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Effect of atomic disorder on transport through magnetic tunnel junctions

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Spin-dependent tunneling through magnetic junctions is sensitive to material properties near the interface and in the barrier. Results of calculations are presented showing how electron transmission through a point contact tunnel junction is affected by atomic disorder in the barrier. Giant variations in the transmission probability are found with limited disorder. Sharp peaks appear in the tunnel current when defects exist at positions in the barrier that facilitate electron hopping across the contact. Consequences for thin film tunnel junction devices are also discussed, with reference to experiments showing strong spatial variations in tunnel current. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1555311]

INTRODUCTION

Magnetic tunnel junctions are thin-film structures comprising a ferromagnet, an insulator, and a second ferromagnet. The large magnetoresistance ratio observed in ferromagnetic tunnel junctions makes them potentially useful in devices such as magnetoresistive recording heads, magnetic field sensors, and nonvolatile random access memories. Interface effects and disorder are important in determining tunnel current in devices.[1–4] Experimental data has shown that the tunneling current through the barrier may be dominated by large current peaks, and thus be difficult to control.[2,5] Measurements by Da Costa *et al.*,[2] for example, show fluctuations of one to two orders of magnitude.

At present, explanations of these large fluctuations have been made qualitatively in terms of structural defects in the barrier, with estimates of spatial density based on the statistics of rare events.[2,6] Some attempts have been made to describe the tunnel current through barrier films with thickness variations.[7–13]

Here, results of calculations are presented that demonstrate how large tunnel current fluctuations can arise through a barrier without pinholes. A small amount of atomic disorder within an insulating barrier is sufficient to create large changes in tunnel current for a junction with a small lateral extent. The calculation is based on a standard approach to ballistic transport in nanoscale structures through the use of a non-equilibrium Green's function technique,[10,14,15] implemented using a tight-binding model, which allows for the specification of the geometry at the atomic structure level in a relatively simple computational scheme.

RANDOM LATTICE MODEL

The junction considered in this calculation consists of a narrow three- dimensional wire with a tunnel barrier separating two magnetic leads. The geometry is sketched in Fig. 1. This model is appropriate for some types of extremely narrow magnetic wire structures and point contacts. It is also relevant to tunneling in structures composed of inhomogeneous films with well-defined granular structure.

Two conduction bands are considered: a band for spin up electrons and a band for spin down electrons. The parameters describing the energy states, E, of electrons in the junctions and leads are $U_{\sigma,i}$, the local potential associated with an atom at site i for a conduction electron with spin σ, and the hopping integral, t_{ij}, representing the overlap integral between wavefunctions of atoms at neighboring sites i and j. The hopping integral is assumed to be spin independent. The wavefunction amplitude of a conduction electron in spin state σ at site i is denoted by $\psi_{\sigma,i}$. A matrix equation for the single particle Schrödinger equation in the tight binding model may be put in the tridiagonal form:

$$E\begin{bmatrix} \vdots \\ \psi_{\sigma,j-1} \\ \psi_{\sigma,j} \\ \psi_{\sigma,j+1} \\ \vdots \end{bmatrix} = \begin{bmatrix} \ddots & -t_{ij} & 0 & 0 & 0 \\ -t_{ij} & U_{\sigma i}+2t_{ij} & -t_{ij} & 0 & 0 \\ 0 & -t_{ij} & U_{\sigma i}+2t_{ij} & -t_{ij} & 0 \\ 0 & 0 & -t_{ij} & U_{\sigma i}+2t_{ij} & -t_{ij} \\ 0 & 0 & 0 & -t_{ij} & \ddots \end{bmatrix} \times \begin{bmatrix} \vdots \\ \psi_{\sigma,j-1} \\ \psi_{\sigma,j} \\ \psi_{\sigma,j+1} \\ \vdots \end{bmatrix}. \quad (1)$$

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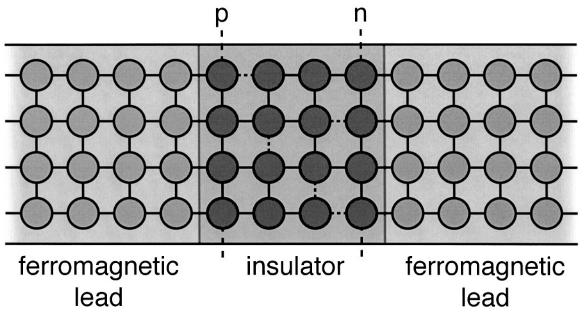

FIG. 1. Schematic of geometry used in model, showing a two-dimensional cross-section of a three-dimensional wire. Solid lines between atoms indicate that hopping is allowed, while dashed lines indicate that coupling between atoms has been disallowed in the model.

Projected onto a basis of atomic orbitals, the matrix operator in Eq. (1) may be written as a matrix, H, of overlap integrals. When inverted this forms a Green's function, $G=(H-E)^{-1}$, which may be used to calculate local densities of states.[10,14,15]

It is convenient to separate the lead regions from the barrier region, as indicated in Fig. 1, and couple the leads to the barrier region through hopping terms to atoms located in positions $i_{x=p}$ and $i_{x=n}$. The Green's functions are then constructed for a finite number of atomic layers ranging from plane p to plane n with the hopping terms between lead atoms and atoms in the planes at $i_{x=p}$ and $i_{x=n}$ contained in the self-energy terms Σ_p and Σ_n.

The current through each lead is defined as the difference between the rate of in-scattering and the rate of out-scattering, summed over all energies in an approximation valid for small bias fields. The total current due to this difference in rates is given by the difference in density of states at layers p and n, weighted by the transition rate into p and out of n.[9] The form of the current, therefore, involves products of Σ and G, which represent the transition rate and density of states, respectively. The current is given by

$$I_n=-\int_{-\infty}^{E_f}\frac{e}{h}\mathrm{Tr}[\overleftrightarrow{\Sigma}{}_p^{\mathrm{in}}(E)\,\overleftrightarrow{G}{}^p(E)-\overleftrightarrow{\Sigma}{}_n^{\mathrm{out}}(E)\,\overleftrightarrow{G}{}^n(E)]dE, \tag{2}$$

summed over all leads, n, at the interface.

The functions $\Sigma^{\mathrm{in/out}}$ describe the transition rates for electrons moving from the states in the leads to states in the junction, and are products of the self-energy terms connecting the lead to the junction at sites in the planes p and n, and the Fermi functions evaluated at these planes. The driving voltage, E_b, is contained in the Fermi functions defined by $f(E)=\{1+\exp[(E-E_F\pm E_b)/k_BT\}^{-1}$ where the ± refers to the planes at positions p and n, respectively.

The conduction states in the leads are calculated analytically for an infinitely long square wire N atoms wide along each side. This is used to construct the self energy terms $\Sigma^{\mathrm{in/out}}$. Next, the matrix H for the tunnel region is inverted numerically in order to find G at each energy and is summed, according to Eq. (2), over all sites in the barrier region for the current. The total current is found for zero temperature by including contributions from all lead energy states less than E_F-E_b.

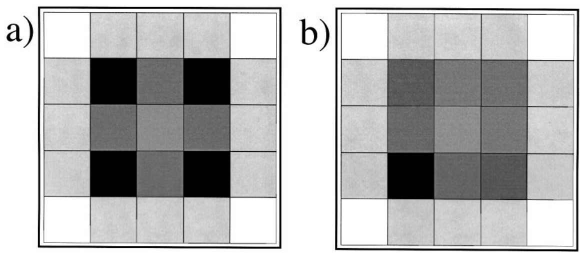

FIG. 2. Schematic showing transmission at lead connected to a system, with cross-section five atoms by five atoms, for a system with (a) no disorder and (b) with coupling between two atoms set to zero. Darker areas indicate lower transmission.

RESULTS AND DISCUSSION

Parameters have been chosen to represent a narrow band of states with moderate splitting between states. The values are not intended to represent a particular material, but instead are convenient for demonstrating features which are common to any magnetic system. The spin up and spin down potentials, U_+ and U_-, are -2.85 and -3.15 eV in the ferromagnetic regions and leads. The Fermi energy E_F is 0 eV. The potential for the insulating barrier is set above E_F at 4 eV. The hopping parameters in the ferromagnetic region are $t_F=0.5$ eV. The hopping parameter in the barrier region is $t_B=0.5$ eV. Defects in the barrier region are represented by setting t_B to zero. Interface hopping parameters are defined as the geometrical mean between the two materials, $t_{\mathrm{int}}=\sqrt{t_F t_B}$. The wire width is $N=3$ unless otherwise specified, and the barrier region is 3 atoms long. The bias voltage is 0.5 V.

Because spin flip processes are not considered in this treatment, the general features of tunneling within a spin channel are similar to those of tunneling though nonmagnetic junctions. In the wire geometry, for example, the barrier separates two regions which are identical if the magnetizations are parallel. As the diameter of the wire is small, energy levels are well separated. Strong resonant transmission effects appear at values of E_B that cause otherwise different energy levels on the two sides of the barrier to become degenerate.

The most sensitive parameters governing the tunnel current in this model are the barrier hopping integral, t_B, and interface hopping parameter, t_{int}. The main effect of modifying these values locally at random locations is to lower symmetries associated with the distribution of wavefunction amplitudes. To clarify what we mean by this, transmission amplitudes are plotted in Fig. 2 for a cross section of the wire. The gray scale is such that white indicates large transmission and black indicates zero transmission. The cross section is taken at plane n shown in Fig. 1. The case shown in Fig 2(a) is that of no disorder, represented by uniform values of t_B in an $N=5$ system, with a barrier 5 atoms wide. The hopping, t_B, between two of the barrier atoms is set to zero

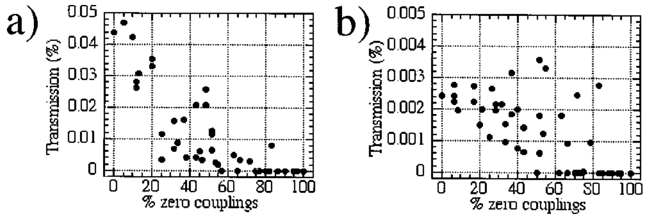

FIG. 3. Variation in transmission events with defect density, where defects are introduced by setting interatomic hopping potentials to zero with (a) parallel ferromagnets, and (b) antiparallel ferromagnets. Note the difference of scale in the two graphs.

in the transmission profile shown in Fig. 2(b). In this case the tunnel current is not symmetrically distributed across the wire.

The effect of more than one defect is illustrated in Fig. 3; transmission is shown as a function of defect density for (a) parallel magnetization of the two ferromagnetic films, and (b) the antiparallel case. Note that the scales on the graphs in Fig. 3 differ by an order of magnitude. These defects are created by setting values for the hopping integral, t_{ij}, to zero between atoms in the insulating layer. The alignment of magnetization in the metals is determined by the majority and minority potentials. In Fig. 3(a) the potentials, and hence, electronic states, on either side of the barrier are similar for each spin channel. The introduction of defects perturbs energy levels within the barrier, such that resonant modes may be enhanced—sometimes causing the transmission to increase. When resonant modes are suppressed transmission decreases. In Fig. 3(b), the antiparallel alignment of magnetization means that the spin dependent electronic states for each metal are very different because of the relative potential difference between metals on either side of the barrier. Resonant effects in this case are unlikely for small values of the bias voltage as large shifts in energy are required to form degenerate states.

These results compare well with those of Tsymbal and Pettifor[11] who demonstrate that the introduction of impurities (in this case changes in the on-site atomic energy levels) in the barrier layer of a single-band tight-binding model leads to a rapid drop in tunneling magnetoresistance with increased impurity concentration. They also demonstrate that the introduction of impurities has dramatic effects on resonant modes.

It is worth considering the effect that the introduction of spin flip scattering might have on the outcome of this model. Generally, spin flip scattering would be expected to increase the tunneling current in the antiparrallel case and decrease the tunneling current in the parallel case. Spin flip scattering is not expected introduce resonant effects in the antiparallel case. However, more work is needed to examine these conjectures.

In summary, the results indicate that large fluctuations in tunnel current through a magnetic tunnel junction of small lateral extent may be attributable to small amounts of disorder in the insulating layer. This may be generalized to an extended thin film if the film is not continuous, but instead a collection of small independent grains, each of which as a considered to be narrow wire. In this case, fluctuations in current through thin film magnetic tunnel junctions may be attributed to atomic disorder. The theory may also have applications to patterned systems and nanocrystals.[16]

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