Reduction of electron tunneling current due to lateral variation of the wave function

W. H. Butler, X.-G. Zhang, and T. C. Schulthess
Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831-6114

J. M. MacLaren
Department of Physics, Tulane University, New Orleans, Louisiana 70018

(Received 8 August 2000; published 29 January 2001)

Electron tunneling in solids is usually envisioned in terms of a simple barrier model based on free electrons tunneling through a region of homogeneous potential. We point out that this model neglects the variation of the wave function in the plane of the interface and show that oscillations of the wave function parallel to the interface increase its rate of decay perpendicular to the interface. This simple observation has important implications for spin-dependent tunneling and may explain why ''*s* electrons'' seem to tunnel much more readily than ''*d* electrons.''

DOI: 10.1103/PhysRevB.63.092402 PACS number(s): 75.45.+j, 72.15.Gd, 73.40.Gk

I. INTRODUCTION

Recently there has been much interest in tunneling between ferromagnetic electrodes.[1–4] This interest has been focused on the dependence of the tunneling current on the relative alignment of the moments of the electrodes on opposite sides of the barrier. This dependence arises because electrons in the two spin channels in a ferromagnet show different tunneling rates through the barrier. In trying to understand this difference in the tunneling rates, one important question that has arisen concerns the relative rates of tunneling by ''*s*'' and ''*d*'' electrons, i.e., those Bloch electrons with symmetries that are best described by ''*s*'' or ''*d*'' orbitals.

Most tunneling theories[5,6] for this type of system predict that the tunneling rate is proportional to the product of the densities of states of the two electrodes on either side of the barrier. Experiments, however, are not consistent with this prediction. In cases in which the spin polarization of the tunneling current has been determined by tunneling into superconductors,[7] it has so far been the case that the observed tunneling spectrum indicates that the tunneling current is carried predominantly by majority electrons. This is true even for cases such as nickel and cobalt in which the minority density of states is an order of magnitude larger than that of the majority.

Some variations of the tunneling theory attempt to avoid such inconsistency by defining a ''tunneling density of states.'' Although the tunneling density of states is identical to the density of states in the case of free electrons, for real materials the concept is difficult to define. Presumably, it is that part of the density of states that is necessary to make the theory agree with experiment. However, the use of such a concept fails to explain why part of the density of states participates in tunneling and other parts, presumably including the typically large ''*d*'' density of states at the Fermi energy for minority spins do not.

Electron tunneling in solids is usually envisioned and modeled in terms of a simple barrier model in which free electrons are incident on a simple repulsive step potential (Fig. 1). The transmission probability as a function of transverse electron momentum for this type of barrier can be calculated simply and is given by[8]

$$T(k_\parallel)=\frac{16k_1\kappa^2k_2\exp(2\kappa d)}{\{\kappa(k_1+k_2)[1+\exp(2\kappa d)]\}^2+\{(\kappa^2-k_1k_2)[1-\exp(2\kappa d)]\}^2} \tag{1}$$

where d is the barrier thickness. The quantities, k_1, k_2, and κ are given by $k_1=\sqrt{(2m/\hbar^2)(E-V_1)-k_\parallel^2}$, $k_2=\sqrt{(2m/\hbar^2)(E-V_2)-k_\parallel^2}$ and $\kappa=\sqrt{(2m/\hbar^2)(V_B-E)+k_\parallel^2}$. The reflection probability, R, is $1-T$. For most tunneling situations, $\exp(2\kappa d)$ is much greater than unity. In this limit, we find that T is given by

$$T(k_\parallel)=\frac{16k_1\kappa^2k_2\exp(-2\kappa d)}{[\kappa(k_1+k_2)]^2+(\kappa^2-k_1k_2)^2}. \tag{2}$$

The tunneling conductance can be calculated directly from the transmission probability[9,10]

$$G=\frac{e^2}{h}\sum_{k_\parallel}T(k_\parallel). \tag{3}$$

Thus, if we consider Bloch electrons incident on a simple step barrier, it would appear naively that there could be only a single decay rate for a given value of $k_\parallel$. That is, the tunneling current should decay with the barrier thickness, d, as $\exp(-2\kappa d)$ where $\kappa=\sqrt{(2m/\hbar^2)(V-E)+k_\parallel^2}$. In previ-

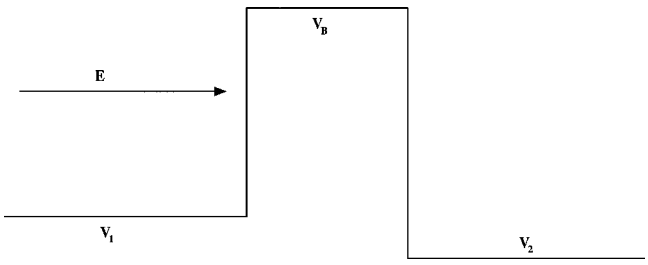

FIG. 1. Free electrons incident on a simple barrier.

ous papers,[11,12] however, we have emphasized different wave function symmetries in the electrodes and showed that they lead to different decay rates in the barrier layer due to the fact that each symmetry will have a minimum decay rate corresponding to that of the slowest decaying complex energy band in the barrier layer with that symmetry. The physical effect, that different types of Bloch states decay at different rates in a barrier is, however, much more general.

The basic physical reason that the different Bloch states decay at different rates in the barrier is that they have different amounts of curvature in the plane parallel to the interfaces. The free-electron model fails to describe this aspect of real metals because it does not include spatial variations in the lateral directions (other than those associated with the lateral components of the wave vector, $k_\parallel$). Consider the simple barrier model with a homogeneous barrier V. If the wave function in the electrode is more realistic than that of a free electron, it may have oscillations in the plane parallel to the interface even when $k_\parallel=0$. As we show below, these oscillations will increase the decay rate perpendicular to the interface.

Assume for simplicity that the boundary conditions at the edge of the barrier can be matched with the separable form $\psi(x,y,z)=\phi(x,y)\exp(-\kappa z)$. Then, the decay perpendicular to the barrier $(k_\parallel=0)$ will be given by

$$\kappa^2=\frac{2m}{\hbar^2}(V_B-E)-\frac{\langle\phi|\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)|\phi\rangle}{\langle\phi|\phi\rangle}. \qquad (4)$$

Because the variation of ϕ is assumed to be oscillatory, the second term above must be positive and correlate with the number of nodes of $\phi(x,y)$.

Thus the additional curvature of the wave function in the plane parallel to the interface causes an increase in the rate of decay perpendicular to the interface (just as a nonzero value of $k_\parallel$ would). In this picture, the role of symmetry is to determine the number of nodes of the wave function in the plane of the interface. This translates into curvature in this plane which affects the decay rate. States that are primarily *s*-like will have little of this curvature, *p*-like states will have more and *d*-like states will typically have even more. For this reason, we argue that our result that the nature of the state in the electrode influences its decay rate in the barrier is quite general. Most of the *d*-derived states, in particular, will be disadvantaged in penetrating the barrier because of their higher curvature due to additional nodes in the plane parallel to the barrier.

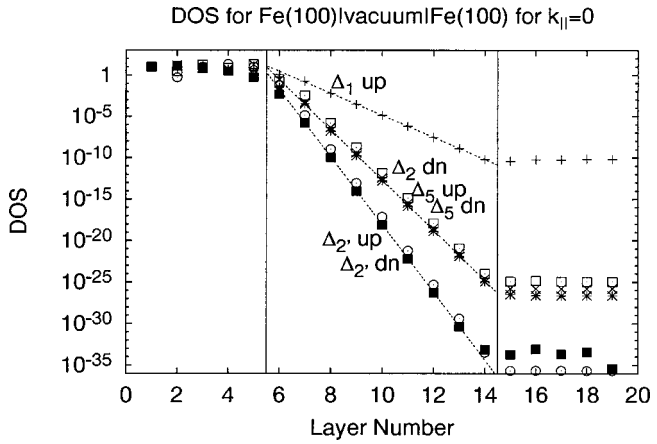

FIG. 2. Calculated Density of States (DOS) for $k_\parallel=0$ for Fe(100)|vacuum|Fe(100). The DOS is calculated using scattering boundary conditions with Bloch waves incident from the left. Vacuum is approximated here by a spatially homogeneous barrier. The straight lines have slopes given by $-2\sqrt{(2m/\hbar^2)(V-E_F)+g^2}$ as described in the text. The moments of the two iron electrodes are assumed to be aligned.

Because the notion of multiple decay rates in a spatially homogeneous barrier layer may seem counterintuitive, we calculated the decay into the barrier of the density of states for each band at the Fermi energy of Fe(100). The density of states was calculated with boundary conditions in which there is a unit flux of incident electrons in a single Bloch state on one side (left side in this case) plus reflected electrons on the same side (left) and transmitted electrons on the opposite side (right). These boundary conditions yield a density of states that decays in the barrier from left to right.

For this calculation we chose the barrier height relative to the Fermi energy to be approximately equal to the work function in order to be an approximate representation of tunneling through vacuum. The calculation employed the layer Korringa Kohn Rostoker (LKKR) technique to calculate the electronic structure and density of states.[13] This calculation must be approached with care when using a technique (such as the LKKR) that employs an atomic sphere approximation (ASA). The ASA is not bad for atoms, but it does not provide a very accurate representation of the vacuum because it attempts to represent a constant barrier potential as a sum of spherical potentials each having a magnitude of about 0.5 Hartree (13.6 eV). In order to better represent the homogeneous vacuum potential, all potentials were recalculated relative to a potential zero equal to the vacuum level. This gives a perfectly homogeneous vacuum at the expense of decreased accuracy for the Fe bands.

The results displayed in Fig. 2 show three decay rates. The majority Δ_1 state (which contains *s*,*p*, and *d* components with 1,*z*, and $2z^2-x^2-y^2$ symmetries, respectively) decays as $\kappa=\sqrt{(2m/\hbar^2)(V-E)}$, exactly as expected for the simple barrier model. The other states, however, decay more rapidly. The minority Δ_2 (*d* character, x^2-y^2 symmetry)

and all of the Δ_5 states (p and d components with x, y, xz, and yz symmetries) decay as $\kappa=\sqrt{(2m/\hbar^2)(V-E)+g_1^2}$, where $g_1=2\pi/a$ for a square lattice of lattice constant a. The majority and minority $\Delta_{2'}$ states that have d character and xy symmetry decay as $\kappa=\sqrt{(2m/\hbar^2)(V-E)+g_2^2}$ with $g_2=\sqrt{2}(2\pi/a)$. g_1 and g_2 are simply the magnitudes of the first two reciprocal lattice vectors of the two-dimensional (2D) lattice parallel to the interfaces.

The Δ_1 state has no node in the xy plane for $k_\parallel=0$. On the other hand, the Δ_5 states on a two-dimensional square lattice have one node per unit cell, with a period of a in either the x or the y direction, which corresponds to a wave vector of g_1. Thus taking linear combinations of the four plane waves with magnitude g_1, $\exp(\pm i2\pi x/a)$, $\exp(\pm i2\pi y/a)$, we can construct functions with Δ_5 symmetry, $\sin(2\pi x/a)$,$\sin(2\pi y/a)$. We can also use them to construct a wave functions with Δ_2 symmetry, $\cos(2\pi x/a)-\cos(2\pi y/a)$. Finally, we can use linear combinations of the plane waves associated with the four reciprocal lattice vectors of magnitude g_2, $\exp(\pm i2\pi x/a\pm i2\pi y/a)$, to construct a wave function with $\Delta_{2'}$ symmetry, $\cos(2\pi x/a+2\pi y/a)-\cos(2\pi x/a-2\pi y/a)$.

For the case of $k_\parallel\neq 0$, the symmetry of the Bloch states and of the decaying evanescent states that they couple to becomes more complicated. The wave function in the barrier region that joins to the incident plus reflected Bloch wave on the left can be expanded in terms of reciprocal lattice vectors in the form[11]

$$\psi(\rho,z)=\sum_g c_g e^{i(\mathbf{k}_\parallel+\mathbf{g})\cdot\boldsymbol{\rho}-\sqrt{\frac{2m}{\hbar^2}(V_B-E)+(\mathbf{k}_\parallel+\mathbf{g})^2}z}. \qquad (5)$$

Here ρ is a vector in the xy plane and we have taken the limit of a thick barrier so that growing evanescent waves are excluded.

For $k_\parallel=0$, the coefficients, c_g must be such that the decaying wave function in the barrier region can match to Bloch states maintaining the proper symmetry as explained above. Because of this symmetry requirement only Bloch states with Δ_1 symmetry can couple to decaying waves that contain the $g=0$ reciprocal lattice vector in their expansion. For $k_\parallel\neq 0$, however, the states in the barrier will typically consist of a linear combination of different reciprocal lattice vectors decaying at different rates. For a relatively thick barrier the component with the slowest decay rate, typically that corresponding to the $g=0$ reciprocal lattice vector, will be the last one surviving so that in that sense, for an arbitrary point in the 2D Brillouin zone there will ultimately be a single decay rate.

The transmission coefficient for thick barriers will then depend on the magnitude of the $g=0$ coefficient of the wave function expansion in Eq. (5). Note that this component of the wave function corresponds to a probability density, $P(\rho,z)=|\psi(\rho,z)|^2$ that is constant in the xy plane. Coefficients for the wave function in the barrier with $g\neq 0$ will be necessary for the probability density to join continuously to that of the metal.

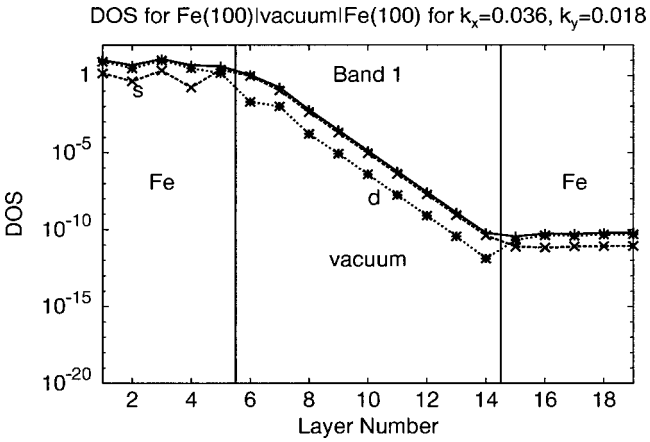

FIG. 3. Calculated DOS for $k_\parallel\neq 0$ for Fe(100)|vacuum|Fe(100) for a Bloch state that has Δ_1 symmetry at $k_\parallel=0$. These calculations employ the same boundary conditions as Fig. 2.

Even when $k_\parallel$ is nonzero, the d component of the wave function with nodes in the xy plane will generate only very small contributions to the $g=0$ expansion coefficients. This means that the d DOS will decay very rapidly in the first few layers of the barrier and that the contribution to the transmission of Bloch states that have d-derived oscillations in the xy plane will typically be several orders of magnitude smaller than those Bloch states that do not have such oscillations. This is illustrated in Figs. 3 and 4 which show the DOS for the same boundary conditions as Fig. 2. In this case, however, $k_\parallel=(0.036,0.018)$ and we show the angular momentum decomposition of the DOS. In the barrier, the angular momentum decomposition is performed around fictitious sites that would form a continuation of the bcc Fe(100) lattice. Figure 3 shows the DOS for the continuation of the majority Δ_1 band at $k_\parallel=(0,0)$ to $k_\parallel=(0.036,0.018)$. The calculated DOS is essentially unchanged for this Bloch state which does not have rapid oscillations in the xy plane. The DOS for the other Bloch states is, however, affected by the loss of symmetry as is shown in Fig. 4. There is an initial rapid decay of the DOS as the parts of the wave function that have in-plane

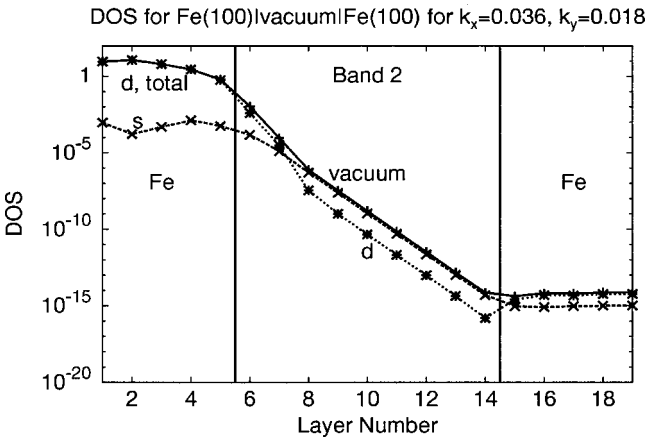

FIG. 4. Calculated DOS for $k_\parallel\neq 0$ for Fe(100)|vacuum|Fe(100) for a Bloch state that has no $g=0$ component at $k_\parallel=0$. These calculations employ the same boundary conditions as Figs. 2 and 3.

oscillations decay according to Eq. (5) with $g \neq 0$. After those terms are gone there is a small residual component that decays at the rate given by Eq. (5) with $g = 0$.

In the case of a real barrier layer, formed from an insulator such as Al_2O_3, similar arguments regarding the decay rate apply. The Bloch states in the metal couple to decaying states of appropriate symmetry and the corresponding decay rates determined by complex bands of the barrier which are no longer simple plane waves. The characteristic decay rates calculated for iron electrodes with MgO barrier layers agreed exactly with those predicted by the imaginary value of the wave vector of the state of appropriate symmetry in the barrier.[12]

In summary, we have shown that the lateral variation of wave functions can dramatically change the rate at which they decay in a barrier. Specifically we show that the decay rate is determined by the symmetry of the Bloch states in the *xy* plane, in particular the number of nodes of the wave function in a unit cell. This understanding points toward possible directions for designing materials with electronic structures optimized to produce greater contrast between the two spin channels in spin-dependent tunneling.

It should be noted for completeness that *d*-derived states suffer an additional disadvantage in tunneling through a barrier. Their band velocity is typically lower than that of free-electronlike states. Since the transmission coefficient that enters the Landauer formula is flux conserving, it incorporates a factor of v_z, the component of the band velocity perpendicular to the interface, compared to the density of states plotted in Figs. 2–4. We note that Mazin has emphasized the importance of the band velocity perpendicular to the interface when interpreting tunneling and Andreev reflection.[14,15]

Work at Oak Ridge was sponsored by the Defense Advanced Research Projects Agency and by the Office of Basic Energy Sciences, Division of Materials Sciences of the U.S. Department of Energy. Oak Ridge National Laboratory is operated by UT-Battelle, LLC, for the U.S. Department of Energy under Contract No. DE-AC05-00OR22725. J.M.M. acknowledges support from the Oak Ridge Institute for Science and Education and DARPA Grant No. MDA 972-97-1-003.

[1] S. A. Rishton, Y. Lu, R. A. Altman, A. C. Marley, X. P. Bian, C. Jahnes, R. Viswanathan, G. Xiao, W. J. Gallagher, and S. S. P. Parkin, Microelectron. Eng. **35**, 249 (1997).

[2] S. S. P. Parkin, K. P. Roche, M. G. Samant, P. M. Rice, R. B. Beyers, R. E. Scheuerlein, E. J. O'Sullivan, S. L. Brown, J. Bucchigano, D. W. Abraham, Y. Lu, M. Rooks, P. L. Trouilloud, R. A. Wanner, and W. J. Gallagher, J. Appl. Phys. **85**, 5828 (1999).

[3] J. S. Moodera, E. F. Gallagher, K. Robinson, and J. Nowak, Appl. Phys. Lett. **70**, 3050 (1997).

[4] C. T. Tanaka, J. Nowak, and J. S. Moodera, J. Appl. Phys. **86**, 6239 (1999).

[5] M. Julliere, Phys. Lett. **54A**, 225 (1975).

[6] J. C. Slonczewski, Phys. Rev. B **39**, 6995 (1989).

[7] P. M. Tedrow and R. Meservey, Phys. Rev. B **7**, 318 (1973); P. M. Tedrow and R. Meservey, Phys. Rev. Lett. **26**, 192 (1971); R. Meservey and P. M. Tedrow, Phys. Rep. **238**, 173 (1994).

[8] J. M. MacLaren, X.-G. Zhang, and W. H. Butler, Phys. Rev. B **56**, 11 827 (1997).

[9] R. Landauer, IBM J. Res. Dev. **1**, 223 (1957).

[10] M. Büttiker, IBM J. Res. Dev. **32**, 317 (1988).

[11] J. M. MacLaren, X.-G. Zhang, W. H. Butler, and Xindong Wang, Phys. Rev. B **59**, 5470 (1999).

[12] W. H. Butler, X.-G. Zhang, T. C. Schulthess, and J. M. MacLaren, Phys. Rev. B **63**, 054416 (2001).

[13] J. M. MacLaren, S. Crampin, D. D. Vvedensky, R. C. Albers, and J. B. Pendry, Comput. Phys. Commun. **60**, 365 (1990).

[14] B. Nadgorny, R. J. Soulen, M. S. Osofsky, I. I. Mazin, R. J. M. van de Veerdonk, A. A. Smits, S. F. Cheng, E. F. Skelton, and S. B. Qadri, Phys. Rev. B **61**, 3788 (2000).

[15] I. I. Mazin, Phys. Rev. Lett. **83**, 1427 (1999).