Spin-dependent tunneling in FM|semiconductor|FM structures

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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. © *2006 American Institute of Physics*.
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Recently, there has been much interest in spin-dependent tunneling between ferromagnetic (FM) electrodes separated by an insulator (I) or a 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.[1–6]

Large magnetoresistance was predicted in recent calculations for certain epitaxial tunneling systems.[7–11] 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 Δ_1 Bloch state for the majority, but not for the minority. For some insulating and semiconducting materials, states with this Δ_1 symmetry will decay much more slowly than states with different symmetries. Recently these predictions have been largely confirmed.[12–15]

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-blende 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.[9,13] 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 the 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 the GaAs lattice.
- Model C: Fully intermixed, i.e., two Fe atoms filling the vacancy sites in the 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

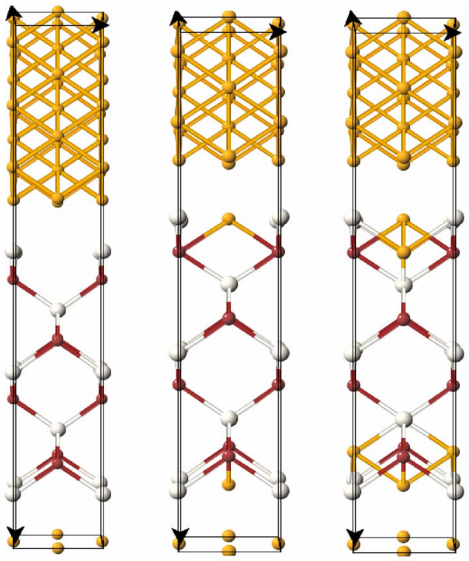

FIG. 1. (Color online) Three interface structures of Fe|GaAs(100) and Fe|ZnSe(100). Models A, B, and C (from the left).

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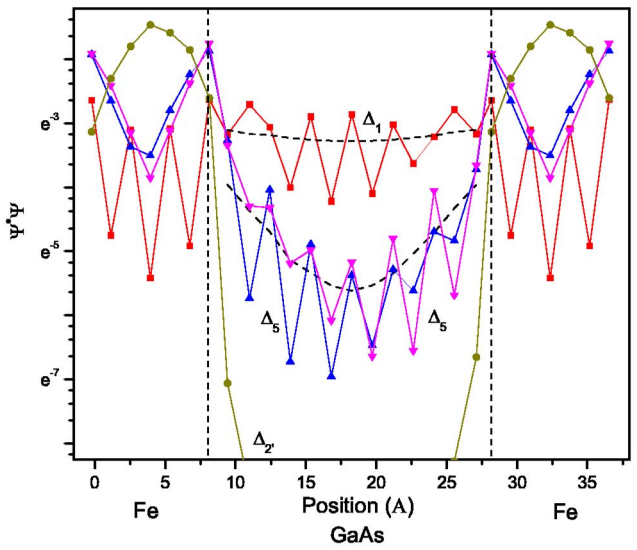

FIG. 2. (Color online) Absolute square of Δ_1 (squares), $\Delta_{2'}$ (circles), and Δ_5 (triangles) wave functions in a Fe|GaAs supercell. The dashed lines without data points indicate the expected decay rate based on Eq. (1).

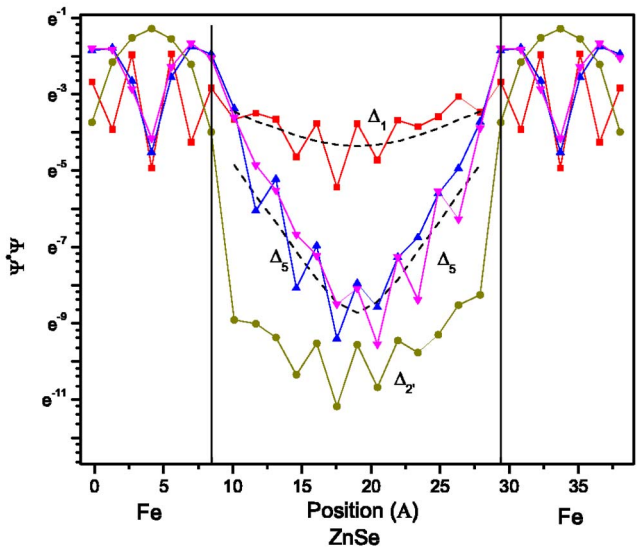

FIG. 3. (Color online) The same quantities as in Fig. 2 for Fe|ZnSe.

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 the Fe layer, we have calculated the bulk Fe energy taking the interlayer distance at the middle of the 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 in Model B ending up with the energy of 14 Fe atoms in Model B. Finally, by comparison of all three models, we found that 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 Figs. 2 and 3, we present layer-resolved wave-function probability density, $\psi^*\psi$ for the majority spin state with $\Delta_1, \Delta_{2'}$ and double degenerate Δ_5 symmetry for Fe|GaAs and Fe|ZnSe structures, respectively. One can see that the slowest decay rate is for states with Δ_1 symmetry. States with Δ_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 quasimomentum k^2 as a function of energy for Bloch states traveling in the (100) direction for GaAs and ZnSe. They are shown in Figs. 4 and 5, respectively. In the vicinity of the gap, k^2 can be represented by

$$\frac{1}{k^2(E)} = \frac{\hbar^2}{2m_v^*(E-E_v)} + \frac{\hbar^2}{2m_c^*(E-E_c)}, \tag{1}$$

where E_v and E_c are the top of the valence band and the bottom of the conduction band, respectively, for the Δ_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 Figs. 4 and 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 pro-

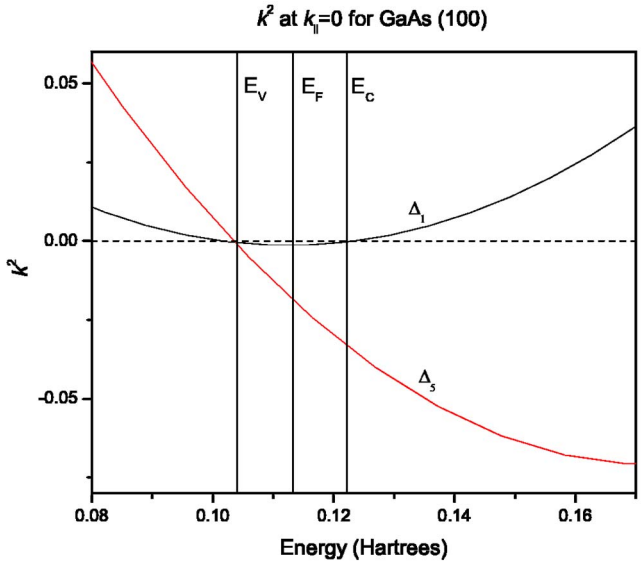

FIG. 4. (Color online) Dispersion $k^2(E)$ for GaAs in the vicinity of the gap along Δ (100). E_v labels the top of the valence band and E_c is the bottom of the conduction band.

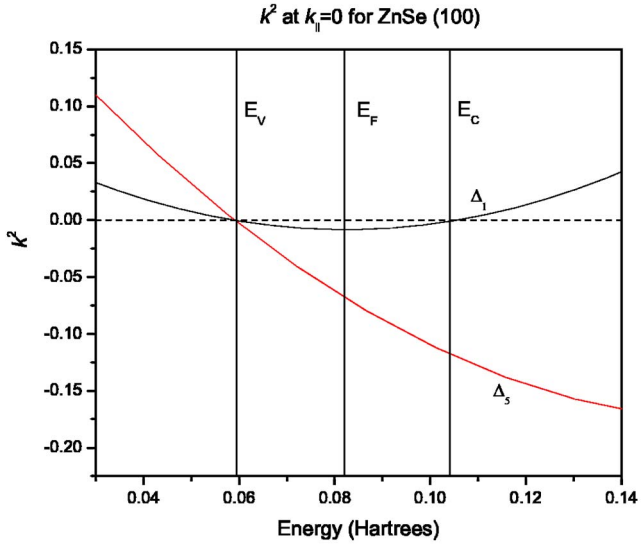

FIG. 5. (Color online) The same as Fig. 4 for ZnSe.

portional to $\exp(-2|k|z)$, where k is obtained from Eq. (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. 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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