Validity of the Julliere model of spin-dependent tunneling

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(Received 20 March 1997; revised manuscript received 27 June 1997)

We consider spin-dependent tunneling between two ferromagnets separated by a simple step barrier, and examine four models for the magnetoconductance ratio $\Delta G/G$: A model due to Julliere which characterizes the magnetoconductance solely in terms of the tunneling spin polarization, a model due to Slonczewski which provides an approximate expression for the magnetoconductance of free electrons tunneling through a barrier, the exact expression for the magnetoconductance of free electrons tunneling through a barrier, and the numerical calculation of the magnetoconductance of band electrons in iron tunneling through a barrier. We find that the Julliere model does not accurately describe the magnetoconductance of free electrons tunneling through a barrier. Although Slonczewski's model provides a good approximation to the exact expression for free electrons in the limit of thick barriers, we find that the tunneling of band electrons shows features that are not described well by any free electron picture and which reflect the details of the band structure of iron at the Fermi energy. [S0163-1829(97)05641-5]

I. INTRODUCTION

Since the discovery of the giant-magnetoresistance effect,[1] there has been a renewed interest in the phenomenon of spin-dependent transport in general. Spin-dependent transport in a tunnel junction composed of two ferromagnetic layers separated by an insulating barrier was first reported in 1975,[2] and it is now possible to reliably deposit tunneling junctions between ferromagnetic materials that show a consistent magnetoresistance.[3–5] The theoretical model that is the most widely used today to describe this phenomenon was proposed by Julliere[2] and was based on arguments of Tedrow and Meservey[6] who had earlier studied tunneling between superconductors and ferromagnets. The Julliere model is based on the assumption that the tunneling current in each spin channel is proportional to the product of the ''effective tunneling density of states'' for the given spin channel for the metals on either side of the barrier. In the free electron model this ''effective tunneling density of states'' would presumably be the Fermi level density of states for each spin channel. However, in a real ferromagnet, since different states have different effective masses and velocities, it might be some suitably weighted average. The change in the conductance between parallel and antiparallel alignment of the moments on the two sides of the barrier relative to that of parallel alignment is

$$\frac{\Delta G}{G}=\frac{2PP'}{1+PP'}, \tag{1}$$

where P and P' are the spin polarization ratios of the effective tunneling density of states in the two magnetic layers

$$P=\frac{N^{\uparrow}-N^{\downarrow}}{N^{\uparrow}+N^{\downarrow}}. \tag{2}$$

$N^{\uparrow}$ and $N^{\downarrow}$ are the effective tunneling densities of states. Although the meanings of $N^{\uparrow}$ and $N^{\downarrow}$ and hence of the ''polarization,'' P are vague in this model, specific values are often obtained from tunneling experiments in which electrons tunnel between a ferromagnet and a superconductor across an oxide barrier.[6] In the case of Ni, values of P obtained from these tunneling experiments are inconsistent with those seen in spin-polarized photoemission.[7] One interesting prediction of the model is the independence of $\Delta G/G$ on both the geometry and the electronic structure of the barrier layer. In our opinion, this prediction seems unrealistic because we expect the electronic structure of the barrier, and of the interface between them, as well as that of the ferromagnet, to play a role in determining the transport.

In this work we will first study the conductance of spin polarized free electrons through a simple barrier, and compare the results of numerical values of the conductance ratio to that expected by the Julliere model[2] and Slonczewski's model[8] (which will be discussed in more detail later on). These results will also be contrasted with predictions of the tunneling conductance ratio between two semi-infinite Fe layers separated by a step barrier, for which the electronic structure of Fe was computed self-consistently within the local-spin-density approximation.

II. TUNNELING OF FREE ELECTRONS

For a single spin channel, the free-electron potentials in the three regions are V_1, V_b, and V_2, respectively, where

$V_1 < E_F$, $V_2 < E_F$, and $V_b > E_F$. Depending on the spin alignment, V_1 and V_2 are taken to be either $V_\uparrow$ or $V_\downarrow$. In this model the exchange splitting is given simply by $V_\uparrow - V_\downarrow$. The z component of the wave vector for an electron at the Fermi level on the left of the barrier is $k_1 = \sqrt{(2m/\hbar^2)(E_F - V_1) - k_\parallel^2}$, and on the right of the barrier is $k_2 = \sqrt{(2m/\hbar^2)(E_F - V_2) - k_\parallel^2}$. Inside the barrier the decaying wave vector is $\kappa = \sqrt{(2m/\hbar^2)(V_b - E_F) + k_\parallel^2}$.

The unitary transmission coefficients for this barrier are given by

$$T(k_\parallel) = \frac{16 k_1 \kappa^2 k_2 \exp(2d\kappa)}{\{\kappa(k_1 + k_2)[1 + \exp(2d\kappa)]\}^2 + \{(\kappa^2 - k_1 k_2)[1 - \exp(2d\kappa)]\}^2}, \tag{3}$$

where d is the barrier thickness. The reflection coefficient R is $1 - T$. For most tunneling situations, T is small, and R is close to unity. In this limit, we find that T is given by

$$T(k_\parallel) = \frac{16 k_1 \kappa^2 k_2 \exp(-2d\kappa)}{[\kappa(k_1 + k_2)]^2 + (\kappa^2 - k_1 k_2)^2}. \tag{4}$$

Finally we use the Landauer-Büttiker formula[9,10] for the tunneling conductance

$$G = \frac{e^2}{(2\pi)^2 h} \int d^2 k_\parallel T(k_\parallel), \tag{5}$$

where we have assumed that there is no diffuse scattering in the barrier region and consequently $k_\parallel$ is conserved. Thus each $k_\parallel$ is an independent conduction channel.

In the free-electron model the two spin channels have different wave vectors $k_\uparrow = \sqrt{(2m/\hbar^2)(E_F - V_\uparrow) - k_\parallel^2}$ and $k_\downarrow = \sqrt{(2m/\hbar^2)(E_F - V_\downarrow) - k_\parallel^2}$ at the Fermi level. Thus the majority conductance for parallel alignment of the moments on opposite sides of the barrier is found from Eqs. (3) and (5) using $k_1 = k_2 = k_\uparrow$, and for the minority conductance $k_1 = k_2 = k_\downarrow$, while the conductance for antiparallel alignment of the moments is obtained by setting $k_1 = k_\uparrow$, $k_2 = k_\downarrow$. The polarization of the tunneling electrons used in the Julliere model, applied to free electrons, is simply that of the Fermi energy electrons, i.e.,

$$P = \frac{k_\uparrow - k_\downarrow}{k_\uparrow + k_\downarrow}. \tag{6}$$

In general, $\Delta G/G$ calculated from Eq. (5) cannot be easily reduced into simple functions of P and P'.

Slonczewski[8] also considered the same free electron model of spin-dependent tunneling. He obtained an expression for the tunneling conductance that can be written in our notation as

$$G = \frac{e^2}{4\pi h} \frac{\kappa_0}{d} T(0), \tag{7}$$

where κ_0 is the decaying wave vector in the barrier at $k_\parallel = 0$. Slonczewski's result is obtained from Eq. (5) by integrating over $k_\parallel$ and keeping only the leading terms in $1/d$.

The final result of Slonczewski's analysis for the conductance ratio is of the same form as that proposed by Julliere, but with an effective polarization in place of P, defined as

$$P_{\text{eff}} = P \frac{\kappa_0^2 - k_\uparrow k_\downarrow}{\kappa_0^2 + k_\uparrow k_\downarrow}, \tag{8}$$

where both $k_\uparrow$ and $k_\downarrow$ are evaluated at $k_\parallel = 0$. Thus, unlike the original Julliere model, the expected conductance ratios would depend quite sensitively on the type of tunnel junction.

III. NUMERICAL EVALUATION FOR FREE ELECTRONS

We evaluated Eq. (5) numerically for various barrier heights and thicknesses, choosing a Fermi energy of 6.8 eV. The results for the conductance ratio are compared with the predictions of the Julliere model using both Eq. (6) as well as Eq. (8), and are shown in Fig. 1. The barrier height was varied in the range 0.25 to 10.0 eV above the Fermi energy, a range which encompasses both semiconducting and insulating bandgaps. For each barrier height, thicknesses of 5 to 100 Å were studied, corresponding to just a few atomic layers all the way to about 50 atomic layers. The conductance ratios are plotted as a function of the Fermi level polarization P. It can be seen that the Julliere model does not describe the conductance ratio well for any of the barriers investigated. Slonczewski's expression provides a much better description for most of the parameters investigated, but has significant errors for some ranges of the parameters. Slonczewski's expression is closest to the true free-electron tunneling result for large barrier thicknesses and for small barrier heights. The errors result from the neglect of all terms except those of order $1/d$ in the expansion of the integral. These can become significant if κ becomes large while d is still not large enough for the exponential factor to be dominant.

As has been shown, the Julliere model does not accurately represent the magnetoconductance ratio in the free-electron model. Although Slonczewski's generalization does provide a reasonable description of free-electron tunneling through a step barrier, it is not simple to apply to experiment because the effective polarization P_{eff} depends on both the ferromagnet moment alignment and the barrier height, and thus cannot be uniquely defined for each material. We also note that the Julliere model was designed to be quite generally appli-

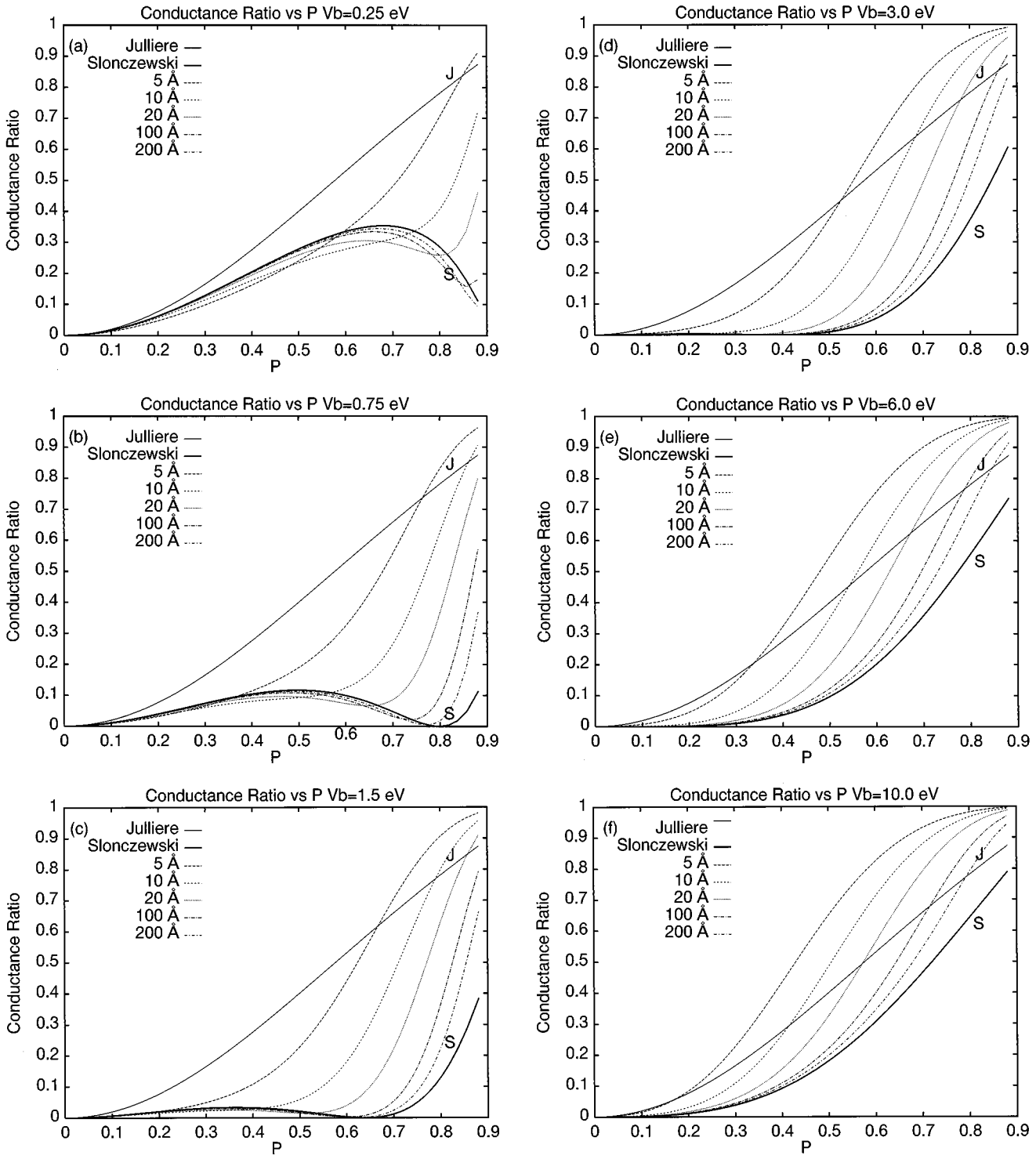

FIG. 1. Conductance ratio ($\Delta G/G$) for free electron spin dependent tunneling for various barrier heights (a) 0.25 eV, (b) 0.75 eV, (c) 1.5 eV, (d) 3.0 eV, (e) 6.0 eV, and (f) 10.0 eV. In each panel, barrier widths of 5, 10, 20, 100, and 200 Å are shown along with the Julliere and Slonczewski results labeled by (J) and (S) respectively.

cable while Slonczewski's model is based on the free-electron approximation.

IV. TUNNELING OF BAND ELECTRONS

In the second part of this work we are interested in how well the Julliere and free-electron descriptions apply to spin-dependent tunneling from real ferromagnets through a simple step barrier. The system that we have chosen to study is an Fe|barrier|Fe tunnel junction, where the barrier was taken to be a simple step of varying height and width. The electronic structure of the bulk ferromagnets was solved self-consistently within the local spin density approximation using the layer Korringa-Kohn-Rostoker (LKKR) approach[11] in the atomic sphere approximation. The barrier consisted of atomic spheres with uniform potential V. As a check of the

TABLE I. Conductance ratios ($\Delta G/G$) for Fe|Barrier|Fe junctions as a function of barrier height, measured with respect to the Fermi energy and barrier width.

Barrier height (eV)	5 Å	10 Å	20 Å
0.8	0.65	0.65	0.71
1.1	0.75	0.75	0.78
3.3	0.91	0.92	0.93
4.4	0.94	0.94	0.97

atomic sphere approximation for the barrier region, we verified that it reproduced the transmission and reflection coefficients of free electrons which we obtained analytically and described in Sec. II. The LKKR method allows an infinite system with only two-dimensional translational symmetry to be built up from its constituent layers. For tunneling of band electrons, the transmission coefficient T describes the scattering of Bloch states through the barrier. The calculation of the Bloch wave scattering S matrix proceeds as follows. First the Bloch states in each lead are computed. In the LKKR method atoms are grouped into layers whose scattering matrices are represented in a plane wave basis. The plane waves are labeled by a two-dimensional reciprocal lattice vector, a wave vector in the two-dimensional Brillouin zone, and a particular energy and direction of travel. The Bloch states are expanded in terms of these plane waves in the region between the layers, and the coefficients are eigenvectors of the layer transfer matrix, i.e., the particular combinations of plane waves that propagates without scattering to the next layer with only a change in phase.[12] The eigenvalue provides the value of k_z, since both the energy and $k_\parallel$ are specified. The Bloch states can also be labeled by their direction of travel which is determined by the z component of the group velocity. The z component of the group velocity can be found by adding a small imaginary part to the energy, and dividing that by the resulting small imaginary part of k_z. The plane wave scattering matrix for the barrier region can be found from the scattering matrices of the constituent layers. Since each Bloch wave can be expressed in plane waves, and the scattering of each of these plane waves is known, the scattering of each Bloch wave into plane waves can be found. These scattered waves can be projected back onto the Bloch waves. If the initial Bloch waves are normalized to unit flux, the resulting S matrix is unitary.

Table I shows the variation in the conductance ratio as a function of barrier height, measured with respect to the Fermi energy, and barrier thickness. It can be seen that for a given barrier height, the conductance ratio is almost independent of barrier thickness, but does depend on barrier height, a result consistent with Slonczewski's solution, but not with the original Julliere model. In fact the current distributions over the Brillouin zone are more localized than in the case of free electrons, as shown in Fig. 2. While the shape of the conductance in the majority channel for parallel alignment of the moments is qualitatively similar to that expected for free electron tunneling, both the minority channel for parallel alignment and both channels for antiparallel alignment appear substantially different from the free-electron conductance. In the minority channel, only certain regions of the Brillouin zone have large conductances and the conductance is not peaked at the zone center as would be expected for free electrons. These peaks reflect the details of the minority band structure of Fe at the Fermi energy. In the case of the antiferromagnetic alignment, the conductance appears similar to that of the minority channel. We can understand this behavior by noting that the majority channel has less structure than that seen in the minority channel, and the the conductance, therefore, is dominated by features of the spin down channel. In the case of Fe, the majority spin Fermi energy passes close

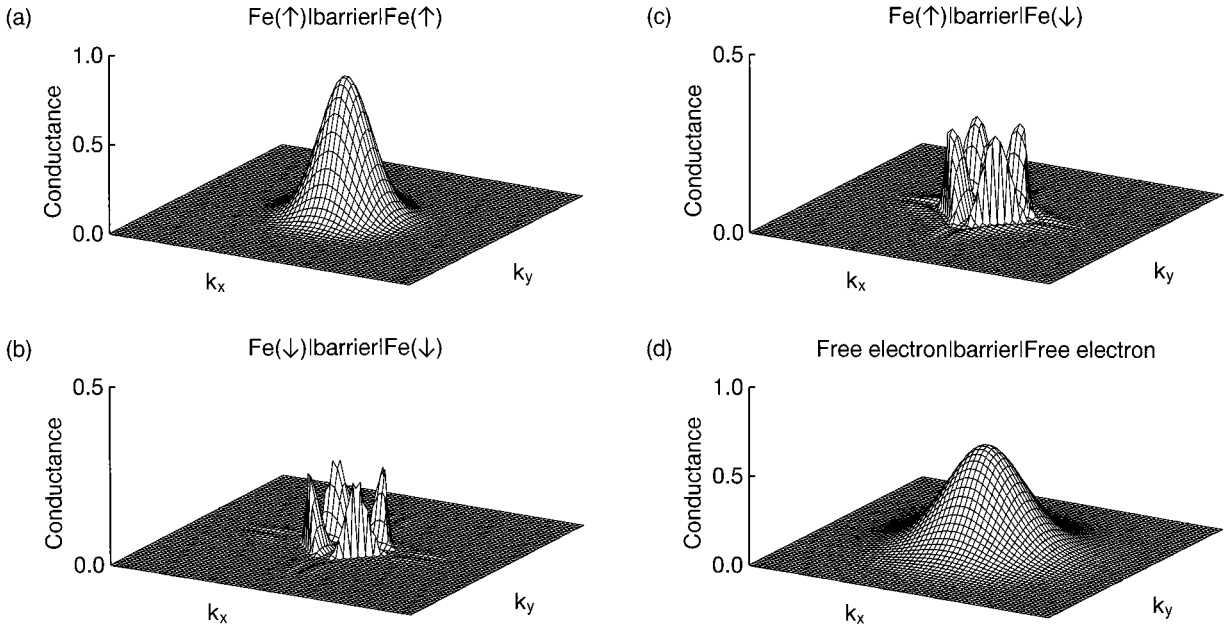

FIG. 2. Calculated tunneling conductance distribution throughout the first Brillouin zone for Fe|Barrier|Fe for (a) majority channel with parallel moment alignment, (b) minority channel with parallel moment alignment, and (c) either channel with antiparallel moment alignment compared with (d) the free-electron distribution. The values of the conductance have been scaled by 1.0×10^{7}.

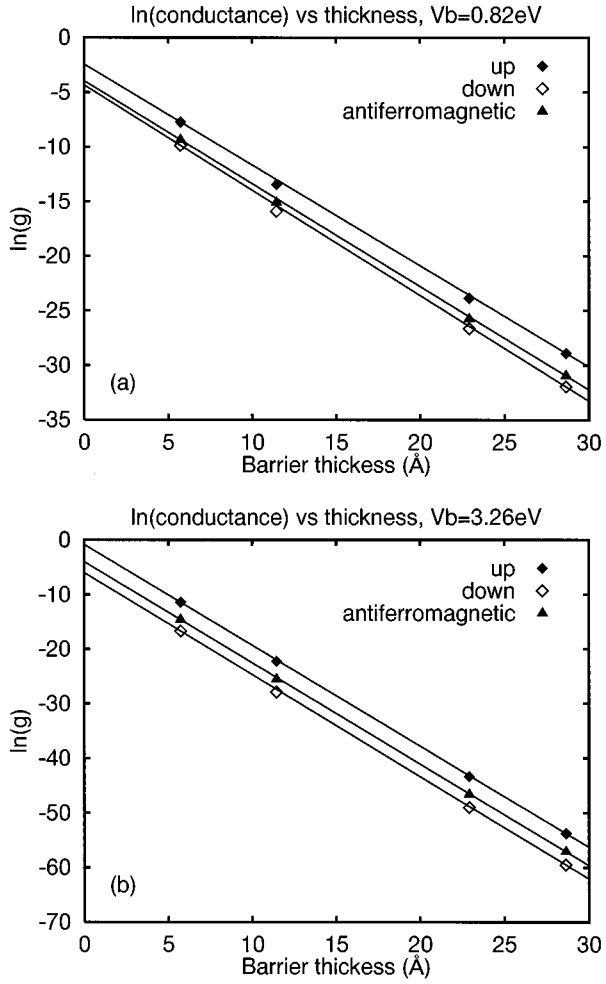

FIG. 3. Conductance of majority and minority channels for parallel moment alignment and either channel for antiparallel alignment as a function of barrier thickness for barrier heights of (a) 0.8 eV and (b) 3.3 eV. The straight lines are fits to the data.

to the top of the *d* bands and the states while still primarily *d* in character have a significant dispersion. For the minority electrons, however, the Fermi energy passes through the middle of the *d* bands.

The spin up, spin down, and antiparallel conductances for two barrier heights are shown as a function of barrier thickness in Fig. 3. For each barrier height the decay observed in each channel is almost identical. Inside the barrier, Slonczewski showed for free-electron tunneling, where the conductance is peaked around $k_{\|}=0$, that the conductance will decay as $\exp[-2\sqrt{(2m/\hbar^2)(V_b-E_F)}d]$. The calculated slopes are in close agreement with this prediction. Since the contributions from up and down electrons come from different parts of the Brillouin zone, the similar decay rates from both spin channels is unexpected. The calculated conductance ratios are much larger than the experimental values that have been reported.[2,3] They are also much larger than would be predicted by the Julliere model using the value of $P=0.44$ for iron obtained from ferromagnet|insulator|superconductor tunneling experiments.[6]

It is clear that neither the Julliere model nor the free-electron model is appropriate for describing the tunneling between two Fe ferromagnets. In our opinion the Julliere model, even in its weakest form which states that there is a number P, which describes a ferromagnet and determines the magnetoconductance ratio through Eq. (1), does not have a firm theoretical foundation. On the other hand, there seems to be a modest amount of experimental evidence that is at least consistent with the model. Parkin has observed[5] that Eq. (1) with values of P taken from Tedrow and Meservey's work[6] provides a reasonable upper bound to the magnetoconductance ratios that he has obtained in spin-dependent tunneling structures.

The calculations which we report here assume that the interfaces are perfect and that $k_{\|}$ is conserved during tunneling. It has been speculated that the breakdown of $k_{\|}$ conservation may restore the Fermi energy density of states as the relevant parameter governing the tunneling probability,[13] although as emphasized previously the P values obtained by Tedrow and Meservey seem to have little relation to the Fermi energy density of states.

V. CONCLUSIONS

In conclusion, we have shown that the Julliere model is not generally appropriate for spin-dependent tunneling. Although Slonczewski's model is a reasonable approximation for free electrons, it is not clear how it should be applied to real materials with more complicated band structures. A successful model needs to incorporate both the true band structure in the presence of the interfaces as well as the dependence of the tunneling current on the barrier height and thickness.

ACKNOWLEDGMENTS

This work was supported by Laboratory Directed Research and Development funds at Oak Ridge National Laboratory and by the Office of Basic Energy Sciences Division of Materials Sciences of the U.S. Department of Energy under Contract No. DE-AC05-960R22464 with Lockheed Martin Energy Research Corp. The work at Tulane University was funded by the NSF Center for Photoinduced Processes, the Louisiana Board of Regents, and by DARPA Grant No. MDA 972-97-1-003.

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