# Spin-Dependent Interface Transmission and Reflection in Magnetic Multilayers

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## Abstract

First-principles calculations of transmission and reflection from Ag/Fe, Au/Fe, Cu/Co, and Cu/Ni interfaces show very strong spin dependence that differs significantly from expectations based on free electron approximations. The results can be used to understand both the giant magnetoresistance and the oscillatory exchange coupling observed in magnetic multilayers of these materials. The spin dependence of the reflection probabilities is strong enough to give a large giant magnetoresistance even if there is no spin dependent defect scattering. The calculated reflection amplitudes determine the strength of the oscillatory exchange coupling.

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## I. INTRODUCTION

Magnetic multilayers, in which magnetic layers are separated by nonmagnetic spacer layers, exhibit two effects in which there has been significant recent interest: giant magnetoresistance (GMR) [1] and oscillatory exchange coupling [2]. The GMR is the change in resistance when the relative orientation of the magnetizations in neighboring layers is switched by applying a magnetic field. When the magnetizations are parallel, there is a "short circuit" effect; electrons of one spin have a lower average resistance. They carry more of the current, lowering the total resistance of the structure compared to the total resistance for antiparallel magnetizations. The spin dependence of the resistance can come from spin-dependent defect scattering or spin-dependent interface reflection. The oscillatory exchange coupling is the coupling between the magnetic layers that oscillates in sign as a function of the spacer layer thickness. In magnetic multilayers, multiple reflection from the interfaces produces quantum well states, which are spin polarized because the reflection amplitudes are spin dependent. The quantum well states increase or decrease in energy as the thickness of the spacer layer increases. When they cross the Fermi level, the energy gained or lost from filling them changes the relative energies of the configurations with parallel and antiparallel magnetizations.

Both GMR and oscillatory exchange coupling have been the subject of many model and first-principles calculations [3]. Model calculations, usually based on the free electron approximation, can be easy to interpret and give insight into the important mechanisms, but many important details, related to neglecting the appropriate band structure, are not included. First-principles calculations implicitly include many of these details, but extracting underlying mechanisms from the results can be difficult. It can be quite useful to combine the best of both approaches and carry out first-principles calculations of the band-structure-related details used in model calculations. Among such details, spin-dependent transmission and reflection probabilities, particularly those for Fermi surface electrons, play an important role in both the GMR and the oscillatory exchange coupling.

Here, I present first-principles calculations of the spin-dependent transmission and reflection probabilities for the (001) interfaces of Ag/Fe, and Au/Fe and the (001), (111), and (110) interfaces of Cu/Co and Cu/Ni. I discuss the implications of the results for the transport properties of these systems and compute the strengths of the oscillatory exchange coupling.

## II. TRANSMISSION AND REFLECTION PROBABILITIES

In structures in which there is a single interface between two materials, an electron propagating toward the interface can either transmit or reflect. If the interface is coherent, that is, the two materials are well lattice matched, then the momentum parallel to the interface is conserved during transmission and reflection. Far enough from the interface, the time-independent scattering states for this process consist of linear combinations of bulk Bloch states. On one side of the interface, it consists of a Bloch state propagating toward the interface plus one or more reflected Bloch states propagating away from the interface, and on the other, it consists of zero or more transmitted Bloch states propagating away from the interface. Close to the interface, the scattering states consist of these Bloch states plus evanescent contributions that decay exponentially with distance from the interface. The transmission and reflection probabilities are just the flux in the transmitted and reflected Bloch states divided by the flux in the incident Bloch state. The two probabilities sum to one.

The calculation [4] of the time-independent scattering states starts by breaking space up into layers. The potential is computed for each layer from a bulk electronic structure calculation (a linearized-augmented-plane-wave implementation of the local spin-density approximation). Generalized Bloch states for a layer are computed from the potential in the layer. Generalized Bloch states are related to Bloch states by allowing the component of the wave vector normal to the interface to be complex. They form a complete set of states, which includes the usual Bloch states and all evanescent states, and consequently describe

any time-independent solution of Schrödinger's equation for arbitrary boundary conditions. The generalized Bloch states for the two materials are matched together across the interface to construct the electron scattering states, giving the reflection and transmission amplitudes directly.

The calculations for Cu/Ni and Cu/Co, where the Co is face-centered cubic, use the bulk lattice constant of Cu for both materials. Face-centered cubic Ag and Au are quite well lattice matched with body-centered cubic Fe if the (001) planes are rotated 45° with respect to each other. The calculations for Au/Fe and Ag/Fe use the bulk lattice constant for Fe and a very slight tetragonal distortion, based on their bulk elastic constants, for Au and Ag.

Figures 1-4 show the transmission probabilities across interfaces between these pairs of materials calculated for states on the Fermi surfaces of both materials. The Fermi surfaces are shaded according to the transmission probability for each state, and then they are projected into the interface Brillouin zone. For simple Fermi surfaces and certain interface orientations, there is only one state moving toward the interface at each parallel wave vector. Grouped together, these states form a sheet of the Fermi surface. For the interfaces with only one sheet of states moving toward the interface, that sheet is shown in the whole interface Brillouin zone. For other interface orientations, or for complicated Fermi surfaces, the Fermi surface has several sheets. That is, at some parallel wave vectors there is more than one state moving toward the interface. For Fe, minority Co and Ni, Cu(110), and majority Co(110), each sheet is shown in a fraction of the Brillouin zone. The behavior over the full Fermi surface is found by rotating each sheet into each fraction of the Brillouin zone and stacking the sheets on top of each other. Table I gives the average over the Fermi surface of the transmission probabilities.

Some general features of these results are straightforward to understand. For example, states reflect completely if there are no states in the other material with the same parallel momentum. In addition, the symmetry of the states is important. Fermi surface states have $s-p$ character for noble metals and majority states in Co and Ni, but they have mainly

TABLE I. Transmission probabilities averaged over the Fermi surface.

| | Into Minority | Into Majority | From Minority | From Majority |
|---|---|---|---|---|
| Ag/Fe(001) | 0.16 | 0.86 | 0.14 | 0.36 |
| Au/Fe(001) | 0.17 | 0.84 | 0.16 | 0.37 |
| Cu/Co(001) | 0.49 | 0.79 | 0.27 | 0.95 |
| Cu/Co(111) | 0.54 | 0.73 | 0.33 | 0.94 |
| Cu/Co(110) | 0.44 | 0.66 | 0.29 | 0.92 |
| Cu/Ni(001) | 0.72 | 0.73 | 0.33 | 0.93 |
| Cu/Ni(111) | 0.80 | 0.67 | 0.38 | 0.92 |
| Cu/Ni(110) | 0.62 | 0.63 | 0.31 | 0.60 |

$d$ character for minority states and Fe majority states. States with $s-p$ character tend to couple well to one another and to states with $dz^2$ character, but couple weakly to other $d$-like states. At high symmetry points, like the zone center, $\bar{\Gamma}$, these symmetry requirements become strict and some states, like the minority states in Au/Fe, reflect completely even though there are states with the same parallel wave vector.

Au/Fe (Fig. 1) and Ag/Fe (similar, but not shown) both show very good transmission into the majority states of Fe and poor transmission into the minority states. In the reverse direction the difference is much smaller, because there are many majority states that have very small transmission probabilities. These systems contain minority electrons that are largely confined to each separate material, majority electrons that transmit freely between them, and majority electrons confined to the ferromagnetic material.

The potentials in Cu are very similar to the potentials for the majority electrons in Co and Ni, but significantly different from those for the minority. This spin dependence leads to strongly spin-dependent scattering from substitutional impurities in these systems [6,7], and strongly spin-dependent transmission across interfaces, Figs. 2-4. The majority Fermi surfaces in Co and Ni are similar to the Fermi surfaces in Cu, but smaller. The similarities

lead to almost complete transmission from the majority states in the ferromagnet into the nonmagnetic material, but the smaller sizes lead to complete reflection for the states in Cu with group velocities parallel to the interface. The transmission from Cu into minority states is not simply characterized. Some electrons transmit well, some completely reflect, but most exhibit intermediate behavior. The complicated behavior arises from the complicated nature of the minority Fermi surfaces of Co and Ni. Overall, the results do not vary much with interface orientation. It seems likely that transport calculations, which average in some way over all of the states, will have only a weak orientation dependence.

These transmission probabilities can be contrasted with those from free electron approximations. Projecting spherical free-electron Fermi surfaces on to the interface Brillouin zone gives circles of different radii. States with parallel wave vectors less than the Fermi wave vectors of the materials on either side of the interface transmit well. When the parallel wave vector becomes close to the smaller of the two Fermi wave vectors, the transmission goes to zero, and reflection is complete for states with a parallel wave vector greater than the smaller Fermi wave vector. This free electron behavior is a reasonable description of the behavior for the majority states in Cu/Co and Cu/Ni, but not for the minority states, nor for Au/Fe(001) or Ag/Fe(001).

## III. GIANT MAGNETORESISTANCE

Strongly spin-dependent interface reflection can lead to a GMR effect even if there is no spin dependence to the defect scattering. For the case of current perpendicular to the interfaces, a contribution to the GMR comes from the spin dependence of the resistance associated with each interface. For current flow parallel to the interface there is no resistance associated with reflection. However, if the defect scattering rates are different in the ferromagnetic layers and nonmagnetic layers, spin-dependent interface reflection will still contribute to the GMR as is discussed below.

GMR is usually observed in samples in which the elastic mean free paths and the thick-

nesses of the layers are comparable and both lengths are much less than the spin diffusion length. The essential physics is most easily understood from semiclassical calculations, which are valid when the layer thicknesses are much greater than the mean free paths. Here, I discuss GMR from such a semiclassical perspective, and note some corrections that are a consequence of the mean free paths being comparable to the thicknesses. I also assume that the spin diffusion length is infinite. Throughout this discussion, GMR is caused by a short circuit effect. When the magnetizations are antiparallel, electrons of both spins have the same average resistance. When the magnetizations are parallel, electrons of one spin have a higher resistance and those of the other a lower resistance. The electrons with the lower resistance carry more of the current, lowering the resistance of both spins taken together. Thus the resistance of the structure is lower when the magnetizations are parallel.

Current flow perpendicular to interfaces that reflect electrons requires that there be a chemical potential difference across the interface, even if there is no defect scattering at the interface [5]. For interfaces separated by much more than the mean free path, the amount of current crossing the interface is proportional to the chemical potential difference across the interface. This proportionality means that there is a resistance associated with each interface even if the momentum randomization occurs elsewhere in the sample. This resistance is independent of the separation of the interfaces and the bulk scattering rates, provided the interfaces are sufficiently far apart.

If the reflection probability is spin-dependent, the resistance of the interface is also. Thus, if electrons of only one spin transmit freely through all the interfaces in the structure, those electrons will have a lower resistance when the magnetizations in the ferromagnetic layers are parallel. They cause the short circuit effect that gives the GMR. The interface resistance is dominated by electrons moving perpendicular to the interface, which tend to be close to the zone center. It is clear from Fig. 1 and Fig. 2 that this effect will give a large contribution to the GMR for Au/Fe(001), Ag/Fe(001) and Cu/Co(001), but from Fig. 3 it will be much smaller for Cu/Ni(001). For most of these systems, the spin dependence of the interface resistance is much greater than it would be in free electron models. In those

models, the electrons close to the zone center reflect only weakly from both the majority and the minority states and do not contribute to the GMR.

When the separation between interfaces becomes comparable to the mean free path in the material between them, interference between electrons reflecting from different interfaces modifies the transport so that the interface resistance is no longer associated with a single interface. For periodic interfaces closer than a mean free path, the Bloch states of the superlattice become the appropriate basis for treating the scattering. In this regime, which has been used in all first principles calculations to date [6–8], the contribution to the resistance from the interfaces becomes obscured, but is still present.

The electronic structure of multilayers and superlattices can be constructed piece-wise from the electronic structures of the bulk materials and the interface reflection amplitudes [9]. Such a construction allows the electronic structure of multilayers and superlattices to be understood in terms of these simpler parts. Where the reflection probability is small, the states tend to propagate readily through the whole structure, but when the reflection probabilities are large, the states tend to localize in one material. In superlattices, reflection from the interfaces produces gaps in the Fermi surface of the superlattice. When states are freely propagating though the superlattice, these gaps are small, but when the states are localized the gaps become large. The results shown in Fig. 2, explain the spin-dependent gaps found for Cu/Co(001) superlattices [10]. That calculation shows that even when there is no defect scattering, this spin dependence leads to a GMR effect in a point contact [10].

For current parallel to the interface, "channeling" can make an important contribution to the GMR, as seen in studies based on free-electron models [11]. Channeling occurs for any multilayer in each layer in which electrons are strongly reflected from both its interfaces. If the scattering rate in that layer is lower than it is in neighboring layers, electrons in that layer which strongly reflect see a lower effective scattering rate than they would in the absence of reflection. In magnetic multilayers, channeling contributes to the GMR only for parallel wave vectors for which there is strong reflection for one spin, but not the other. In this case, channeling does not occur for electrons of either spin in antiferromagnetic

alignment because both transmit through one or the other interface. On the other hand, for ferromagnetic alignment, electrons of one spin are confined to the layer, and if that layer has a lower scattering rate, these electrons cause a short circuit effect, giving a GMR.

In the Cu/Co and Cu/Ni systems, the electrons in Cu with the largest velocities parallel to the interfaces reflect completely from the majority states due to the mismatch in the Fermi surfaces. Since the same states transmit well into the minority states, channeling by these electrons will give a large contribution to the GMR if the scattering rate in Cu is much smaller than it is in Co. Closer to, but not at, the zone center, there are additional channeling contributions to the GMR from states that are strongly reflected from the Co minority states, but are readily transmitted into the Co majority states.

Free electron models will not correctly describe these channeling effects. In free electron models, the minority Fermi surface is smaller than the majority Fermi surface. Thus, the electrons in Cu with the largest velocities parallel to the interfaces will reflect completely from both the majority and the minority states and not contribute to the GMR. On the other hand, there will be a contribution, not found in the present results, from electrons with parallel wave vectors between the majority and minority Fermi wave vectors. Finally, free electron models will not include the contribution for electrons closer to the zone center found in the present results.

For the Au/Fe(001) and Ag/Fe(001), the difference in reflectivity is so large over the Fermi surface that channeling will be a very big effect, even though the electrons in the noble metal that are moving parallel to the interface reflect strongly from both majority and minority states and do not give a channeling contribution to the GMR.

There is an additional interface contribution to the GMR for parallel transport in supercell calculations [8,10]. Here, the group velocities of the states at the Fermi surface *of the supercell* are modified by the multiple reflection at the interfaces. This effect is related to the gaps in superlattice Fermi surfaces discussed above. The different group velocities at the spin-dependent Fermi surfaces in different configurations lead to a GMR.

The results presented here make it clear that free-electron models will not accurately

predict the size of either the interface resistance or the channeling effect. Free electron descriptions are reasonable only for majority electrons in Cu/Co and Cu/Ni, but the contribution to the GMR depends on the difference in reflection between majority and minority systems.

## IV. OSCILLATORY EXCHANGE COUPLING

The exchange coupling between ferromagnetic layers separated by nonmagnetic spacer layers is a product of geometrical properties of the Fermi surface of the spacer layer material and the reflection amplitudes from the interfaces [12,13]. There are oscillatory contributions to the coupling from parallel wave vectors where two sheets of the Fermi surface are parallel to each other and have opposite group velocities in the interface direction. For large spacer layer thicknesses, $D$, each of these critical spanning vectors, indexed by $\alpha$, makes a contribution, $J^\alpha$ of the form

$$\frac{J^\alpha}{D^2}\sin(q_\perp^\alpha D+\phi^\alpha)=\frac{\hbar v_\perp^\alpha \kappa^\alpha}{4\pi^2 D^2}\mathrm{Im}\left[\Delta r_A^\alpha \Delta r_B^\alpha e^{iq_\perp^\alpha D}e^{i\chi^\alpha}\right], \tag{1}$$

where $v_\perp^\alpha$ is the component of the effective group velocity in the interface direction, $\kappa^\alpha$ is the radius of curvature of the Fermi surface, $\Delta r_{A(B)}^\alpha$ is the spin difference in the reflection amplitude for the left (right) interface, $q_\perp^\alpha$ is the critical spanning vector, which determines the period of the oscillation $L^\alpha = 2\pi/q_\perp^\alpha$, $\chi^\alpha$ is a phase from the type of critical point (maximum, minimum, saddle point), and $\phi^\alpha$ is the resulting phase (The reflection amplitudes are complex.) [14]. Table II gives the coupling strengths for all of the critical points for these systems. These critical points are the same as those identified from experimental Fermi surfaces by Bruno and Chappert [15].

For Ag/Fe and Au/Fe the critical point at $\bar{\Gamma}$ (the interface zone center) gives a long period oscillation. Here the reflection probability for the minority spins is exactly one and for the majority spins it is close to zero. The other critical points, along the $\bar{\Delta}$ line close to the zone boundary, produce a short period oscillation. At these points, the reflection probability is

TABLE II. Coupling strength due to various stationary points on the spacer layer Fermi surfaces, see Eq. 1.

| Interface | $k_x$ ($\mathrm{nm}^{-1}$) | $k_y$ ($\mathrm{nm}^{-1}$) | Period (nm) | Period (layers) | $J^\alpha/(1.0\ \mathrm{nm})^2$ ($\mathrm{mJ/m}^2$) |
|---|---|---|---|---|---|
| Ag/Fe(001) | 0.00 | 0.00 | 1.34 | 6.5 | 3.1 |
| Ag/Fe(001) | 9.41 | 0.00 | 0.50 | 2.44 | 0.36 |
| Au/Fe(001) | 0.00 | 0.00 | 2.12 | 10.3 | 1.1 |
| Au/Fe(001) | 9.12 | 0.00 | 0.51 | 2.49 | 2.0 |
| Cu/Co(001) | 0.00 | 0.00 | 1.16 | 6.4 | 0.12 |
| Cu/Co(001) | 9.92 | 0.00 | 0.47 | 2.58 | 11 |
| Cu/Co(111) | 14.22 | 0.00 | 0.90 | 4.3 | 0.67 |
| Cu/Co(110) | 0.00 | 0.00 | 0.26 | 2.07 | 27 |
| Cu/Co(110) | 0.00 | 12.31 | 0.34 | 2.65 | 0.029 |
| Cu/Co(110) | 8.71 | 12.31 | 0.32 | 2.52 | 0.16 |
| Cu/Co(110) | 8.71 | 12.31 | 1.23 | 9.7 | 1.3 |
| Cu/Ni(001) | 0.00 | 0.00 | 1.16 | 6.4 | 0.005 |
| Cu/Ni(001) | 9.92 | 0.00 | 0.47 | 2.58 | 10 |
| Cu/Ni(111) | 14.22 | 0.00 | 0.90 | 4.3 | 0.26 |
| Cu/Ni(110) | 0.00 | 0.00 | 0.26 | 2.07 | 1.2 |
| Cu/Ni(110) | 0.00 | 12.31 | 0.34 | 2.65 | 0.003 |
| Cu/Ni(110) | 8.71 | 12.31 | 0.32 | 2.52 | 0.008 |
| Cu/Ni(110) | 8.71 | 12.31 | 1.23 | 9.7 | 0.07 |

increasing rapidly as a function of parallel wave vector for the majority states and decreasing rapidly for the minority states. These rapid changes lead to a large uncertainty in the coupling strengths for these critical points. For Au/Fe, the ratio of the strengths for the two periods happens to be close to the experimentally determined ratio of 2.1 [16], but for Ag/Fe the ratio is very far from the experimental ratio of 1.0 [17]. All the coupling strengths are roughly an order of magnitude larger than measured values [18].

The Cu/Co systems have been extensively studied experimentally [19] and theoretically [20–24]. Previous theoretical results are similar to the results found here. For the (001) interface, the critical points along $\bar{\Delta}$ give a strong short period oscillation and the critical point at $\bar{\Gamma}$ gives a long period oscillation that is weak because both spins reflect weakly. For the (111) interface the critical points at the necks along the zone boundary give strong coupling. For the (110) interface, there are four critical spanning vectors, including one at the zone boundary which gives a strong long period oscillation and one at $\bar{\Gamma}$ which gives an extremely strong short period oscillation. The Cu/Ni systems have received much less attention. The differences in coupling strength compared to Cu/Co are due to the differences in reflection amplitudes.

As was the case for the Au/Fe and Ag/Fe systems, the calculated coupling strengths for Cu/Co are much stronger than those measured experimentally. In my opinion, the difference results from calculations being done for ideal interfaces while measurements are made on systems with interdiffusion and steps and other defects at the interfaces. Interface defects reduce reflection amplitudes by scattering electrons into all parallel wave vectors. Reduced reflection amplitudes lead to reduced coupling strengths. The experimental determination of the structural properties of the interfaces will allow a more detailed comparison between theory and experiment.

The major source of error in this work is the deviation of the Fermi surfaces calculated in the local spin-density approximation from the actual Fermi surfaces. Comparing predicted periods with those found from the measured Fermi surfaces [15] gives an estimate of this error. Differences range up to $\pm 20\%$. Lee and Chang [23] compute coupling strengths for

Cu/Co using empirical tight-binding and Eq. (1). Since they fit their band structures for Cu to de Haas-van Alphen data, the contributions to the coupling from the geometrical factors are more accurate in their calculations. On the other hand, the reflection probabilities, which they calculate in a parameterized tight-binding approach, are less reliable. Their results disagree with the present calculations by up to a factor of two. A less significant source of error in this work is the neglect of self-consistency in the interface potential. Experience [4] suggests that introducing a self-consistent potential leads to only small changes in the reflection and transmission amplitudes.

## V. SUMMARY

First-principles calculations of transmission and reflection from Ag/Fe, Au/Fe, Cu/Co, and Cu/Ni interfaces show very strong spin dependence. The behavior of the spin-dependent transmission and reflection probabilities is significantly more complicated than expected from free electron models. The complications arise because many of the relevant Fermi surfaces are significantly more complicated than spheres. The spin dependence of the reflection from interfaces is enough to give a large GMR even if there is no spin dependent defect scattering. For perpendicular transport, it leads to a spin-dependent resistance associated with each interface. For parallel transport, it leads to channeling, which gives a GMR if the scattering rates are different in the two materials. The calculated reflection amplitudes predict strengths of the oscillatory exchange coupling which are much greater than those observed experimentally. This disagreement is probably due to the assumed perfection of the interfaces.

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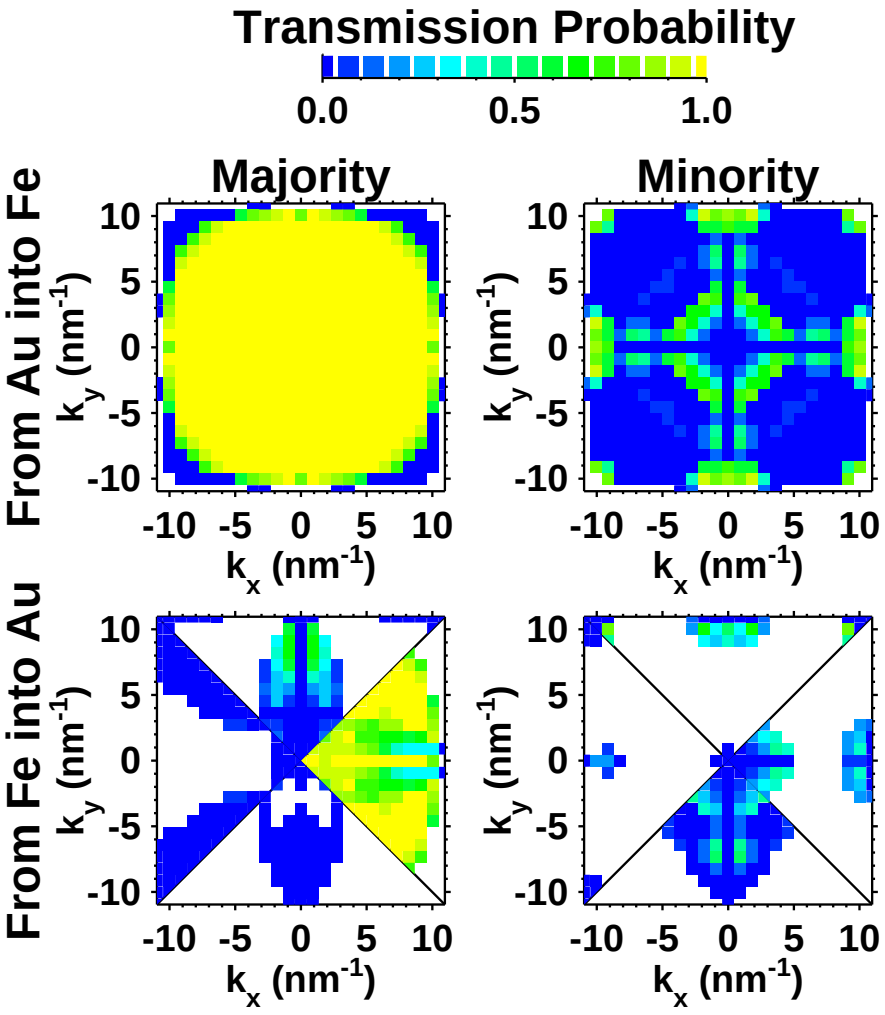


FIG. 1. Spin-dependent transmission probabilities for Au/Fe(001). The transmission probabilities are shown for various points on the Fermi surface projected onto the interface Brillouin zone. The color scale for the transmission probability is at the top. The top (bottom) two panels show the transmission for electrons incident from the Au (Fe) into the Fe (Au). The two right (left) panels show the transmission probabilities for the minority (majority) electrons.

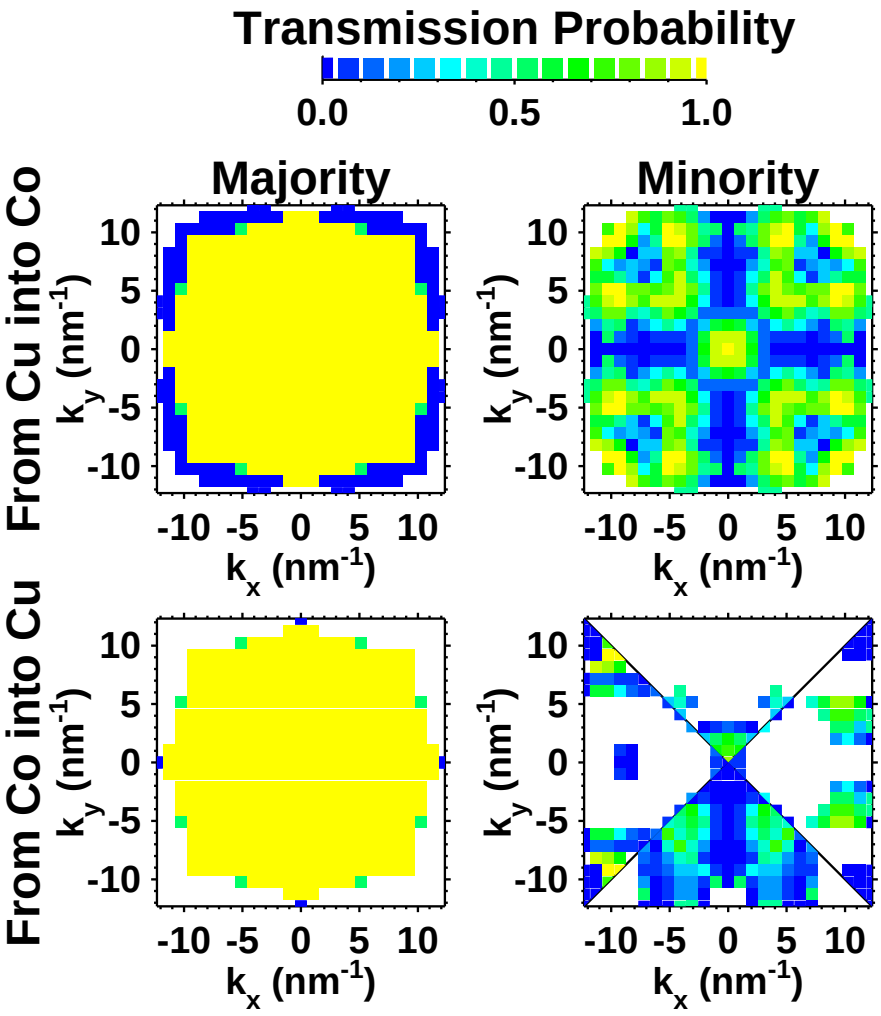


FIG. 2. Spin-dependent transmission probabilities for Cu/Co(001). See Fig. 1.

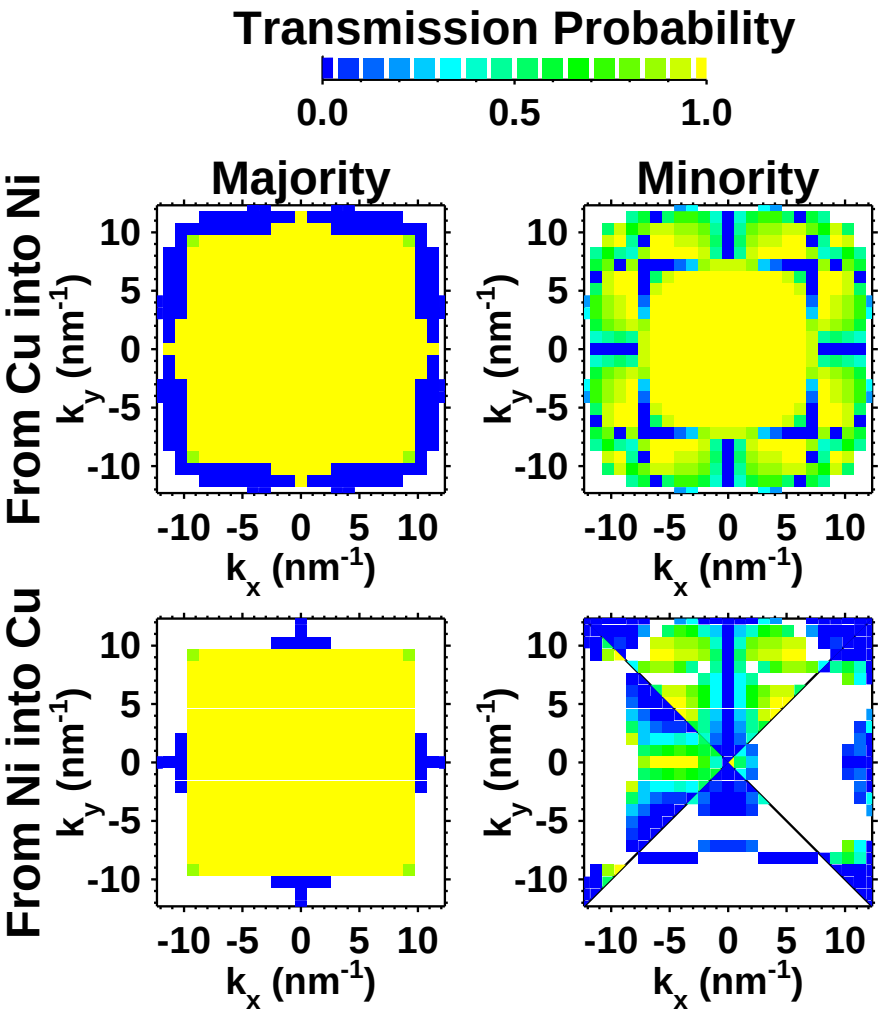


FIG. 3. Spin-dependent transmission probabilities for Cu/Ni(001). See Fig. 1.

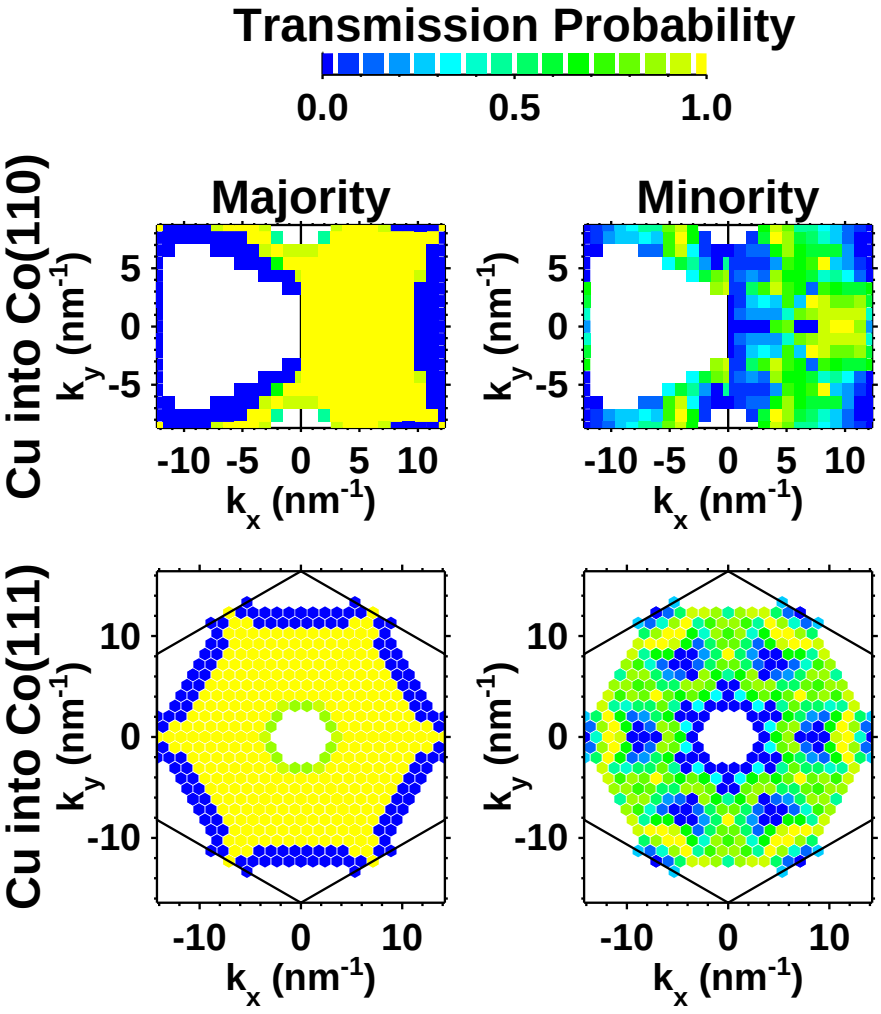


FIG. 4. Spin-dependent transmission probabilities for Cu/Co(110) and Cu/Co(111). See Fig. 1.