rate based on Equation (1).
respectively, for the $\Delta_1$ band. For both of these systems we find that the effective masses $m_v$ and $m_c$ are approximately equal at the band edges so that the $k^2$ as a function $E$ has the form of a parabola. We have calculated the effective mass $m^*/m$ for both GaAs and ZnSe by fitting the above formula to the curves in Fig. 4 and Fig. 5. The calculated effective mass, $m^*/m$ is 0.0353 for GaAs and 0.0993 for ZnSe. The decay of the absolute square of the wave function of a given symmetry in the gap will be proportional to $\exp(-2|k|z)$, where $k$ is obtained from equation (1). Note that $k^2$ is negative in the gap so $k$ is imaginary.

In summary, we have shown that Bloch states of only certain symmetries are able to propagate through the barrier and the wrong symmetry cannot propagate in a metallic electrode. Coherent spin-injection across an Fe(100)|GaAs(100) and Fe(100)|ZnSe(100) interface can be understood using ordinary band structure codes, providing an efficient tool to screen material combinations for spin-injection. It should be noted that the energy gaps given by DFT based codes tend to significantly underestimate band gaps. An alternative approach would be to use electronic structure calculations to identify the symmetries of the complex energy bands at the top and bottom of the gap and then to use experimental band masses and energy gap measurements to estimate decay rates.

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FIG. 4: Dispersion $k^2(E)$ for GaAs in the vicinity of the gap along $\Delta$ (100). $E_v$ labels the top of the valence band and $E_c$ is the bottom of the conduction band.

FIG. 5: The same as Fig. 4 for ZnSe.

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