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Interlayer exchange coupling

M.D. Stiles*

Electron Physics Group, National Institute of Standards and Technology, Bldg 220 Rm B206 Gaithersburg, MD 20899, USA

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Abstract

The extensive research done on interlayer exchange coupling in transition metal multilayers has resulted in a deep understanding of this coupling and a remarkable agreement between theoretical results and measurements. The coupling between two magnetic layers separated by a non-magnetic spacer layer is mediated by the electrons of the spacer layer. The coupling, which oscillates in sign as a function of the thickness of the spacer layer, is closely related to the well-known RKKY interaction between magnetic impurities. Due to the existence of many high-quality measurements, it has been much more fully developed theoretically than the interaction between impurities. Theory predicts that the periods of the oscillatory coupling should depend on critical spanning vectors of the Fermi surface belonging to the spacer-layer material. There is remarkable agreement for the measured periods and those predicted from the Fermi surfaces. There is also substantial agreement between theory and experiment on the strength of the coupling. This review presents the comparison between theory and experiment in some detail. © 1999 Published by Elsevier Science B.V. All rights reserved.

Keywords: Interlayer exchange coupling; Spacer-layer thickness; Fermi surfaces; RKKY interaction

1. Introduction

When magnetic films are separated by a non-magnetic spacer layer, the magnetizations of the layers are coupled to each other by an exchange interaction through the electrons of the spacer layer. As the thickness of the spacer layer is varied, the coupling can oscillate in sign; as many as 60 sign changes have been observed as a function of thickness. This coupling is closely related to the oscillatory coupling, known as the RKKY interaction [1–3], between magnetic impurities in a non-magnetic host. It was first observed in 1986, both in transition metal multilayers [4] and in rare-earth multilayers [5,6]. Shortly thereafter, a large change in resistance with changing alignment of the layer magnetizations, known as giant magnetoresistance, was discovered in Fe/Cr multilayers [7,8]. This discovery led to a great deal of interest because of commercial applications. In 1990, systematic studies of the giant magnetoresistance in several transition metal multilayers found that the coupling oscillates as a function of spacer-layer thickness [9]. This review article will describe our current understanding of the interlayer exchange coupling in transition metal multilayers, based on the extensive research done since 1990.

Much has been written about interlayer exchange coupling, including several reviews [10–13]. This review emphasizes the current status of the comparison between theory and experiment. I will

* Corresponding author. Tel.: +1-301-975-3745; fax: +1-301-926-2746.

E-mail address: mark.stiles@nist.gov (M.D. Stiles)

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not attempt to describe the related coupling found in rare-earth multilayers, which have been the subject of several reviews [14,15]. Similarly, I will not discuss quantum-well states in magnetic multilayers, even though their observation has played an important role in confirming our understanding of interlayer exchange coupling. These results have been recently reviewed in Refs. [16,17]. Finally, I will only consider the bilinear coupling in these systems. I will not describe the biquadratic coupling which is almost always present in addition to the bilinear coupling. The biquadratic coupling is believed to arise from extrinsic effects [18], like interface roughness, and the comparison between theory and experiment is much more ambiguous. A recent review [19] describes what is known. Particular forms of biquadratic coupling are associated with antiferromagnetism in the spacer layer, Cr and Mn being two examples. These effects are described elsewhere in this volume [20] and will not be considered here.

In the next section, I will describe the physical origin of interlayer exchange coupling. This understanding is embodied in several different models for the coupling. I will describe these models, emphasizing their common features. Some experimental predictions, like the periods of the coupling, are common to all of the models. Others, like the coupling strength, vary from model to model. In Section 3, I will describe some of the difficulties in comparing theory to experiment. Finally in Section 4, I will compare experimental results with theoretical results on a system by system basis.

2. Bilinear coupling models

Interlayer exchange coupling between magnetic layers mediated by a non-magnetic spacer has essentially the same physical origin as the RKKY coupling between magnetic impurities in a non-magnetic host. In both cases, localized and spin-polarized disturbances, interfaces in one case and impurities in the other, are coupled to each other by their influence on the electrons in the spacer or host, respectively. First consider a single interface or impurity. It sets up an oscillatory polarization in the non-magnetic spacer or host. This polarization is essentially a single-particle effect. All electrons scatter from the interface or impurity. The interference between the incoming and scattered waves gives rise to oscillatory probability densities for each electron. Since the interfaces and impurities are magnetic and scatter spin-up and spin-down electrons differently, filling all states below the Fermi energy gives an oscillatory spin density. Since different waves are characterized by vectors for all the states, each of their states contributes to oscillations with different periods. However, all of the oscillations cancel out, except for those at the Fermi energy, where there is a sharp cut-off from completely filled states to completely unfilled states, leaving an oscillation characterized by the Fermi surface. The second interface or impurity couples to the spin density set up by the first. Since the spin density oscillates as a function of the spacer-layer thickness or impurity separation, the coupling oscillates as well.

Several early models [21–25] of the interlayer exchange coupling were based explicitly on using the RKKY interaction for impurities. These models consider the interaction between two two-dimensional sheets of impurities embedded in a non-magnetic host. This model is based on a local-moment approximation to describe the magnetic material. While such an approximation may [26,27] or may not [28] be valid for magnetism in rare-earth multilayers, it is not valid for magnetism in transition metals where the bandwidths of the d-electrons, which make up the magnetic moments, are on the order of 10 eV wide.

While RKKY-based models may not use an appropriate description of the magnetism in transition metals, they point out some important general features of models for the interlayer exchange coupling. They point out that the periods of the oscillatory coupling are determined by critical spanning vectors of the Fermi surface of the material that makes up the spacer layer [22,29]. Critical spanning vectors, see Fig. 1, are vectors in the direction of the interface normal, that connect two sheets of the Fermi surface that are parallel to each other at the endpoints of the vector. Critical spanning vectors determine the coupling periods in all models of interlayer exchange coupling. Comparing measured periods with those predicted by

various models is the most robust aspect of comparing theory and experiment in these systems.

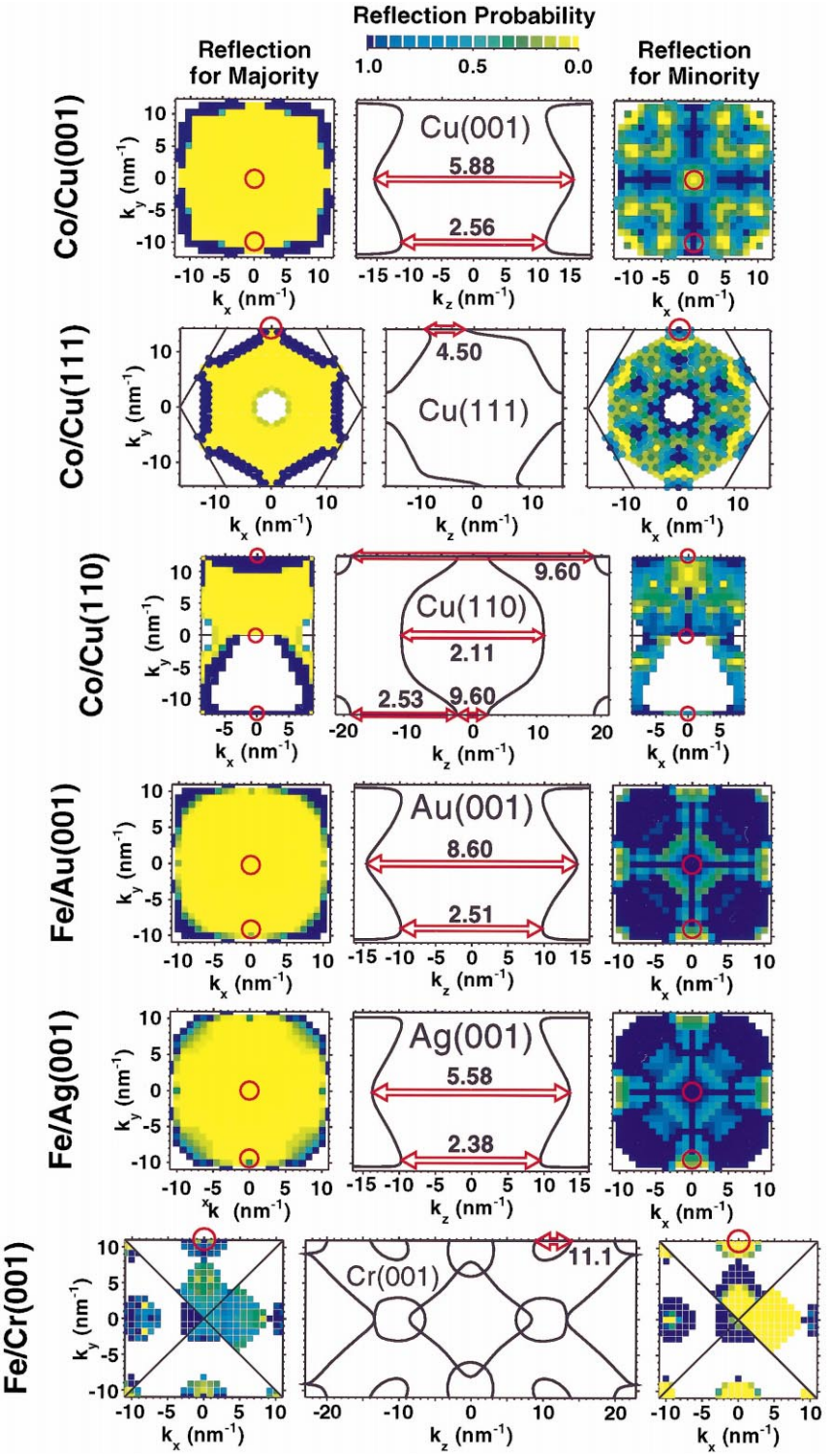
In these models, the critical spanning vectors are properties of the Fermi surface of the bulk material that makes up the spacer, rather than the Fermi surface of the spacer layer itself. The fact that the spacer layer is part of a multilayer, and cannot have an independent Fermi surface is beside the point. The (possibly fictitious) bulk material that makes up the spacer does have a well-defined Fermi surface that is useful for understanding the interlayer exchange coupling. The electron states in the multilayer can be described in terms of linear combinations of bulk states of the material that makes up each layer. These states are matched together at the interfaces to construct the scattering states of the full system. Even though the bulk materials may be artificial constructs, they still provide a useful basis for a description of the states in the system.

Soon after the discovery of the interlayer exchange coupling, it was thought, based on free-electron models, that oscillation periods would be much shorter than those that were observed experimentally. It was quickly pointed out by several groups [30–32] that it is important to account for the lattice of the spacer layer. With a lattice, it is impossible to talk of oscillations that are faster than the lattice spacing. Such oscillations get 'aliased' with the lattice spacing to produce oscillations that are slower than the lattice spacing. The period of an oscillation on a lattice with layer spacing d is determined from a critical spanning vector $q_\perp$ by finding the shortest possible equivalent spanning vector, $|q_\perp - 2\pi n/d|$, where n is some integer.

While models based on the RKKY interaction capture much of the essential physics and correctly predict possible coupling periods, they do not correctly predict the strength of the coupling because they do not adequately describe magnetism in transition metals. An alternate approach, which is also not quantitative but captures much of the essential physics, is to make a free-electron approximation in each layer with exchange split bands in the ferromagnetic material [33–36]. The two simple models, RKKY and spin-split free-electron bands, represent two extremes in the description of magnetism, local-moment models and itinerant models respectively.

One feature of free-electron models is that the strength of the interlayer coupling depends on the spin difference of the reflection amplitudes for electrons in the spacer layer reflecting from the interfaces with the magnetic material. This dependence transfers to models with general band structures [37–39]. Spin-dependent reflection from the interfaces gives quantum confinement in the spacer layer [29], setting up spin-dependent quantum-well states, both true bound states and resonances, due to the interference resulting from multiple reflection from the interfaces. As mentioned above, these quantum-well states have been seen experimentally in photoemission and inverse photoemission [40–43]. The filled quantum-well states give rise to the oscillatory polarization described earlier. As the thickness of the spacer layer is changed, the quantum-well states move up or down in energy depending on the details of the spacer-layer band structure. The oscillatory interlayer exchange coupling is determined by the energy changes associated with filling and emptying these states as they cross the Fermi energy when the thickness of the spacer layer is varied. The stronger the spin-dependent reflection, the stronger the confinement and the stronger the oscillatory coupling.

Fig. 1. Critical spanning vectors and interface reflectivities. For a series of spacer layers, magnetic materials, and interface orientations, organized in rows, the middle panels show slices though the Fermi surface of each spacer layer material for $k_x = 0$. The interface normal is the z direction in all cases. Superimposed in red on the Fermi surfaces are some of the critical spanning vectors. Each critical spanning vector is labeled by its associated coupling period in monolayers as determined from the experimental Fermi surfaces [22,114]. In the left and right panels, the Fermi surface is projected onto the $k_z = 0$ plane. It is color-coded based on the probability for an electron incident from the spacer layer material to reflect from the interface with the magnetic material. Probabilities for electrons with spins parallel to the majority and minority spin directions are shown in the left and right panels, respectively. The locations of the critical spanning vectors are labeled by red circles centered at the critical point. The Cu Fermi surface projected into a (1 1 0) interface and the Cr Fermi surface projected into a (0 0 1) interface have multiple sheets. To present these overlapping sheets, each is only shown in a faction of the interface Brillouin zone. The full Fermi surface can be reconstructed by rotating the various partial sheets into to the other symmetric parts of the zone.


Reflection Probability
1.0
0.5
0.0
Reflection for Majority
Reflection for Minority
Co/Cu(001)
Cu(001)
5.88
2.56
Co/Cu(111)
4.50
Cu(111)
Co/Cu(110)
9.60
Cu(110)
2.11
2.53
9.60
Fe/Au(001)
Au(001)
8.60
2.51
Fe/Ag(001)
Ag(001)
5.58
2.38
Fe/Cr(001)
Cr(001)
11.1
k_x (nm^-1)
k_y (nm^-1)
k_z (nm^-1)

All these models, RKKY [22], quantum-confinement [29], free-electron [33–36], and interface-reflection [37–39] predict that for large spacer-layer thicknesses, D, the coupling should be given by a sum of terms of the form

$$J(D) = \sum_{\alpha} \frac{J^{\alpha}}{D^2} \sin(q_{\perp}^{\alpha} D + \phi^{\alpha}). \quad (1)$$

There is a contribution from each critical point, labeled by α, with critical spanning vector $q_{\perp}^{\alpha}$, coupling strength, J^{α} and phase ϕ^{α}. For large thicknesses, this *form* is independent of the model used to describe the interlayer coupling. For small thicknesses, other terms, called pre-asymptotic corrections, become important. In all models, the periods are determined by the critical spanning vectors of the spacer-layer Fermi surface, $L^{\alpha} = 2\pi/q_{\perp}^{\alpha}$. Thus, the best way to compare measured coupling periods with theory is to use the critical spanning vectors found from analyzing experimental measurements of the Fermi surfaces [22].

Model-independent comparisons are not possible for comparing coupling strengths. Two main approaches have been used for computing coupling strengths. The first approach is to calculate the total energy of the multilayer by computing and filling all the electron states below the Fermi energy. These calculations can be self-consistent, allowing the potential to vary in response to variations in the densities, or not. Even if not done self-consistently, these calculations are computationally very demanding. They have been implemented using different approximations for the band structure. The two most common approximations are tight-binding (TB) approximations or the local-density approximation (LDA).

The second approach is to calculate the coupling strength, J^{α}, in the asymptotic expansion for each contribution to the sum, Eq. (1) from

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

where $v_{\perp}^{\alpha}$ is the component of the effective group velocity in the interface direction, κ^{α} 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, and χ^{α} is a phase from the type of critical point (maximum, minimum, saddle point). In this approach, the critical spanning vectors are identified, and the spin-dependent reflection amplitudes for the states at those points on the Fermi surface are computed (see Fig. 1). These calculations are much less demanding computationally and give insight into what aspects of the band structures, Fermi surfaces, and electronic wave functions are important. The asymptotic form results from an approximation that ignores the energy and parallel wave-vector dependence of the reflection amplitudes and assumes that the Fermi surface is strictly quadratic near the critical points of the Fermi surface. These approximations may not be appropriate for particular systems [44–46], as will be discussed below. For small thicknesses, the pre-asymptotic corrections both can change the decay of the oscillations and can modify their effective period. However, the simple asymptotic form provides a useful context in which to understand the further details. All pre-asymptotic corrections are automatically included in total-energy calculations that are adequately converged.

A final theoretical issue is related to self-consistency in the electronic structure calculations. All of the asymptotic calculations and many of the total-energy calculations ignore the effect of the electron–electron interaction in the spacer layer on the spin-density wave that gets set up there. Ignoring the electron–electron interaction is analogous to using the bare susceptibility, χ_0, as opposed to the Stoner enhanced susceptibility, $\chi = \chi_0/(1 - J\chi_0)$. For noble metal spacer layers, this approximation appears to be good. For transition metal spacer layers, the situation is less clear. In Fe/Cr multilayers, the coupling is found to be a superposition of a short period and a long period. As discussed elsewhere in this issue [20], ignoring the electron–electron interaction is not a good approximation for the short-period component of the coupling. On the other hand, it may be a good approximation for the long-period contribution, as discussed below. Unfortunately, it is difficult to determine the importance of the electron–electron interactions in other systems. No other transition metals are well lattice-matched to transition-metal ferromagnets, a condition that is necessary for meaningful determinations. Several calculations

based on the local-density approximation have tried various approximations for turning off the electron–electron interaction [47,48] and compared the results with those from treating the electron–electron interactions self-consistently within the local-density approximation.

3. Difficulties in comparing theory and experiment

Several issues complicate the comparison between theory and experiment for interlayer exchange coupling. Many of these are related either to growing an experimental structure that is close enough to ideal that the system can be treated theoretically or to doing a calculation that is sufficiently complicated that it provides an adequate description of the actual experimental system. The most difficult issue to address theoretically is a lack of periodicity in the interface plane. Without this periodicity, the asymptotic approximations are not valid and the total-energy calculations are intractable. Thus, good comparisons between theory and experiment are only possible for systems that are close enough to lattice matched that is possible to grow coherent structures, structures in which all layers have the same in-plane lattice net. Unfortunately, this consideration greatly restricts the number of systems for which meaningful comparisons are possible.

Other possible types of disorder can at least be treated theoretically at some level of approximation. However, to do so it is necessary to know what the disorder is, and how much of it there is. For all but a few measurements, this information is not available. The simplest type of disorder to account for is the presence of fluctuations in the thickness of the spacer layer. While there are additional effects due to diffuse scattering at the steps, the gross effect of thickness fluctuations can be accounted for by averaging the coupling over the distribution of thicknesses due to the growth front [21]. It is possible to vary the roughness of the interface by varying the growth conditions, to measure the growth front with scanning tunneling microscopy, and to compare the resulting coupling with averages over the growth front [49]. In this case, the comparison appears to be quite good.

The coherent-potential approximation can be used to treat more localized and uniformly distributed defects, like bulk defects, including alloying [50,51], or interdiffusion at interfaces [52,53]. Physically, scattering from defects reduces the coherent scattering fraction, this scattering reduces the amplitude of the quantum-well states, reducing in turn the size of the oscillatory coupling. Only in the case of intentional alloying is the concentration of defects known well enough that quantitative comparisons between theory and experiment can be made. These will be discussed below.

Finite temperature also reduces the amplitude of the interlayer coupling. Most models predict a specific form of the temperature dependence [22,29], an additional factor of the form

$$\frac{(2\pi k_B TD/\hbar v_\perp^\alpha)}{\sinh(2\pi k_B TD/\hbar v_\perp^\alpha)} \tag{3}$$

associated with each critical spanning vector. However, none of these models include an accurate description of the temperature dependence of the ferromagnetic magnetization. Since the primary temperature dependence in ferromagnets at low temperature comes from the thermal excitation of spin waves, the temperature dependence of the exchange coupling will depend on the behavior of correlated spin waves in both materials. The spin waves in both materials become correlated by the exchange coupling across the interface. I am unaware of any quantitative treatment of this temperature dependence for interlayer exchange coupling (see Ref. [54] for a treatment of tunneling magnetoresistance). There have been some studies in which the form of the measured temperature dependence is consistent with that predicted by various models. In many systems the temperature dependence is weak, so the comparisons discussed below will ignore the temperature for the most part.

A theoretical difficulty is that the local-density approximation only reproduces the band structure to within some unknown accuracy. Where the Fermi surface is known experimentally, the accuracy can be checked. However, this inaccuracy is impossible to correct for within total-energy calculations. Thus the periods of the oscillations in these calculations will have some inherent inaccuracy,

and because the Fermi surfaces of the constituent materials are also slightly inaccurate, there is an unknown uncertainty in the resulting coupling strengths that cannot be eliminated. Most tight-binding band structures are constructed by fitting to band structures computed within the local-density approximation [55]. It is possible to adjust the tight-binding parameters to bring the Fermi surface into better agreement with experiment [56], but this is an uncontrolled approximation and may make other aspects of the tight-binding description worse.

Asymptotic calculations give J^{α}, total-energy calculations give $J(D)$, and experiments give $J(D)$ modified by whatever disorder is present. Even if there were no disorder in the experiment, the coupling at large thicknesses cannot be directly compared with that from a total-energy calculation because the periods in the calculation will be different than those in the physical system. Ideally, both total-energy calculations and experiment are fit to parameterized forms, like the asymptotic form, Eq. (1), and the parameters compared. In this case, the parameters are also easily compared with the results of asymptotic calculations. Unfortunately, it has been shown that the asymptotic form is not always a good description of at least the theoretical results (see the discussion below for Co/Cu(0 0 1)). If the results are not fit, experimental periods are usually determined from the separation of several peaks in the coupling. Without fits, coupling strengths are compared through the strengths of a peak at small thickness. These coupling strengths are different dimensionally from the parameters found in asymptotic calculations, J^{α}. To make meaningful comparisons it is useful to report the results of asymptotic calculations in the form of $J^{\alpha}/(1\ \mathrm{nm})^2$, as will be done below.

A final experimental difficulty is determining the coupling strengths from whatever properties are measured. The coupling strength is determined by computing the properties from a model and varying the parameters of the model, including the coupling strength, to fit the measured properties. This procedure is strongly dependent on having the correct model for all of the important energies in the system. In many model calculations, there are sharp features in the calculated properties that would aid in determining the parameters. However, in most measurements these sharp features are broadened out, presumably by disorder. The determination of the model parameters is sensitive to how the disorder is treated [57,58]. If the measurement involves reversal of the magnetization, it is also necessary to have a model for the reversal process. Most often, the models for reversal are solved in one of two limits, either the global minimum energy limit, which gives no hysteresis, or the Stoner–Wohlfarth limit, which gives maximal hysteresis. Reality is usually in between. Accurate determinations of the coupling require accurate determinations of the magnetic moments of each of the layers. Often, the magnetic moment is estimated from the thickness of the ferromagnetic films and the bulk magnetization. Then, the accuracy depends on how accurately the thickness is known, and how close the thin-film magnetization is to that of the bulk.

4. Comparison between theory and experiment

In this section, I describe the comparison between theory and experiment for specific systems. Overall, the agreement between theory and experiment is quite substantial, much more so than for similar comparisons for the bulk RKKY interaction between impurities. One of the outstanding points of agreement comes from the periods predicted from the experimental Fermi surfaces [22] and their precise experimental determination for the Ag/Fe(0 0 1) [58] and the Au/Fe(0 0 1) [59] systems. The coupling periods for other systems have been found less precisely, but all are in substantial agreement with critical spanning vectors of the experimental Fermi surfaces. The coupling strengths for Cu/Co(0 0 1) which have been measured [60–64] and calculated [39,44–46,65–71] by several groups are in qualitative agreement when some of the difficulties in the comparison are taken into account. Comparisons for the coupling strength of Cu/Co(1 1 1) [56,71–76] and Au/Fe(0 0 1) [71,77] are also in agreement, although studied less extensively. Several alloy studies [78,82] show agreement between periods predicted from approximate calculations of the alloy Fermi

surfaces and the measured periods as the alloy concentration is varied. Finally, the models described above predicted that the strength of the interlayer coupling should oscillate as a function of the thickness of every layer in the multilayer, e.g. not only the spacer-layer thickness, but also the thicknesses of the magnetic layers, and any capping layers. All these variations have been observed.

4.1. Lattice-matched noble-metal spacers

4.1.1. Co/Cu(0 0 1)

The most extensively studied system, both theoretically [39,44–46,56,65–71,83] and experimentally [60–64,84], has been FCC Co grown on Cu(0 0 1). These two materials are quite well lattice-matched and high-quality multilayers can be grown. However, there are substantial complications in the comparison between theory and experiment. Perhaps these complications are apparent simply because this system has been so extensively studied. The coupling is expected to involve a combination of two periodicities [22]. One period is long and is associated with the belly of the free-electron-like Cu Fermi surface. The other is short and is associated with the necks of the Fermi surface. Experimentally, the ratio of the two coupling strengths depends quite strongly on the growth [64,84]. Theoretically, it has been found [44–46] that the asymptotic approximation does not hold in the region of experimental interest. Finally, in both calculations and experiment [85,86] the coupling strength is found to depend on the thickness of the Co layers and even Cu capping layers [87,88].

In Co/Cu(0 0 1), theoretical difficulties arise for several reasons [46]. For the long period, which is associated with a critical point at the zone center, $\bar{\Gamma}$, the reflection amplitude is small for both minority and majority electrons. So the resulting asymptotic coupling strength is small for infinitely thick Co. However, for the minority electrons, the reflection amplitude increases rapidly with parallel momentum around the critical point up to nearly complete reflection at points still close to the zone center [71,89] (see Fig. 1). Thus, for thinner spacer layers, in which the coupling is sensitive to larger areas of the Fermi surface, the coupling is much stronger than would be expected from the asymptotic result [46]. In fact, the apparent period changes as well. In addition, the reflection amplitude for finite Co thickness is very sensitive to the Co thickness [83].

For the short period, there is a gap for the Co minority electrons with the same symmetry as the Fermi surface electrons in the Cu at the critical point. However, the gap is narrow in energy. Since the phase of the reflection amplitude changes by π across the gap, the reflection amplitude is strongly energy dependent, even though its modulus is constant [45,46,90]. The energy dependence of the reflection amplitude in this case gives a large reduction of the coupling for thin spacer layers compared to the value expected from the asymptotic result. These deviations from the asymptotic behavior for both critical points are born out in total-energy calculations [45,66–68].

The periods measured experimentally are in good agreement with those expected from the critical spanning vectors of the experimental Fermi surface [22]. Johnson et al. [62] measured the coupling as a function of thickness and fit the results to a combination of two periods with the asymptotic form, Eq. (1). Since the theoretical models indicate that the asymptotic behavior is not expected to hold for the thicknesses measured in the experiment, these fits need to be treated with caution. The resulting fits give periods of 2.60 ± 0.05 ML and 8.0 ± 0.5 ML, while the periods extracted from the experimental Fermi surfaces are 2.56 and 5.88 ML. The short periods are in good agreement, and the increase of the long period in the pre-asymptotic region is seen in total-energy calculations [45,66–69], and expected based on analysis of the pre-asymptotic corrections [46]. Weber et al. [64] measure the sign of the coupling and fit the zero crossing to the sum of two asymptotic contributions. With the same caution about the applicability of such fits they find short periods in the range of 2.58–2.77 ML and long periods in the range 6.00–6.17 ML over the four samples they studied. In all four samples, the zero crossings were very different, showing the sensitivity of the results to the quality of the growth.

Given the large pre-asymptotic behavior in this system, there is substantial agreement between different calculations of the coupling strength.

Table 1
Coupling energies in Co/Cu(0 0 1) multilayers. All coupling energies are in mJ/m^2. The asymptotic values are given at a spacer thickness of 1 nm. Entries with a * have been estimated by the author from figures in the given references. The total-energy calculations are compared with each other and experiment by determining the coupling energy at a peak close to 1 nm spacer thickness. The position of the peak, D_{peak} is given in ML

Reference	Method	$J^L/(1\ \mathrm{nm})^2$	$J^S/(1\ \mathrm{nm})^2$	D_{peak}	$J(D_{\mathrm{peak}})$
[71]	Asymptotic (LDA)	0.12	11		
[56]	Asymptotic (TB)	0.021	6.7		
[89]	Asymptotic (TB)	0.14	0.57		
[44]	Total-energy (TB)	0.01*	12*	6	1.2*
[69,70]	Total-energy (LDA)		13*	9	4.6*
[66–68]	Total-energy (LDA)			7	1.42
[63]	Experiment			5.2	0.39
[85]	Experiment			5.2	0.24
[61]	Experiment			6	0.16

Representative values of coupling energies are compared in Table 1. It is possible from some of the total-energy calculations to calculate or estimate the asymptotic behavior, which is found to agree with strictly asymptotic calculations. The total-energy calculations can be compared with each other in terms of the strength of the coupling at a peak close to 1 nm spacer thickness. The calculated coupling strengths are at least a factor of three larger than the measured values. This difference is likely due to the (unmeasured) thickness fluctuations in the samples. Lang et al. [66–68] demonstrate that they can average the calculated coupling over a reasonable growth front and get values very close to what is measured.

There have been several studies of the phase of the interlayer coupling as a function of the alloying in the magnetic layers [91,92]. However, these studies only observed the long-period contribution to the coupling. Since the short-period coupling may contribute for thin films, and the amount it contributes may vary as a function of the alloy composition of the magnetic layers, any comparison with theory is difficult.

4.1.2. Co/Cu(1 1 1)

The growth of FCC Co on Cu(1 1 1) has also been studied extensively [72–76,93–95], in part to understand the differences in growth by sputtering and molecular beam epitaxy. For a review of growth studies see Ref. [96]. The problem arises because the energy difference during growth between FCC-like and HCP-like structures is very small. It is easy to nucleate islands of both structures during growth. These different growth structures lead to highly defective multilayers. Theoretically, this system is interesting because there is not a free-electron-like critical spanning vector for this orientation of the Cu Fermi surface, only one spanning vector that bridges the neck at an oblique angle [22] (see Fig. 1). There is only weak evidence of an oscillatory coupling. In most experiments, one strong antiferromagnetic coupling peak is seen and evidence for another peak at some greater thickness is seen. Asymptotic calculations of the coupling strength give $J/(1\ \mathrm{nm})^2 = 0.59$ [56] and 0.67 mJ/m^2 [71]. These values compare well with the coupling strengths measured at thicknesses of about 1 nm of 0.54 [74], 1.1 [72], and 0.4 mJ/m^2 [76].

4.1.3. Co/Cu(1 1 0)

For the (1 1 0) orientation of FCC Co on Cu, the coupling is expected to be a superposition of four periods [22]. Three of these are short periods, one of which is expected to be stronger than those from all other critical spanning vectors for all orientations of Co/Cu [56,71]. However, only the long period has been observed [72,97]. The coupling strength at about 1 nm is measured to be 0.7 mJ/m^2 [72], which is close to the asymptotic values of 1.0 [56] and 1.3 mJ/m^2 [71] for the long-period

coupling strength, but much smaller than the coupling strength calculated for the short-period, 38 and 27 mJ/m^2, respectively, in the two calculations.

While the coupling strengths calculated for the (1 1 1) and the (1 1 0) orientations of Co/Cu multilayers appear to be in good agreement with measured coupling strengths, these orientations have not been studied as extensively as has the (0 0 1) orientation. The growth of these multilayers is not as well controlled as it is for the (0 0 1) orientation. Theoretically, only asymptotic calculations have been done. Either total-energy calculations need to be done, or at least an analysis of the pre-asymptotic corrections.

4.1.4. Fe/Cu(0 0 1)

If Cu is grown on Fe, it can be forced to grow in a BCC structure up to some thickness. There have been several studies of this system which is of interest because the BCC Cu Fermi surface, while still free-electron-like, has very different critical spanning vectors than the FCC Cu Fermi surface. Calculations [62,98,99] show that the coupling is a combination of two short-period components and a long period, with one of the short periods dominant. The experimental results are at odds with each other. Johnson et al. [62] find a short-period oscillation for spacer-layer thicknesses between 11 and 18 ML. Celinski et al. [100] find much stronger coupling but with at least a strong contribution from a component with a much longer period.

4.1.5. Fe/Au(0 0 1)

While BCC Fe and FCC Au have very different lattice constants, when the (0 0 1) orientation of Au is rotated by 45° with respect to the (0 0 1) orientation of Fe, the two layers have an in-plane lattice match that is better than 1% [101,102]. This close lattice match allows for very good growth of multilayers of these materials, particularly on Fe whiskers [59,77]. While the in-plane lattice is well matched, out-of-plane there is a huge mismatch. Thus, any steps on the substrate lead to growth defects that propagate through the layer. The very low step densities of iron whisker surfaces make them quite useful substrates for these systems.

By growing a wedge of Au on an iron whisker and using RHEED oscillations to calibrate the thickness of the wedge as a function of position, Unguris et al. [59] were able to observe 60 changes in sign of the coupling as the Au thickness varied over 80 monolayers. This allowed them to determine the periods of the two oscillatory contributions quite precisely. The measured periods of 2.48 ± 0.05 and 8.6 ± 0.3 ML are in remarkable agreement with those predicted for the system based on the critical spanning vectors of the experimental Fermi surface by Bruno and Chappert [22] 2.51 and 8.60 ML.

In a subsequent experiment, Unguris et al. [77] measured both the coupling strength as a function of the spacer-layer thickness and, through the RHEED intensity oscillations, the width of the growth front. This allowed them to correct the measured coupling strength for the averaging of the thickness fluctuations. They fit the resulting coupling strength to a combination of two oscillations assuming the asymptotic form, Eq. (1), holds for all thicknesses. The resulting coupling strengths, $J^S/(1\text{ nm})^2 = 1.29 \pm 0.16$ and $J^L/(1\text{ nm})^2 = 0.18 \pm 0.02$ mJ/m^2, are reasonably close to calculated asymptotic coupling strengths [71], 2.0 and 1.1 mJ/m^2. While this agreement is comparable to that for Co/Cu(0 0 1), the measured results for this system have been corrected for thickness fluctuations. Thus the agreement is not completely satisfactory. The strength of the short-period oscillation is in good agreement, but that of the long period is off by a significant amount. At the critical point associated with the short-period oscillation, the reflection amplitudes for both minority and majority electrons are significant, and varying with parallel wave vector [71] (see Fig. 1). The errors in the alignment of the Fermi surface due to the local-density approximation are likely to lead to significant uncertainty in the value of this contribution to the coupling. On the other hand, at the critical point associated with the long-period oscillation, only the reflection probability for the minority electrons is significant. However, the reflection probability does vary with parallel wave vector, and since it is in a symmetry gap, its phase does change with energy. It remains to be seen whether pre-asymptotic corrections [46] of the type important for Co/Cu(0 0 1), will also be important in this case. Additionally, there have also been indications

[103] that the coupling strength for this system can depend on Fe thickness.

There have been several total-energy calculations for the Fe/Au(0 0 1) system [104,105]. Both find coupling energies that are the same order as expected from the asymptotic calculation [71]. Costa et al. [104] find a strong short-period oscillation and a weaker long-period oscillation. While it is difficult to make quantitative comparisons based on the published results, this trend is closer to what is seen experimentally than the asymptotic results. The authors compare their results with those of an earlier experiment for Au/Fe multilayers grown on GaAs [107]. While the overall scale factor disagrees by about an order of magnitude, the calculations give excellent agreement of peak heights and positions. Unfortunately, neither the measured peak positions, nor their strength agree with the later measurements on Fe whiskers. This disagreement highlights the difficulty in comparing total-energy calculations directly with experiment. Since the local-density approximation makes some error in the Fermi surface, these calculations necessarily get the oscillatory periods wrong, and hence the peaks in the wrong places.

4.1.6. Fe/Ag(0 0 1)

Since silver has a lattice constant very close to that of gold, the same considerations hold for the growth of Ag on Fe(0 0 1) as for Au. There is the similar agreement between the oscillation periods measured on Fe whiskers [58], 2.37 ± 0.07 and 5.73 ± 0.05 ML, and those predicted based on the experimental Fermi surface [22], 2.38 and 5.58 ML. Measurements [106] of the coupling strength have not been analyzed in terms of two asymptotic contributions, but both sets of measurements [58,106] show that the long-period oscillation is relatively stronger for Ag spacers than it is for Au spacers. This same trend is seen in both asymptotic calculations [71] and total-energy calculations [104]. While direct comparison is difficult, the measured coupling strengths [106] are consistent with the magnitudes of the coupling found in both calculations.

There has been one study of the hexagonal (1 1 1) face of Ag grown on the pseudo-hexagonal face of Fe (1 1 0) [107]. That measurement found oscillations consistent with those expected from the critical spanning vector of the Fermi surface [22].

4.2. Other lattice-matched spacer layers

4.2.1. Fe/Cr(0 0 1)

Fe/Cr multilayers, particularly in the (0 0 1) orientation, have been quite widely studied. They were the first transition-metal multilayers to show antiferromagnetic coupling [4], giant magnetoresistance [7,8], oscillatory coupling [9], and short-period oscillatory coupling [108–110]. Cr is the only transition metal that is well lattice matched to either Fe or Co, so Fe/Cr multilayers are particularly interesting to test whether the understanding of interlayer exchange coupling extends beyond noble metal spacer layers. Unfortunately, high-quality Fe/Cr multilayers are dominated by the antiferromagnetic order in the Cr, which masks the coupling of the type that applies to noble metals. The short-period coupling in these systems and the antiferromagnetism in the Cr are discussed elsewhere in this issue [20] and will not be discussed further here.

The long-period coupling in Fe/Cr(0 0 1) is still controversial. Experimentally, it is well established [49,97,108,110,111], that in samples where the thickness fluctuations are large enough that the short-period coupling is averaged out, a long-period component with a period of about 12 ML is observed. Theoretically, the origin of this long-period oscillation is controversial. Even among authors who believe that the coupling comes from essentially the same mechanism as the coupling in noble metal spacer layers, there is disagreement over what part of the Fermi surface is responsible. Several different parts of the Fermi surface have been suggested. Mirbt et al. [48] suggest that the long-period contribution comes from a short-period contribution at the center of the interface Brillouin zone. This short-period oscillation gets aliased to a long-period oscillation by beating against the doubled unit cell due to antiferromagnetic order. Based on supercell calculations with Fe layers two atomic layers thick, van Schilfgaarde et al. [79,112] suggest that the long period comes from an aliasing of the second harmonic of the short-period coupling. From analyses of the critical

spanning vectors of the paramagnetic Cr Fermi surface, Koelling [113] has suggested that a spanning vector of the lens part of the Fermi surface has the correct size. Several calculations [114–116] of the asymptotic contributions to the coupling have found that the strongest coupling comes from spanning vectors of the ellipsoids at the N-points of the Brillouin zone (see Fig. 1). These various mechanisms have been discussed in detail in Refs. [114,117].

There are no definitive experiments that distinguish between the different suggestions. Perhaps the best evidence comes from alloy studies [82] in which the Cr is doped with V. The period of the coupling is found to change with alloying. The different spanning vectors that have been suggested all change differently with doping. The changes in the spanning vectors of the N-centered ellipsoids are the most consistent with the experiment. This evidence is indirect. Ideally, this issue could be settled by photoemission experiments like those of Li et al. [118]. Unfortunately, establishing the important part of the Fermi surface by photoemission is quite difficult. To *establish* a part of the Fermi surface as the origin of the coupling requires demonstrating that there are quantum-well states there, that they are spin-polarized, that they are at a critical point, and most difficult, that there are no quantum-well states on some other part of the Fermi surface that fit these criteria. No photoemission studies of interlayer exchange coupling on any system have systematically studied the whole Fermi surface.

4.2.2. Fe/Cr(2 1 1)

Several studies of Fe/Cr(2 1 1) multilayers [97,111] have found remarkable similarities between the long-period coupling for these systems and the Fe/Cr(0 0 1) multilayers. The period found in both systems is very close to that found in sputtered multilayers that are believed to be predominantly (1 1 0) textured [9]. This orientation independence suggests that there might be a different mechanism for the coupling than the quantum-well mechanism described above. However, calculations of the asymptotic contributions to the coupling show that for both the (2 1 1) [114] and (1 1 0) [114–116] interface directions, the dominant long-period contribution to the interlayer coupling comes from the N-centered ellipsoids and that the periods, when extracted from the experimental Fermi surfaces are very close to what is measured in all three cases.

4.2.3. Fe/V(0 0 1) and Fe/Al(0 0 1)

Fe and V are close enough to being lattice-matched that there is some hope of growing coherent multilayers that could be compared with theory. Oscillatory coupling has been seen in V/Fe(0 0 1) multilayers grown on Fe whiskers [119], but the growth is significantly worse than for Cr, Au, or Ag, and the oscillatory coupling is only observed over a much smaller range of spacer thicknesses. The coupling that is observed in this system bears little resemblance to that calculated [47] for it. It may be that the strain in the V is great enough that the structure considered in the calculation differs too significantly from that present in the measurement. It is also possible to observe antiferromagnetic coupling in multilayers grown with thin layers of Fe, so that the V is less strained [120]. However, since only one antiferromagnetic coupling peak is observed, it is impossible to discuss oscillatory coupling. Multilayers of this type can be reversibly loaded with atomic hydrogen [121]. This changes the lattice somewhat, but also significantly changes the electronic structure. At the same time the coupling in these multilayers changes quite significantly [122].

While Al is also close to lattice matched with Fe, it does not grow well [107,119]. There are indications of oscillatory coupling in some measurements [107] and biquadratic coupling in others [123] but nothing to compare with theoretical calculations.

4.3. Alloy studies

Additional evidence that the coupling is determined by the spacer-layer Fermi surface comes from comparing measurements [78,79,82,102,124] and calculations [79–82] of the oscillatory periods as a function of alloy concentration in the spacer layer. Alloying in the spacer layer changes the oscillatory coupling in two ways. First, it changes the band structure, the Fermi surface, and hence the critical spanning vectors. These changes can be

captured in models based on the virtual-crystal approximation. In these models, the material is imagined to have no disorder, but a fictitious, fractional, nuclear charge on each site. Second, the alloy disorder leads to diffuse scattering, which reduces the amplitude of the coupling. These changes can be captured in models based on the coherent-potential approximation. In these models, the electronic states gain a width due to the diffuse scattering.

For small concentrations of Ni in Cu, the Ni remains non-magnetic, and the Fermi surface contracts due to the lower electron density in Ni compared to Cu. For (1 1 0) and (1 1 1) oriented multilayers, Ni doping gives an increase in the oscillation period of the long period, while for (0 0 1) multilayers, it gives a decrease. An increase, consistent with the Fermi surface properties has been observed for (1 1 0) multilayers [124] and for sputtered multilayers with a (1 1 1) texture [78].

Alloying Cu and Au only weakly changes the oscillation periods because both are noble metals. However, there is still alloy scattering due to the disorder. Annealing an alloy with 55% Au [102] gives a large increase in the coupling energy. Presumably this is due to ordering in the alloy which reduces the diffuse scattering. On the other hand, the increase in the unit cell size in the interlayer may give rise to additional critical spanning vectors that can change the coupling in less systematic ways.

Alloying the Cr in Fe/Cr(1 1 0) multilayers with V [79] gives an increase in the period of the oscillatory coupling that matches an increase found in total-energy calculations of supercells of this orientation. There is good agreement over the whole alloy range between the results of the calculation and the measured periods. The alloying of V in to Cr in Fe/Cr(1 0 0) multilayers [82] has been discussed above.

4.4. Lattice mismatched systems

There have been many studies of multilayers that are not as well lattice matched as those described above. Multilayers studied include Co/Au [125,126], Co/Ru [127–129], Co/Rh [130], Co/Ir [131], Co/Re [132,133], Co/Os [134], in addition to the systematic study by Parkin of most of the transition metals sandwiched between Co and grown by sputtering [135]. There have been fewer studies of multilayers with Fe as the magnetic layer, Fe/Pd [136,137], Fe/Nb [138], and Fe/Mo [139].

There are two trends that come out of these studies that demand explanation. First, with the exception of Os (1.5 nm) and Cr (1.8 nm), all of the observed periods are in the range 0.9–1.2 nm. Second, there is a very strong trend of increased coupling strength as the spacer material moves to the right in the periodic table. For any interface orientation, the Fermi surfaces of transition metals have many critical spanning vectors. Assuming that the sputtered multilayers have the low-index orientation, there are critical spanning vectors that match the observed periods for all of the measured systems [38]. The issue then becomes why are other periods not observed. A possible explanation is that a common period is observed because the experimental sensitivity function is peaked for periods with the observed value. Shorter-period oscillations are averaged out by thickness fluctuations as has been observed for lattice matched systems. Longer-period oscillations are obscured both by the small range of thicknesses measured and by measurement of properties, like magnetoresistance, that do not change sign. While this explanation may be correct, a more physical explanation would provide more insight.

Mathon et al. [140] explain the trend in the coupling strengths as coming from trends in the band structure as a function of position in the periodic table. They consider a simple cubic d-band tight-binding model and consider trends as a function of band filling. For band fillings close to the filling of the ferromagnet they find strong reflection for one spin and weaker reflection for the spin for which the band structure is aligned with that of the spacer material. The resulting large spin asymmetry gives rise to strong coupling. Then, moving left in the periodic table, as the band filling becomes very different from that of the ferromagnet, both spins have strong reflection, and the coupling is weaker. An alternative explanation may be related to trends in structural quality as a function of position in the periodic table.

5. Summary

The extensive research on interlayer exchange coupling has led to a deep understanding of the phenomena, as is evidenced by the detailed agreement between theory and experiment. All models for the coupling predict that it should oscillate with periods set by critical spanning vectors of the spacer-layer Fermi surface. The predicted periods based on analysis of measured Fermi surfaces are in good, in some cases remarkable, agreement with measured periods. The measured strengths of the coupling for the few lattice-matched systems that have been extensively studied agree well with the strengths that have been calculated. There is also substantial agreement between theory and experiment as to the variation of the coupling periods with alloy composition.

There are still some open questions. While the agreement between theory and experiment is good for many systems, none have been studied as extensively as Co/Cu(0 0 1). Most of the agreement is for noble-metal spacer layers. It is not clear how well the models work for transition-metal layers. The one transition metal, Cr, which is well lattice-matched to a transition-metal ferromagnet, is complicated by the presence of antiferromagnetism. Establishing whether or not the models so successful for noble metals apply to the long-period interlayer coupling found in Fe/Cr would indicate whether or not these models might apply to other transition-metal spacer layers. There is not a good model for coupling in systems that are not well lattice-matched. Even though there have been many measurements on such systems, we still do not have a quantitative understanding of the coupling in them.

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