ELSEVIER

Journal of Magnetism and Magnetic Materials 189 (1998) L131–L135

Journal of magnetism and magnetic materials

Letter to the Editor

Role of electronic structure in magnetic tunneling

Kuising Wang[a], Shufeng Zhang[a], Peter M. Levy[a,*], Laszlo Szunyogh[b], Peter Weinberger[b]

[a] *Department of Physics, New York University, 4 Washington Place, New York, NY 10003, USA*
[b] *Institute of Technical Electrochemistry, TU Vienna, A-1060 Vienna, Austria*

Received 29 June 1998

Abstract

To assess the effect of electronic structure of magnetic electrodes on the magnetoresistance of tunnel junctions (JMR) we made ab initio calculations of the electronic structure of BCC(1 0 0) Fe, and FCC(1 0 0) Co and Ni electrodes. We treat hopping to and propagation in the barrier as adjustable parameters and discuss features of the JMR attributable to the electronic structure of the electrodes.

PACS: 73.40.-c

Keywords: Tunneling; Magnetoresistance; Band; Coupling

For an ab initio calculation of transport in magnetic tunnel junctions (MTJ) we resort to a Transfer Hamiltonian-like approach developed by Caroli et al. [1]. To determine the tunneling current we need the electrode Green's functions, the hopping integrals between the electrodes and the barrier, and the electron propagator inside the barrier. Here we focus on the role of the electronic structure of the electrodes in determining magnetoresistance of the MTJ, called JMR, and treat the latter two ingredients as adjustable parameters. The electrode Green's functions are obtained by using a layered version of scalar relativistic screened Korringa–Kohn–Rostoker (SKKR) Green's function method [2]. Our present study, while similar in spirit, differs from the one by Tsymbal [3].

We have extended Caroli's approach to a two-band s–d model. Tunneling conductance for each spin channel is

$$G = \frac{4\pi^2\,\mathrm{e}^2}{h}\mathrm{Tr}[\rho_\alpha \tau_{\alpha\beta} \rho_\beta (\tau_{\alpha\beta})^\dagger], \tag{1}$$

where all quantities in the brackets are 2×2 matrices; α is the last layer of the left electrode, β is the first layer of the right electrode, and $\rho \equiv (g^\dagger - g)/(2\pi\mathrm{i})$ is the density of states (DOS) where g and $g^\dagger$ are retarded and advanced Green's functions of the *isolated* electrodes at the Fermi level which can be 'backward' derived from ab initio free surface Green's functions:

* Corresponding author: Tel.: + 1 212 998 7737; fax: + 1 212 995 4016; e-mail: levy@nyu.edu.

0304-8853/98/$19.00
PII: S0304-8853(98)00290-X

$g_{\alpha\alpha} = G_{\alpha\alpha} - G_{\alpha a} G_{aa}^{-1} G_{a\alpha} \tau_{\alpha\beta}$; the transfer matrix element, see Bardeen [4], is written as

$$\tau_{\alpha\beta} = T^{L}_{\alpha a}[1 - g_{aa} T^{L}_{a\alpha} g_{\alpha\alpha} T^{L}_{\alpha a}]^{-1} \times g_{ab}[1 - T^{R}_{b\beta} g_{\beta\beta} T^{R}_{\beta b} g_{bb}]^{-1} T^{R}_{b\beta}, \quad (2)$$

where the T's are hopping integrals between sites in the electrodes (α; β) and the barrier (a, adjacent to α; b, adjacent to β), g_{ab}, g_{aa} and g_{bb} are unperturbed propagators for the barrier. We take all these as phenomenological constants, and model the barrier as a single, nominal s band at 0.4 Ry above the Fermi level. From our ab initio calculations [5] typical values are $g_{aa} = g_{bb} = -2.0\,\mathrm{Ry}^{-1}$ and $g_{ab} = -0.01\,\mathrm{Ry}^{-1}$, and we determine JMR as a function of the hopping integrals $T^{L} = T^{R} \equiv T_{s,d}$ for s and d electrons. The primary effect of the electronic structure of the electrodes on the conductance of MTJ comes through the DOS factors ρ_α and ρ_β; however, it also enters the denominator of the transfer matrix element as self-energy corrections, (see Eq. (2)); these depend on spin configuration and change the conductance by up to 50% in the range we considered.

We calculated JMR for BCC(1 0 0) Fe, FCC(1 0 0) Co and Ni tunnel junctions in both the specular (ballistic) and diffusive limits. JMR is defined as $(G_{\uparrow\uparrow} + G_{\downarrow\downarrow} - G_{\uparrow\downarrow} - G_{\downarrow\uparrow})/(G_{\uparrow\uparrow} + G_{\downarrow\downarrow})$, where $G_{\sigma\sigma'}$ are conductances of each spin channel when the two electrodes are aligned in parallel or antiparallel. For perfect epitaxial growth (specular limit), two-dimensional translational symmetry in the planes of the layers requires that transverse momentum $k_\parallel$ be conserved, therefore all the quantities in Eq. (1) are $k_\parallel$ resolved ones and summation over $k_\parallel$ for the conductance is implied. When the growth is not ideal or if the interfaces are rough we have diffusive transport, and Eq. (1) reduces to a quasi-one-dimensional formula with all the partial quantities replaced by ones summed over $k_\parallel$.

In Table 1 we list the spin-polarized s and d DOS at the Fermi level for the first two surface layers of *isolated* Fe, Co and Ni electrodes; what we did not show are the *bulk* DOS. For Fe, the s band DOS is strongly and positively polarized (in the same direction as the magnetization) in all layers because of s–d mixing, the Fermi level is inside both majority and minority d bands. While the d band DOS is positively polarized in the bulk of Fe it is negatively polarized in the surface layer. For Co and Ni, at the surface as well as in the bulk, the s DOS polarization is positive albeit very small, the d DOS is always strongly and negatively polarized because the Fermi level lies above the majority d band but within the minority d band. While these characteristics of the *isolated* electrodes that enter Caroli's formalism are similar to those corresponding to the free surface situations, there are significant differences.

Table 1
Electrode s and d DOS for the layer adjacent to the surface $\alpha - 1$ and the surface layer α. The upper two rows are for majority electrons; lower ones for minority electrons

	Fe (s)	Fe (d)	Co (s)	Co (d)	Ni (s)	Ni (d)
$\rho^{\uparrow}_{\alpha-1}$	0.1618	11.277	0.1636	1.8381	0.1699	1.9495
$\rho^{\uparrow}_{\alpha}$	0.2106	7.5483	0.2815	1.4138	0.3193	1.4440
$\rho^{\downarrow}_{\alpha-1}$	0.0168	2.7511	0.0419	8.9444	0.1096	27.282
$\rho^{\downarrow}_{\alpha}$	0.0778	16.222	0.2408	22.045	0.2095	17.717

In Fig. 1 we plot changes in the JMR of an Fe tunnel junction as we increase the d electron contribution to the tunnel current with $T_s = 0.1$ Ry. Results in the diffusive limit mirror the DOS results in Table 1; those for the specular limit reflect appropriate sums over the transverse momentum resolved DOS. They produce higher JMR ratios, but are more difficult to understand. To go beyond hopping between nearest neighbors in an approximate way, we mixed the surface layer Green's function $g_{\alpha\alpha}$ with different proportions of $g_{\alpha-1\alpha-1}$ from the layer adjacent to the surface, as was done in Ref. [3]. When only the surface layer is included, JMR has a dip around $T_d/T_s = 0.1$ because s and d DOS have opposite polarizations. By including more from the adjacent layer this dip accentuates and moves to higher ratios of T_d/T_s because the d DOS is positively polarized for this and all other layers in the metallic electrode. Results in the diffusive limit are similar but the dips go to zero.

In Fig. 2 we show results for a Co junction. The situation is similar to Fe but there are significant

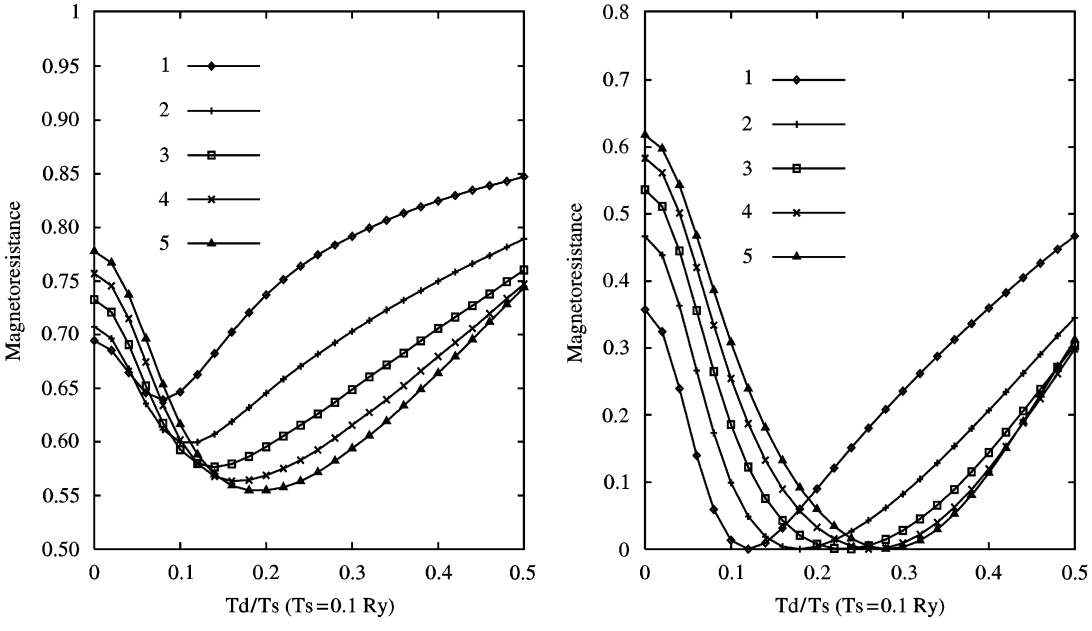

Fig. 1. JMR change with T_d/T_s for the Fe junction in specular (left panel) and diffusive (right panel) limits, 1–5 denotes that electrode Green's functions for the surface layer $g_{\alpha\alpha}$ is mixed with 0, 0.5, 1.0, 1.5 and 2.0 times that for the layer adjacent to the surface $g_{\alpha-1\alpha-1}$.

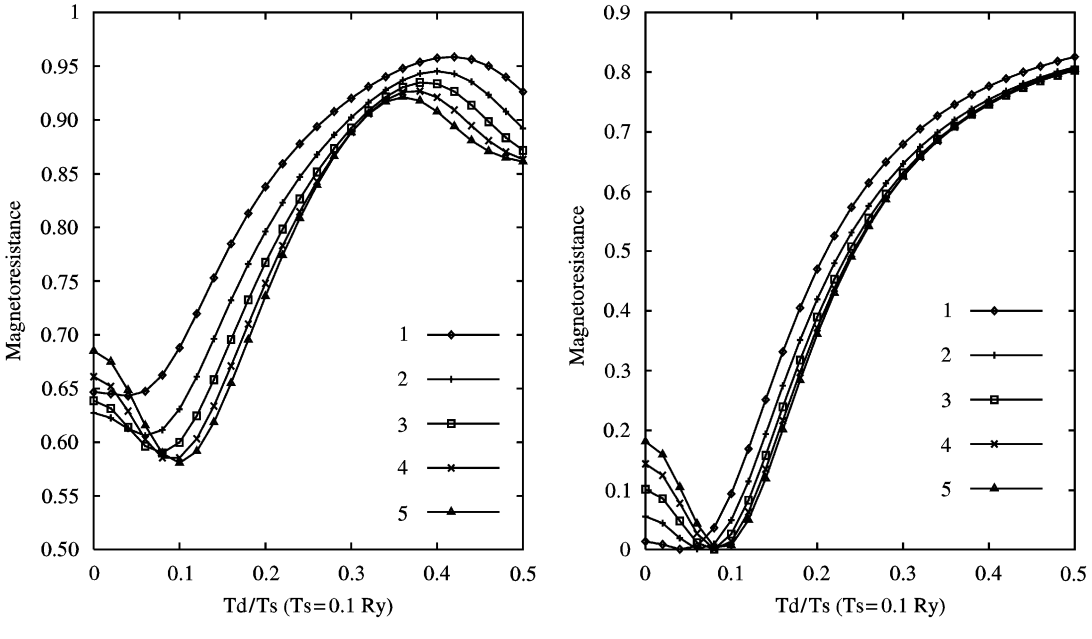

Fig. 2. JMR change with T_d/T_s for the Co tunnel junction. Same labeling as in Fig. 1.

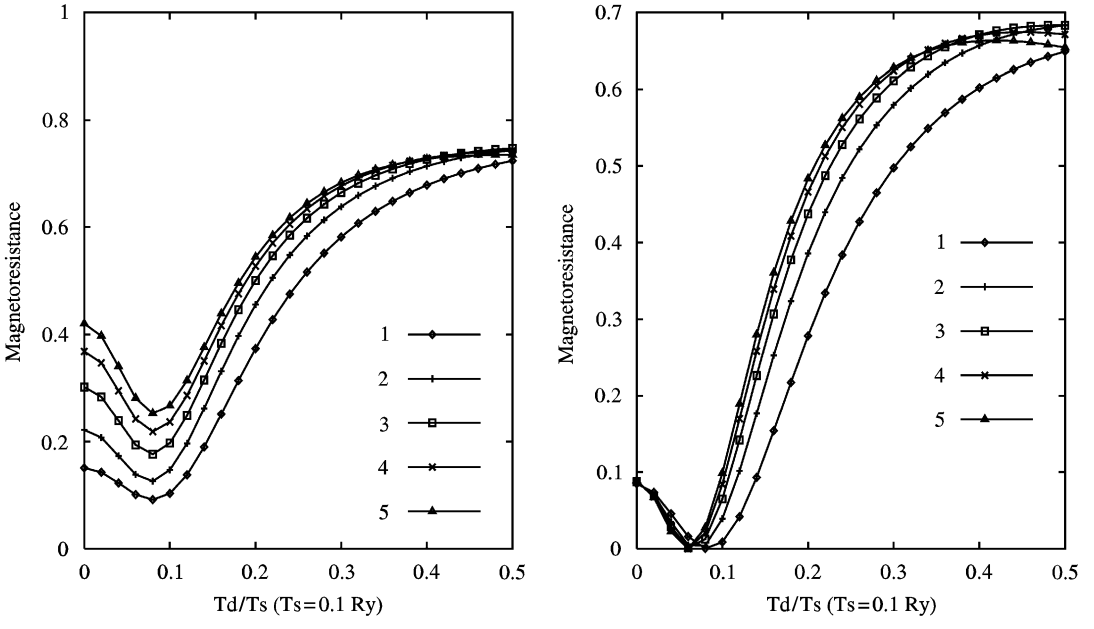

Fig. 3. JMR change with T_d/T_s for the Ni tunnel junction. Same labeling as in Fig. 1.

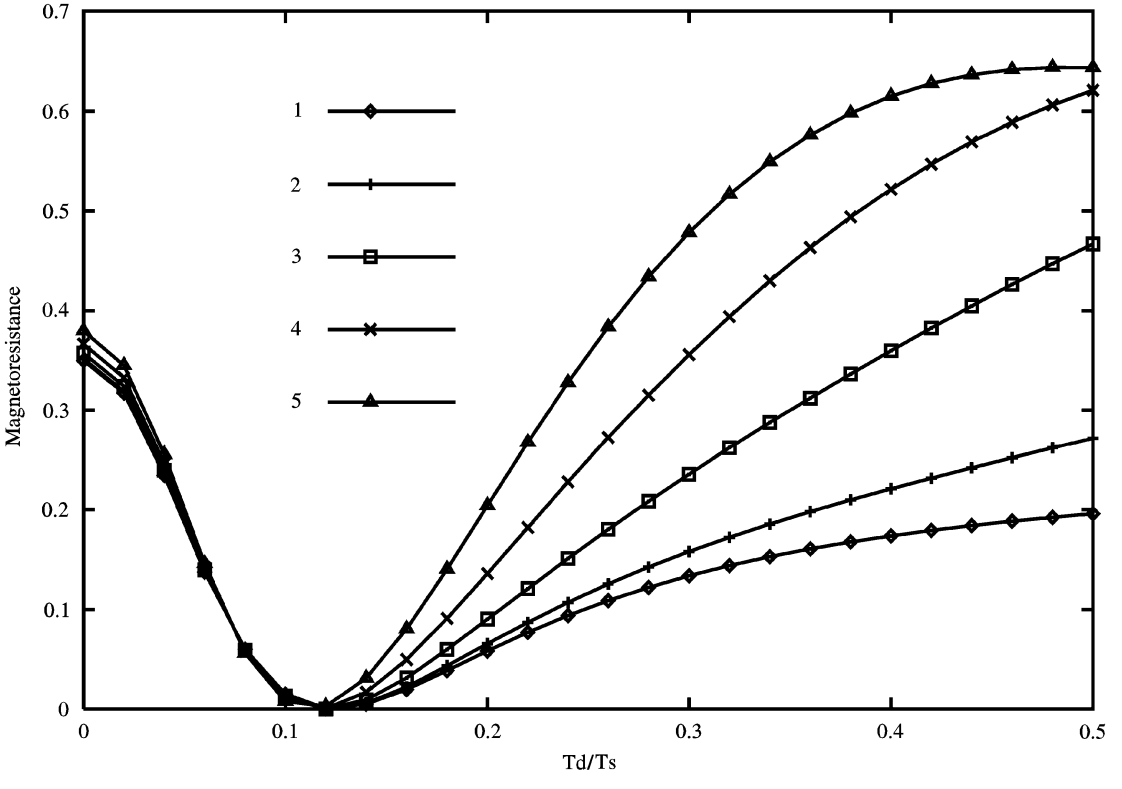

Fig. 4. JMR change with T_d/T_s for different T_s in the Fe junction in the diffusive limit. Here 1–5 means $T_s = 0.01$, 0.05, 0.1, 0.15, and 0.2 Ry.

differences: as the d DOS is more strongly (negatively) polarized than the s DOS, by increasing the d contribution to tunneling, JMR approaches a much higher value than that for pure s electron tunneling. When hopping from the layer adjacent to the surface is included, the dip changes little as d and s DOS are oppositely polarized in all layers. In the diffusive limit JMR is smaller when the s electron dominates, mainly because of the small s DOS polarization in the surface layer. Fig. 3 shows the results for the Ni junction, they are very similar to the Co results.

Finally we have checked how the conclusions drawn above depend on the choice of T_s. In Fig. 4 we show JMR change with T_d/T_s ratio for different T_s values for Fe junctions in the diffusive limit when only the surface layer is included. For s electron dominated tunneling, JMR changes very little because the self-energy corrections to τ are very small. For d electron dominated tunneling JMR increases with T_s in the range studied.

In our discussion we used spin-independent hopping integrals; in this way we emphasized the role of electrode band structure on JMR. In reality, JMR may be enhanced or diminished depending on the relative strengths of these hopping integrals for the two spin channels, but the qualitative features are expected to survive.

Acknowledgements

This work was supported by the Office of Naval Research (N00014-96-1-0203), together with the Defense Advanced Research Projects Agency (MDA972-96-C-0014), the National Science Foundation (INT-96 02192), and NATO (CRG 960340).

P.M.L. thanks Professor Albert Fert and the Laboratoire de Physique des Solides in Orsay, France for their hospitality during his sabbatical stay there.

References

[1] C. Caroli, R. Combescot, P. Nozieres, D.J. Saint-James, J. Phys. C 4 (1971) 916.
[2] L. Szunyogh, B. Újfalussy, P. Weinberger, J. Kollár, Phys. Rev. B 49 (1994) 2721.
[3] E.Yu. Tsymbal, D.G. Pettifor, J. Phys.: Condens. Matter 9 (1997) L411.
[4] Bardeen, Phys. Rev. Lett. 6 (1961) 57.
[5] K. Wang, S. Zhang, P.M. Levy, to be published.