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TUNNELING TRANSPORT IN FERROMAGNET/ INSULATOR/FERROMAGNET JUNCTIONS

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We study the spin-dependent transport in expitaxial Ferromagnet/Insulator/Ferromagnet junctions. Firstly we show that the tunneling through the insulator can be described by the complex band structure of the insulator in the gap region, i.e. by the metal-induced gap states. Since the imaginary part of the Bloch vector describes the decay of the wave function, we calculate the spectrum of the decay parameters κ for several semiconductors. For large thicknesses the state with the smallest κ-value dominates the current. In the second part we present the results of ground state calculation for Fe/ZnSe/Fe(001) and related junctions. We obtain a rather localized charge transfer from the interface Fe layer to the neighbouring semiconductor layer, which is largest for the low-valent termination. Moreover we find that the local moments at the interface depend sensitively on the lattice parameter chosen. Finally, we show that in the minority band at E_F an Fe interface state exists, which deeply penetrates into the barrier.

Keywords: Tunneling junctions; Tunneling magnetoresistance; Complex band structure; Interface states

1. INTRODUCTION

Tunnel junctions consisting in ferromagnet/insulator/ferromagnet (FM/I/FM) layers are at present intensively studied because of the potential application as non-volatile magnetic random access memory (MRAM). Jullière (1975) first showed that in such junctions the transmission is spin-dependent and thus the conductance is different for the parallel and antiparallel orientation of the magnetization of the two FM leads, leading to the so-called *tunneling magnetoresistance* (TMR) effect. More recently (Tezuka and Miyazaki, 1996) and Moodera *et al*. (1995) were able to obtain in room temperature experiments TMR ratios of up to 20% and at present room temperature values of 40% are reported by various groups. The understanding of the TMR and the electronic structure of the junctions has not progressed equally fast. Theoretical calculations based on models (Slonczewski, 1989; MacLaren *et al*., 1999; Zhang and Levy, 1998) have shed some light on various aspects of the effect, but only recently *ab-initio* calculations of the electronic structure and the spin-dependent transmission have been reported (Butler *et al*., 1997; MacLaren *et al*., 1999; Oleinik *et al*., 2000).

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In this paper, we will consider the tunneling through epitaxial systems, so that the whole junction is characterized by a two-dimensional periodicity. Two particular aspects will be treated. Firstly, we demonstrate that the tunneling through insulators can be understood in terms of the metal-induced gap states (MIGS) introduced by Heine (Heine, 1963, 1964, 1965) and that the framework to investigate them is the complex band structure of the insulator in the gap region. Secondly, we will present calculations for the ground-state properties of the junction, discussing in particular the charge transfer, the magnetic profile and the local density of states at the interface. In both cases, we consider as model system Fe/I/Fe(001) sandwiches, where I refers to the semiconductors ZnSe and GaAs, growing expitaxially on Fe.

2. COMPLEX BAND STRUCTURE AND TUNNELING

In the bulk of a crystal, the periodicity demands that the Bloch $\boldsymbol{k}$-vectors are purely real. But near a crystal surface or interface one can match a bulk wave function of complex $\boldsymbol{k}$ in the insulator with the solution outside the half-crystal (Heine, 1963). For the interface between a metal and an insulator the most important of such states are MIGS, being itinerant in the metal but exponentially decaying in the insulator (for energies in the gap). Such solutions for complex $\boldsymbol{k}$-vectors form the complex band structure of the insulator. Although they only occur at surfaces or interfaces, they are solutions of the bulk Schrödinger equation, since the interface-induced changes of the potential are confined in their greatest part to the first one or two monolayers.

For the considered transport problem, under an infinitesimal applied voltage metallic electrons with energies at the Fermi level E_F impinge on the insulator interface. Due to the assumed perfect epitaxy the in-plane component $\boldsymbol{k}_\parallel$ of the incident wave vector $\boldsymbol{k} = (\boldsymbol{k}_\parallel, k_z)$ is conserved. Therefore in the insulator only evanescent states with a given (real) energy E_F and a real $\boldsymbol{k}_\parallel$-component are allowed, so that only the perpendicular component $k_z = q + i\kappa$ can be complex, with the "decay parameter" κ describing the exponential decrease of the wave function in the insulator.

As pointed out in a recent letter (Mavropoulos *et al.*, 2000) the central problem for tunneling is therefore the determination of these decay parameters κ, in particular the search for the smallest possible κ-value $\kappa_{\min}$ for a given Fermi energy in the gap. In fact in the limit of large barrier thickness only the state with the smallest decay parameter, $\kappa_{\min}$, survives and contributes to the tunneling current. The determination of $\kappa_{\min}$ can proceed in two steps. Firstly for given values of $\boldsymbol{k}_\parallel$ and E_F one has to determine, out of the infinitely many solutions with different decay parameters, the one with the smallest $\kappa > 0$ value. In the second step one can then vary $\boldsymbol{k}_\parallel$, and search for the absolute minimum $\kappa_{\min}$ compatible with E_F. Of course, states with κ close enough to $\kappa_{\min}$ will be also important.

The method used for the calculation of the complex band structure is the simplest possible: we apply the local pseudopotential plane-wave technique with empirical form factors. Since these form factors have been fitted to spectroscopic data, this method gives a reasonably good description of the band structure in the gap region, this being the most important for the tunneling. Clearly local density functional calculations give a much better overall description of the band structure, but they have the well-known deficiency of underestimating the band gap by about 50%. Thus the above method is well suited for our purpose.

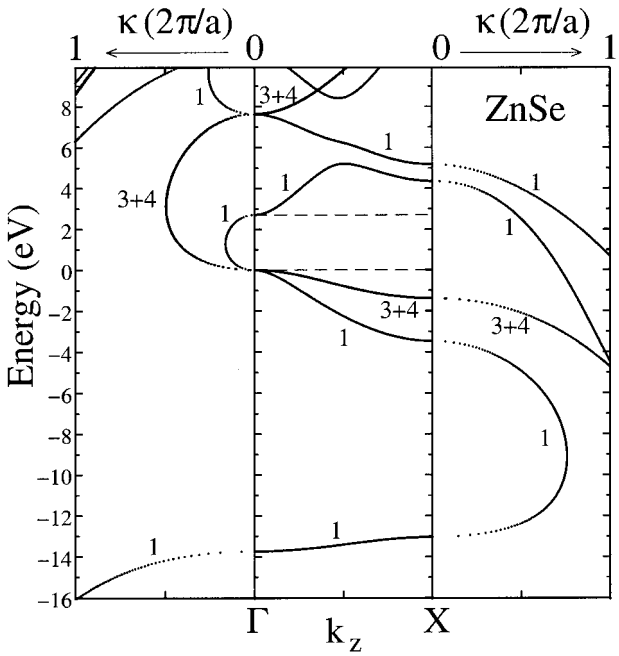

FIGURE 1 The complex band structure of ZnSe, for $\boldsymbol{k}_{\parallel} = 0$, at $q = 0$ (left panel) and $q = 2\pi/a$ (right panel). The real lines are forming loops and free-electron-like parabolas.

In the following we can only shortly sketch some of our results. For more details we refer to (Mavropoulos *et al.*, 2000). Figure 1 shows the band structure of ZnSe for perpendicular incidence ($\boldsymbol{k}_{\parallel} = 0$) on a ZnSe(001) interface, the real bands with k_z real in the middle panel and the complex parts for $q = 0$ in the left and for $q = 2\pi/a$ in the right panel. Here directly the dispersion of the decay parameter κ as a function of energy is plotted. For a given energy in the band gap the one with the smallest κ is that of symmetry Δ_1 (the identity representation) connecting the top of the Δ_1 valence band to the bottom of the Δ_1 conduction band. We expect this to be true quite generally when we are dealing with a direct gap characterized by a Δ_1 valence band maximum and a Δ_1 conduction band minimum. Then the loop connecting these particular extrema will be smaller than any other one, and so will be the corresponding value of the decay parameter.

The next larger κ-values arise from the degenerate Δ_3 and Δ_4 bands, and, additionally, infinitely many other inverse-parabolic states exist starting from higher bands, having much larger κ-values. Departing from the $\bar{\Gamma}$-point, we know that the valence states are lowered energetically, the conduction states are raised and the gap increases. For this reason it is expected that the loops at $q = 0$ become larger for non-zero $\boldsymbol{k}_{\parallel}$ values, and the corresponding values of κ increase.

Thus, by proceeding the search for $\kappa_{\min}$, one can scan the whole two-dimensional surface Brillouin zone at a given energy. One would thus form a constant-energy surface in the $(\boldsymbol{k}_{\parallel}, \kappa)$-space. This consists of many branches, corresponding to the (infinitely) many different complex bands for any given $\boldsymbol{k}_{\parallel}$, but our attention should be focused on the lowest-lying one. This is shown in Fig. 2 for two materials, namely

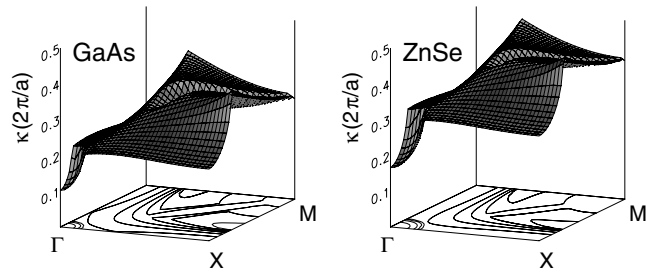

FIGURE 2 The constant-energy surfaces $\kappa = \kappa(\boldsymbol{k}_\parallel)$ drawn in one-fourth of the surface Brillouin zone for GaAs, and ZnSe. Only the lowest positive branches of the decay parameter κ are drawn for an energy in the middle of the band gap. The decay parameter has its minimum at the $\bar{\Gamma}$-point in both cases.

GaAs, and ZnSe, for a typical value of E_F in the middle of the gap. We see that in both cases the decay parameter is minimized at the $\bar{\Gamma}$-point. We also see that the difference of κ at the flatter part of the branch and at $\boldsymbol{k}_\parallel = 0(\kappa_{\min})$ increases monotonically with the band gap, in the order GaAs < ZnSe. However other cases can also occur. For instance, for Si the $\kappa_{\min}$-state is determined by the complex band structure close to the X-point, if the Fermi energy approaches the conduction band minimum. The above results have important consequences for tunneling. In the metal only states of Δ_1-symmetry (in the nomenclature of the ZnSe T_d-symmetry group) can couple to the Δ_1-states in the semiconductor and thus for large insulator thicknesses only metallic states at the $\bar{\Gamma}$-point and with Δ_1-symmetry determine the tunneling currents. The different availability of these Δ_1-states in the majority and minority bands leads to magneto-resistance. Our analysis is fully consistent with the *ab initio* results of (MacLaren *et al.*, 1999).

3. GROUND STATE PROPERTIES OF Fe/ZnSe/Fe(001)

The results reported in this section are based on density functional theory in the local density approximation. We use the tight-binding version of the KKR-Green's function method (Wildberger *et al.*, 1997), which allows N-scaling calculations for layered systems. Moreover we assume spherically symmetric ASA potentials and cut-off the wave functions at $l_{max} = 2$, while the full charge density is included. The investigated geometry consists of two Fe(001) half-spaces being separated by 7 monolayers of ZnSe or GaAs. The half-space Green's functions are calculated by the decimation technique (Sancho *et al.*, 1985). We assume a perfect matching of the bcc lattice of Fe with the zinc-blende lattice of the semiconductors, so that no lattice relaxations are allowed and all atoms are fixed at the positions as determined by the lattice constant of Fe, for which we take the experimental value. For this structure, the zinc-blende lattice constant is twice as large as the bcc constant of Fe, so that each Fe layer contains two non-equivalent Fe atoms. The potentials of 4 Fe layers on both sides of the junction are calculated self-consistently, while all other Fe potentials are replaced by the bulk values.

Charge Transfer All calculations show an interfacial charge transfer from the Fe atoms to the semiconductor atoms. For the Fe/7 ML ZnSe/Fe(001) junction with a

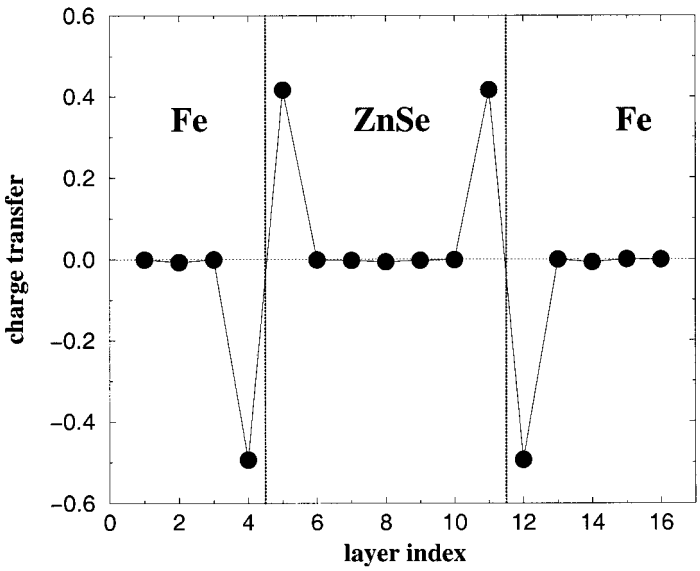

FIGURE 3 Charge transfer per monolayer in an Fe/7 ML ZnSe/Fe(001) junction with Zn terminated interfaces.

Zn-terminated interface the charge transfer per Fe monolayer is shown in Fig. 3. About 0.5 electrons (0.25 electrons per interfacial Fe atom) are transferred from Fe layer and mostly deposited on the interfacial Zn layer, leading to a very localized charge transfer affecting basically only two interface layers. For a Se-terminated interface a somewhat smaller transfer of 0.31 electrons is obtained, despite of the layer electronegativity of Se as compared to Zn. Qualitatively similar results are also obtained for a GaAs interlayer.

Local Moments at the Interface The moment profile of a Fe/ZnSe/Fe(001) junction with 7 ZnSe monolayers is shown in Fig. 4, for both a Zn and a Se terminated interface. The moments induced in the semiconductor is very small and strongly decreasing with the distance from the interface. For the Se-termination the Fe moments at the interface are practically the same as in the bulk, while for the Zn-termination the interfacial moments are increased by about $0.25\mu_B$. However, these results depend strongly on the choice of the lattice parameter used in the calculation. When we change from the experimental value ($a = 10.85$ a.u.) of Fe to the value calculated within the LDA from the minimum of the total energy, i.e. $a = 10.41$ a.u., the interface moments are drastically reduced, for the Se termination to about $1.5\mu_B$, and for the Zn-termination to $2.11\mu_B$, while the bulk moment changes from $2.32\mu_B$ to $2.12\mu_B$. Thus the moments at the interface do not only depend on the termination, but also on the lattice parameter used in the calculation. For these reasons we also expect a sensitive dependence on the relaxations at the interface, which are not included in the present calculations. A satisfactory solution of this problem can presumably be achieved if an improved exchange correlation functional like the generalized gradient approximation (GGA) is used. Furthermore relaxations at the interface should be taken into account.

Density of States at the Interface Figure 5 shows the local densities of states (LDOS) of the layers close to the interface for the Zn-terminated Fe/7 ZnSe/Fe(001) junction.

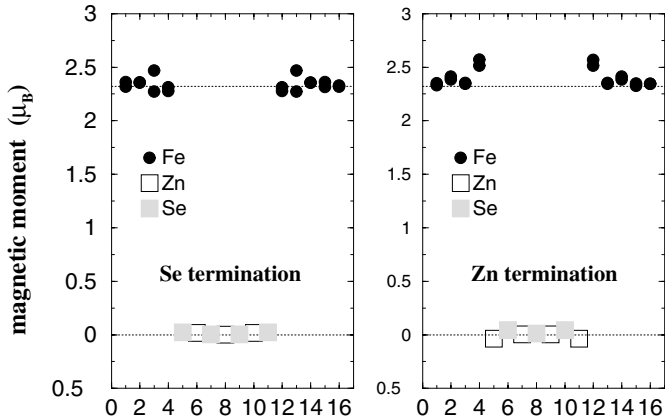

FIGURE 4 Magnetization profile in Fe/7ZnSe/Fe(001) junction with Zn termination, using the experimental lattice parameter of Fe.

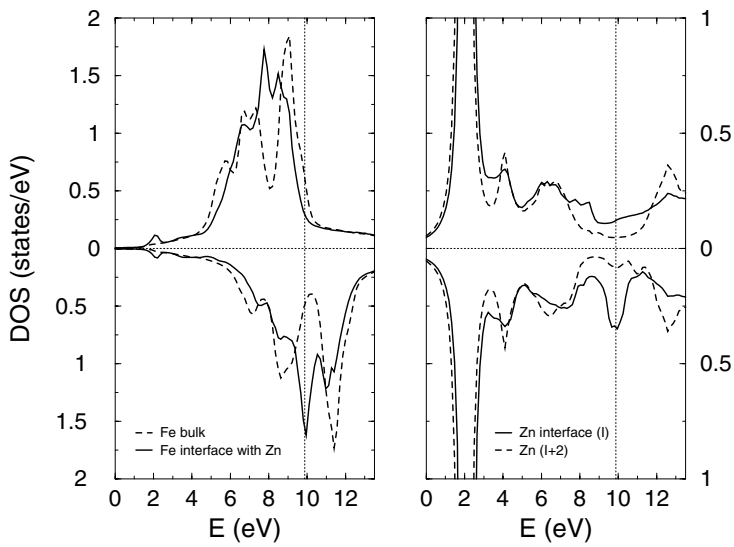

FIGURE 5 Spin-splitted local density of states in an Fe/ZnSe/Fe(001) junction with Zn-terminated interfaces. Left pannel: LDOS of interfacial Fe layer (full line) as compared to the DOS of bulk Fe (dashed). Right pannel: LDOS of interface Zn layer (full line) and the Zn atom two layers away from interface (Zn(I+2), dashed).

The left figure shows the LDOS of the interface Fe layer (solid line) in comparison to the DOS of bulk Fe (dashed), the right one the LDOS of the interface Zn atom (solid line) in comparison to the LDOS of a Zn atom two layers away from the interface (dashed). The LDOS of the interface Fe atom shows a familiar feature known from the Fe(001) surface, i.e. an interface state in the pseudogap of the bulk DOS, which in the minority band is directly located at E_F. As for the surface, this is basically a non-bonding peak, arising from the lack of hybridization with the missing Fe partners on the other side of the interface.

Characteristic for the LDOS of the interfacial Zn atom is the absence of a bandgap. Both for the majority and the minority bands the energy gap is filled with metal-induced gap states (MIGS) which decrease exponentially into the barrier so that only asymptotically, in very thick barriers, a true gap exists. While the MIGS in the gap region of the majority band show very little structure, one sees that in the minority band the Fe interface state also shows up at the interfacial Zn side and penetrates as a MIGS into the semiconductor. The MIGS and in particular the interface states can also be traced up in the two-dimensional Brillouin zone. Here the minority interface state shows up at the Γ point as a state of Δ_1-symmetry at around the Fermi level. The very weak decay of these states, as explained in Section 2, ensures a deep penetration into the semiconductor. As pointed out by Tersoff (1984) the MIGS play an important role in pinning the Fermi level in the gap. In short, charge neutrality should be achieved, if only the lower half of the MIGS are occupied, since these states have valence band character. For the interface states one expects therefore that the Fermi energy coincides with the peak of the interface states, which is indeed the case.

4. SUMMARY

We have presented a theoretical study of tunnel junctions consisting of epitaxial Ferromagnet/Insulator/Ferromagnet layers. As demonstrated, the tunneling process can be described by the complex band structure of the insulator in the gap region, i.e. by the metal-induced gap states. Asymptotically for thick barriers the tunneling is dominated by those Bloch states, which have the smallest imaginary part of the Bloch vector. For the systems considered (Si, Ge, GaAs and ZnSe) these are states of Δ_1-symmetry of the Γ point, making the tunneling process extremely state-selective. *Ab-initio* calculations for the ground state properties of Fe/ZnSe/Fe(001) and similar junctions yield a sizeable charge transfer from the interface Fe layer to the neighboring semiconductor layer. The magnetic moments at the interface depend sensitively on lattice relaxations. For all the investigated junctions an Fe interface state exists in the minority band at E_F which strongly penetrates into the barrier.

References

Butler, W.H., Zhang, X.-G., Wang, X., van Ek, J. *et al.* (1997). Electronic structure of FM/semiconductor/FM spin tunneling structures. *J. Appl. Phys.*, **81**, 5518.

Heine, V. (1963). On the general theory of surface states and scattering of electrons in solids. *Proc. Phys. Soc.*, **81**, 300.

Heine, V. (1964). Some theory about surface states. *Surf. Sci.*, **2**, 1.

Heine, V. (1965). Theory of surface states. *Phys. Rev. A*, **138**, 1689.

Jullière, M. (1975). Tunneling between ferromagnetic films. *Phys. Lett. A*, **54**, 225.

MacLaren, J.M., Zhang, X.-G., Butler, W.H. and Wang, X. (1999). Layer KKR approach to Bloch-wave transmission and reflection: Application to spin-dependent tunneling. *Phys. Rev. B*, **59**, 5470.

Mavropoulos, P., Papanikolaou, N. and Dederichs, P.H. (2000). Complex band structure and tunneling through ferromagnet/insulator/ferromagnet junctions. *Phys. Rev. Lett.*, **85**, 1088.

Moodera, J.S., Kinder, L.R., Wong, T.M. and Meservey, R. (1995). Large magnetoresistance at room temperature in ferromagnetic thin film tunnel junctions. *Phys. Rev. Lett.*, **74**, 3273.

Oleinik, I.I., Tsymbal, E.Y. and Pettifor, D.G. (2000). Structural and electronic properties of $Co/Al_2O_3/Co$ magnetic tunnel junction from first principles. *Phys. Rev. B*, **62**, 3952.

Sancho, M.P.L., Sancho, J.M.L. and Rubio, J. (1985). Highly converged schemes for the calculation of bulk and surface green functions. *J. Phys. F: Met. Phys.*, **15**, 851.

Slonczewski, J.C. (1989). Conductance and exchange coupling of two ferromagnets separated by a tunneling barrier. *Phys. Rev. B*, **39**, 6995.

Tersoff, J. (1984). Schottky barrier heights and the continuum of gap states. *Phys. Rev. Lett.*, **52**, 465.

Tezuka, N. and Miyazaki, T. (1996). Magnetic tunneling effect in $Fe/Al_2O_3/Ni_{1-x}Fe_x$ junctions. *J. Appl. Phys.*, **79**, 6262.

Wildberger, K., Zeller, R. and Dederichs, P.H. (1997). Screened KKR-Green's-function method for layered systems. *Phys. Rev. B*, **5**, 10074.

Zhang, S. and Levy, P.M. (1998). Magnetoresistance of magnetic tunnel junctions in the presence of a nonmagnetic layer. *Phys. Rev. Lett.*, **81**, 5660.