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Ab initio local-spin-density study of oscillatory exchange coupling in Fe/Au multilayers

R Hafner, D Spišák, R Lorenz and J Hafner

Institut für Materialphysik and Centre for Computational Materials Science, Universität Wien, Sensengasse 8/12, A-1090 Vienna, Austria

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Abstract

Fully self-consistent *ab initio* local-spin-density calculations of the interlayer exchange coupling (IEC) in Fe/Au multilayers have been performed. The thickness of the ferromagnetic body-centred cubic Fe layers has been kept fixed at five monolayers (ML), the thickness of the face-centred cubic Au spacer layers has been varied between 2 and 30 ML. Agreement of the calculated and observed oscillation periods of the interlayer exchange coupling has been obtained. To verify the Rudermann–Kittel–Kasuya–Yoshida and quantum-well (QW) pictures for the IEC, detailed investigations of the Fermi surface of Au and of the modulation of the Bloch states in the spacer layer by means of QW oscillations have been performed.

1. Introduction

Since the discovery of the giant magnetoresistance exhibited by Fe/Cr magnetic multilayers [1], intensive investigation of the interlayer exchange coupling (IEC) has continued with unabated fervour. Also IEC was soon discovered in other multilayer systems with non-magnetic spacers like Fe/Au. The IEC between the magnetic layers is mediated by the coherent tunnelling of the electrons through the spacer [1–3]. The first theoretical explanation was given in terms of the Rudermann–Kittel–Kasuya–Yoshida (RKKY) interaction [4], relating the oscillation periods to the nesting vectors (calipers) of the Fermi surface of the spacer, in this case Au. Other explanations are based on electronic Fabry–Pérot-like interference effects [5] or quantum-well (QW) theories, i.e. the spin-dependent confinement of electrons within the spacer layers [6]. It is important to emphasize that these explanations are not mutually exclusive, but differ only in emphasizing different aspects of the same fundamental mechanism: the band offset between the non-magnetic spacer metal and the ferromagnetic metal leads to the confinement of electronic states within the thin film. Essentially, bulk-like eigenstates are modulated by a slowly varying envelope function which ensures that the boundary conditions are met at the interfaces (the boundaries of the QW). The wavelength of the envelope functions may be derived from the oscillations of the inverse photoemission intensity with the thickness of the

spacer [7], which are analogous to the interference fringes in a Fabry–Pérot interferometer. The interlayer exchange coupling is transmitted by spin-polarized QW states at the Fermi level, its periodicity being determined by the wavelength of the spin-polarized QW states. As this wavelength is in turn determined by the cross sections of the Fermi surface of the spacer, the predictions based on the QW mechanism agree with RKKY theory. As regards the periods of the oscillations in the IEC, reasonable agreement has been found between model calculations based on either QW or RKKY model calculations and experiment for nearly all ferromagnet–noble-metal systems, although experiment and calculation sometimes disagree on the phase of the oscillations. This has been tentatively attributed to interface roughening and/or intermixing changing the effective number of spacer layers. The situation is less clear as regards the strength of the coupling which depends crucially on the degree of matching of the energy bands at the interface, which must be determined by *ab initio* calculations. The QW picture also becomes problematic in the limit of ultrathin spacers. The QW wavefunctions extend into the classically forbidden region outside the well with an exponentially decaying envelope and this will lead to deviations from a bulk-like electronic structure in the limit of spacers or magnetic films consisting of only a few atomic monolayers (ML). In the extreme case of alternating ML, the multilayer system becomes equivalent to a layered intermetallic compound. Attempts have been made to determine the IEC by *ab initio* local-spin-density calculations, using either straightforward total-energy calculations or the 'force theorem' which allows one to estimate first-order energy differences on the basis of one-electron energies calculated in a fixed reference potential. At best partial agreement with experiment has been achieved, and the correlation between the model studies and the *ab initio* calculations remains unclear.

In the present work we use *ab initio* local-spin-density calculations to investigate the interlayer exchange coupling and QW-like electronic structure of the Fe/Au multilayers. This system continues to be of particular interest for several reasons:

(i) At an (100) interface, the interatomic distances of face-centred cubic (fcc) Au and body-centred cubic (bcc) Fe match within 1%. This allows the growth of trilayers and multilayers with nearly perfect atomically flat interfaces. The structure of the multilayers with bcc(100) Fe between fcc(100) Au layers has recently been confirmed by medium-energy ion-scattering (MEIS) experiments [8].

(ii) Whereas for metals with identical crystal structures, the band offset is of the order of 1–2 eV, the different topologies of the bands of bcc Fe and fcc Au lead to a difference of nearly 9 eV between the eigenstate of Au at the X point and of Fe at the H point. The large band offset leads to a decay constant of the QW state of the order of the interplanar spacing, so the physical mechanism for the oscillatory IEC can be expected to hold even for ultrathin spacers.

(iii) For Fe/Au multilayers very accurate experimental values for the IEC are available from magneto-optic Kerr-effect [9] and Brillouin-scattering experiments [10]. QW oscillations in the empty sp band of the spacer layer have been found by inverse photoelectron spectroscopy [7].

(iv) Since Fe/Au is a model system, a number of local-spin-density studies have been performed [10–18]. These calculations range from empirical tight-binding approaches [13] to *ab initio* Kohn–Korringa–Rostoker (KKR) Green-function calculations using the force theorem to determine the IEC energies [11, 12, 14] and to fully self-consistent linearized augmented-plane-wave (LAPW) calculations [10, 17].

However, only in the work of Opitz *et al* [11, 12] was the change for a bcc structure in the iron layers to a fcc lattice in the spacer properly taken into account. All other calculations assume that the fcc parent lattice of the spacer extends throughout the multilayer system.

This is important, since the magnetic properties of fcc α-Fe and bcc γ-Fe are known to be widely different. While the most recent self-consistent calculations report quantitative agreement between the calculated and measured IEC strength for ultrathin $Fe_N Au_N$ ($N \leqslant 5$) multilayers, where the QW picture is eventually no longer legitimate [10], for thicker layers ($N \geqslant 20$) good agreement for the oscillation periods, but disagreement on the phase and substantial disagreement for the interaction strength was reported. Opitz *et al* [11, 12] have attempted to attribute these discrepancies to the mesoscopic roughness necessarily present at the Fe/Au interface. However, a simple averaging of the calculated coupling strengths over a distribution of spacer thicknesses turns out to be insufficient for modelling the effect of interface roughness: the strong damping of the short-range periodic component of the coupling would shift the extrema, worsening agreement with experiment. For spacers of intermediate thickness, the results are found to depend in a quite sensitive way on the computational approach—in particular, quite important differences between calculations using the force theorem and total-energy calculations have been reported [14]. Fully self-consistent calculations [10, 17] were only performed for small Au spacer thickness up to 5 ML.

In this paper we present the first fully self-consistent study which treats bcc Fe(100) /fcc Au(100) superlattices with Au spacer thicknesses up to 30 ML. We consider Fe/Au multilayers with the same structure as reported from experiments. The lattice constant of bulk bcc Fe matches the nearest-neighbour distance d of fcc Au within less than 1%. This allows growth with low-stress interfaces. The fcc Au(100) planes are stacked rotated by 45° relative to the Fe(100) planes (bcc–fcc transition). The distances between the fcc(100) planes in Au are $\approx\sqrt{2}$ times the bcc Fe(100) interplane spacing. The experimental lattice constant for Fe is $a_{Fe} = 5.416$ au and for Au $a_{Au} = \sqrt{2}a_{Fe}$. We report detailed results on the electronic and magnetic structure and of the IEC for Fe_5Au_N multilayers with N ranging from 2 to 30. The thickness of the magnetic layers is, at 5 ML, just sufficient to decouple the QW states in the spacers. The variation of the IEC with the spacer thickness is examined using discrete Fourier analysis, allowing us to extract the long and the short periods and amplitudes of the IEC. The results are discussed in terms of RKKY and QW theories.

2. Methodology

Our calculations are based on a k-space tight-binding linear-muffin-tin-orbital method [19] in the atomic-sphere approximation. We use the local exchange–correlation functional proposed by Perdew and Zunger [20] and the spin interpolation suggested by Vosko *et al* [21], adding non-local corrections in the form of the generalized gradient approximation (GGA) [22]. In the case of Fe layers, the use of the GGA is essential since only with the gradient corrections is there correct prediction of the structure and magnetic ground state [23]. LDA calculations predict the non-magnetic hexagonal form of Fe to be lower in energy than the ferromagnetic bcc structure and lead to much smaller energy differences between the magnetic phases of bcc α-Fe.

The calculations are fully self-consistent as regards charge densities, spin densities and total energies. For the Fe/Au multilayers a sampling of ten special k-points on an $(8 \times 8 \times 2)$ grid in the irreducible Brillouin zone, combined with a modest Gaussian smearing of the one-electron energies, was found to be adequate (final energy differences are extrapolated to zero smearing). For Au spacers with 15 and 20 ML, increasing the number of k-points from 10 to 210 resulted in a decrease of the exchange coupling from 0.081 to 0.069 mRyd/atom for 15 ML and in an increase of the IEC from 0.091 to 0.094 mRyd/atom for 20 ML. The electronic structure of bulk Au has been calculated with 770 special k-points. The calculations were performed for Fe_5/Au_N ($N = 2, \ldots, 30$) multilayers to study the interlayer exchange

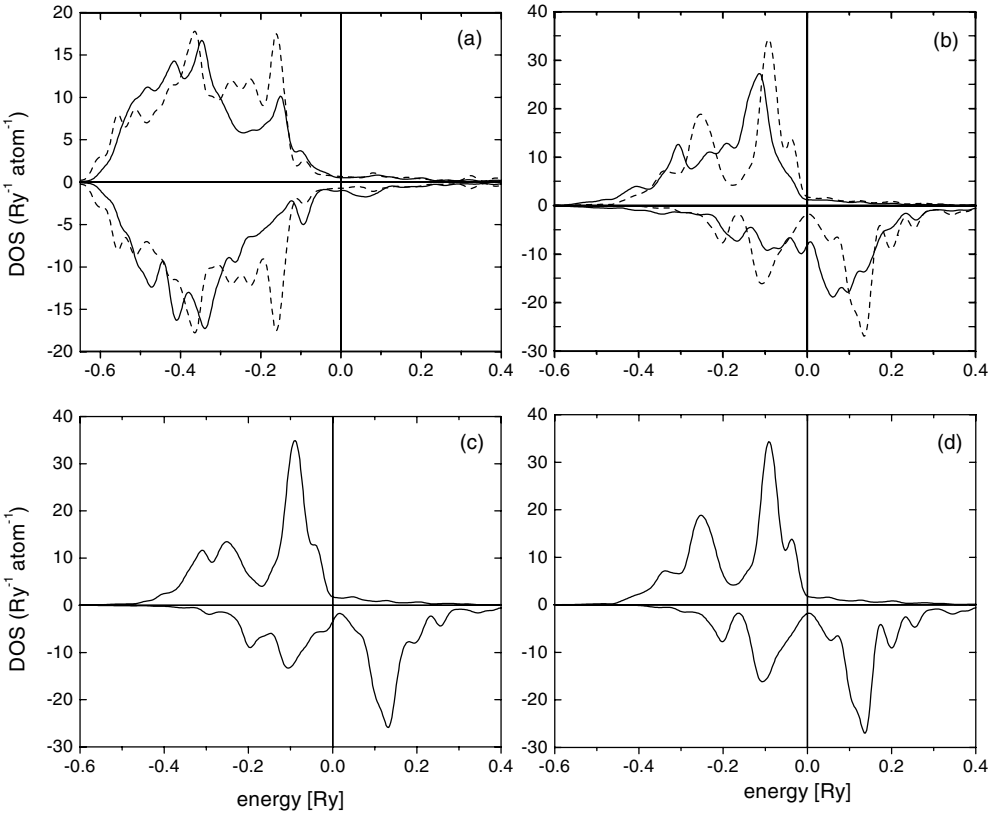

Figure 1. The local layer-resolved spin-polarized electronic DOS in Fe/Au multilayers: (*a*) a Au layer at the interface, (*b*) an Fe layer at the interface, (*c*) a second Fe layer and (*d*) a central Fe layer in the Fe_5Au_5 film. For comparison, the dashed curves in panels (*a*) and (*b*) depict the DOS of bulk fcc Au and bcc Fe.

coupling as a function of the thickness of the spacer layer. The Fe/Au superlattice is described as a periodic system composed of cells extending over $2(N + 5)$ atomic layers. To obtain reliable energy differences between ferromagnetic (FM) and antiferromagnetic (AF) ordering, the unit cell of the AF structure is also used for the FM structure. We started our calculations with parallel iron moments within a layer, aligned ferromagnetically or antiferromagnetically in neighbouring iron layers. The Au moments were initially set to zero.

3. Results

3.1. Electronic structure and momentum profile

Figure 1 shows the layer-resolved local densities of states at the Au/Fe interface and in the inner Fe layers (the result is quite independent of the thickness of the Au spacer). At the interface, the peak of the Fe 3d majority band is shifted away from the Fermi level due to the strong Fe/Au hybridization, whereas the occupied minority band is shifted to lower binding energies. The strong bonding–antibonding splitting characteristic for the bands of bulk bcc Fe has largely disappeared at the interface, but in the central layer of the five-layer film the density of states (DOS) is already quite similar to that of the bulk. In the Au DOS the hybridization gap is clearly apparent in the majority DOS.

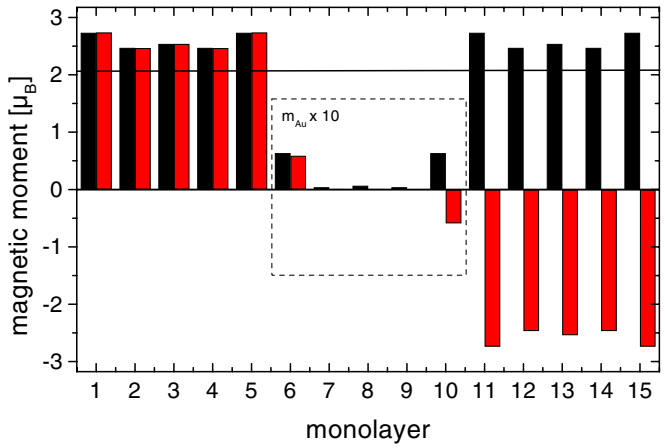

Figure 2. The profile of the magnetic moments in the Fe_5Au_5 multilayer. Black bars represent the results for a FM alignment, grey bars for an AF alignment of neighbouring Fe films. Au moments are multiplied by a factor of ten for clarity. The horizontal line marks the value of the magnetic moment in bulk bcc Fe.

(This figure is in colour only in the electronic version)

The Fe moments lead to a small magnetic polarization of the order of 0.06 μ_B at the Au interface. The coupling between Fe and Au atoms at the interfaces is always parallel. The moments of the iron atoms at the interface, typically about 2.73 μ_B, and the moments of the central Fe atoms, of about $m_{Fe} = 2.54\ \mu_B$, are enhanced compared to the bulk value of 2.31 μ_B. The enhancement of the Fe moments is a consequence of reduced Fe–Fe coordination and the d-band narrowing at the Fe/Au interface (see figure 1). A typical profile of the magnetic moments is shown in figure 2 for the example of an Fe_5Au_5 multilayer. The small moments in the Au layers as well as the enhancement of the Fe moments have been observed in experiments [24,25]. Our magnetic moment profile is also in good agreement with the LMTO calculations of Boehm and Krey [18].

3.2. Interlayer exchange coupling

The IEC is calculated in terms of the difference in total energy $E_{tot}^{FM}(N) - E_{tot}^{AF}(N)$ between two distinct magnetic configurations, where the alignment of the magnetic moments in the neighbouring Fe layers is either parallel or antiparallel. According to our definition of the energy difference, a positive value favours AF coupling and a negative value a FM coupling. The results for a spacer thickness of up to $N = 30$ Au ML are summarized in figure 3. For comparison we have included in the graph the sign of the IEC as determined from the MOKE experiments of Unguris *et al* [26]. Even without artificial phase shift, agreement on the sign of the IEC is excellent—the only relevant exceptions occur for $N = 10$ and 22. The oscillation periods for the IEC are obtained by a discrete Fourier analysis with the results shown in figure 4. In this way long ($\lambda_1 \approx$ 7–9 ML) and short ($\lambda_2 \approx 2.5$ ML) oscillation periods were determined. The results are in agreement with experimental work, which has confirmed the existence of two oscillation periods, $\lambda_2 = 2.5$ ML and $\lambda_1 = 8.6$ ML, of the IEC, as well with other theoretical studies [11, 13, 14]; see table 1 for details.

The coupling strength for the long period (IEC_1) is about 5.9 mJ m^{-2} and for the short period (IEC_2) about 3.2 mJ m^{-2}. The coupling strengths obtained are a factor of 5.6 for the long period and a factor of 3.7 for the short period stronger, as reported by Opitz *et al* [11,12].

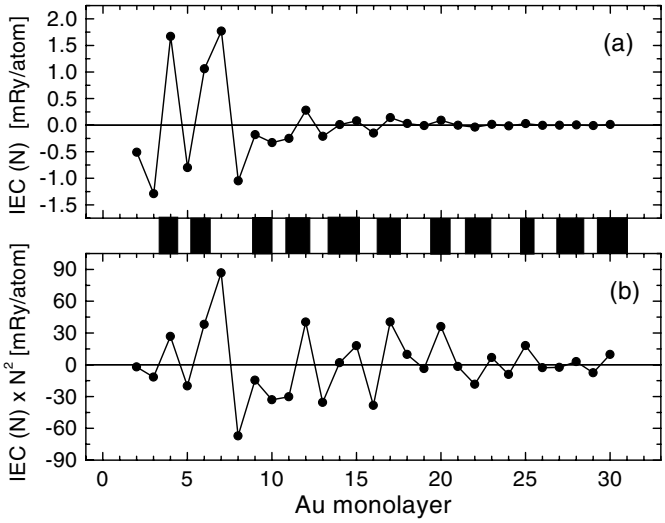

Figure 3. Interlayer exchange coupling in an Fe_5Au_N multilayer as a function of spacer thickness (*a*). Part (*b*) shows IEC $\times N^2$ versus N in order to illustrate the behaviour at large spacer thickness. The black and white bars mark favoured AF and FM coupling according to the experiments of Unguris *et al* [26].

Table 1. Periods and amplitudes of the oscillations in the IEC of Fe/Au multilayers.

	Experiment (MOKE) [26]	Experiment (FS diameter) [29]	Theory (Fourier analysis) This work	[11]	Theory (FS diameter) This work	[11]
		Long (λ_1) and short (λ_2) periods in ML units				
λ_1	8.6 ± 0.3	7–8	7–9	8.2	8.3	8.03
λ_2	2.48 ± 0.05	2	2.5	2.5	2.5	2.64
		Experiment (MOKE) [26]	This work		Theory [11]	
		Comparison of the coupling strengths and amplitudes of the IEC components				
	IEC_1 (mJ m^{-2})	0.038	3.2		0.57	
	IEC_2 (mJ m^{-2})	0.30	5.9		1.57	
	IEC_2/IEC_1	7.7	1.8		2.8	

This difference is probably to be attributed to the use of the force theorem in the calculations of Opitz *et al*—similar discrepancies between non-self-consistent calculations using the force theorem and fully self-consistent total-energy calculations have been reported before by Szunyogh *et al* [14]. The amplitude of the short-period coupling is stronger by a factor of 1.8 than that of the long period, which is in line with other theoretical calculations [12, 16]. The overestimation of the strength of the IEC is found in all spin-density calculations, and also in all QW model calculations. As Opitz *et al* [12] have pointed out, two different damping mechanisms affect the QW states: mesoscopic roughness and defect scattering. A combination of the two should explain the difference between the experiments on imperfect interfaces and the calculations performed for ideal interfaces. However, a fully consistent *ab initio* treatment would require a theoretical treatment of interdiffusion effects (see e.g. [27]).

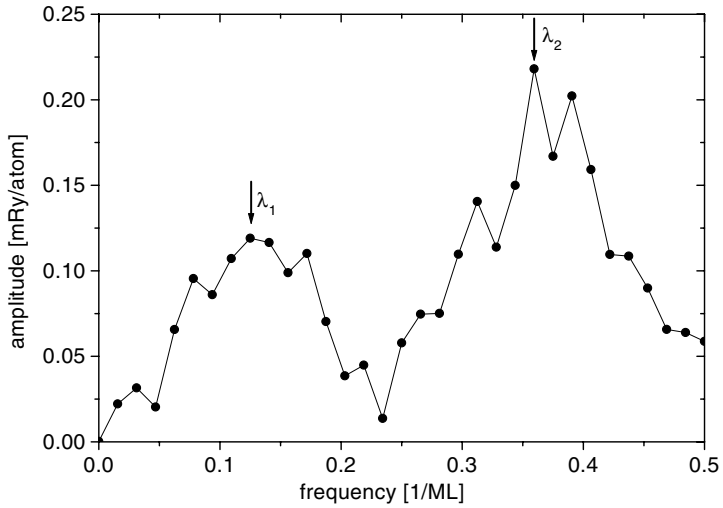

Figure 4. Fourier analysis of the interlayer exchange coupling as a function of the spacer thickness.

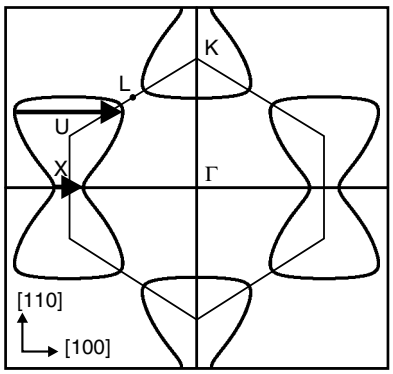

Figure 5. The cross section of the Fermi surface, for a fcc Au(100) spacer. The wavevectors giving rise to oscillatory interlayer coupling along the [100] direction are indicated by the horizontal bold arrows.

3.3. RKKY analysis

The RKKY approach predicts the oscillation periods of the interlayer exchange coupling versus spacer thickness just from inspection of the bulk Fermi surface of the spacer material. As regards providing an experimental test of these predictions, noble-metal spacer layers appear to be the best-suited candidate system. The Fermi surfaces of noble metals are known very accurately from de Haas–van Alphen and cyclotron resonance experiments [28]. Since only the sp bands intersect the Fermi level, the Fermi surface is rather simple, and does not depart very much from the free-electron Fermi sphere. Figure 5 shows a cross section of the Fermi surface of fcc Au, indicating the spanning vectors for the (100) crystalline orientation, $k_1 = 0.76$, $k_2 = 2.54$ in units of the wavevector $k_{ZB} = \pi/d$ at the Brillouin-zone boundary, for which a long period $\lambda_1 = 8.3$ ML and a short period $\lambda_2 = 2.5$ ML are predicted, in good agreement with the result of the Fourier analysis of the IEC versus N relation.

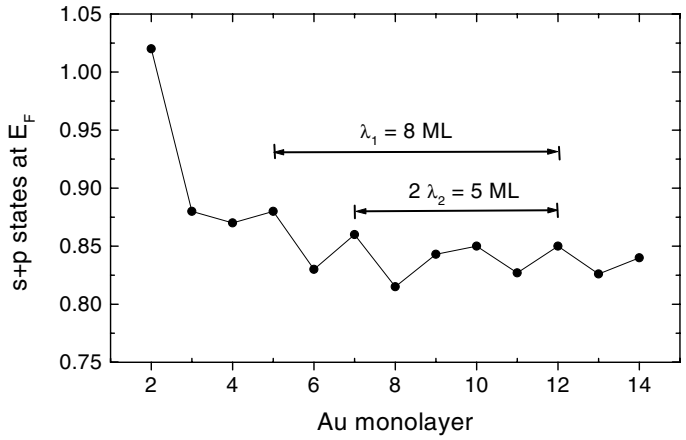

Figure 6. Variation of the density of s and p states in the Au spacer with the spacer thickness between 2 and 14 ML. The two oscillation periods of 2.5 and 8 ML are indicated.

3.4. Spectroscopy of quantum-well states

A QW state consists of a rapidly oscillating Bloch function modulated by an envelope function that ensures that the boundary conditions are met at the interface. For a single band edge this modulation of a Bloch function with a wavevector k_{edge} by an envelope with a wavevector k_{env} produces a total wavevector $k_{\mathrm{tot}} = k_{\mathrm{edge}} \pm k_{\mathrm{env}}$ (considering only the components perpendicular to the interface). The wavelength λ_{env} of the envelope is equal to twice the thickness of the spacer layer, $\lambda_{\mathrm{env}} = 2Nd$, where N is the number of spacer ML and d is the interlayer spacing; thus $k_{\mathrm{env}} = 2\pi/\lambda_{\mathrm{env}} = \pi/(Nd)$. For the (100) interface, the band-edge wavevector $k_{\mathrm{ZB}} = \pi/d$ and this leads to a simple relation between the periodicity of the QW state (measured in terms of the number of ML) and the band wavevector measured in units of k_{ZB}, $k = k_{\mathrm{tot}}/k_{\mathrm{ZB}}$:

$$k = 1 - \frac{1}{N} \tag{1}$$

$$N = \frac{1}{1-k}. \tag{2}$$

The QW states are produced by total reflectivity at the interfaces; partial reflectivity leads to an energy-dependent phase shift, which would have to be included in analysing the peak positions of QW states in the electronic density of states. The phase shifts arising from the two interface reflections can be eliminated if one examines the modulation at a constant energy of the electrons as a function of the thickness of the spacer layer. At the Fermi energy, the period of the oscillation can be calculated from the simple relation given above, with $k = k_{\mathrm{F}}/k_{\mathrm{ZB}}$. For the nesting Fermi wavevector k_1 one calculates a long period of $N \approx 8.3$ ML which agrees with the periodicity resulting from the RKKY treatment of the exchange coupling given by an oscillation wavevector $2(k_{\mathrm{ZB}} - k_{\mathrm{F}})$. A similar agreement leads to the short period.

Figure 6 shows the variation of the s and p density of states in the Au layer at the Fermi level as a function of the number of ML. Both the long (≈8 ML) and the short (≈2.5 ML) periodicity are clearly recognizable up to about 15 ML, although the amplitude of the QW oscillations is quite weak.

4. Comparison with previous theoretical studies

One of the most recent articles about Fe/Au multilayers was published by Yoshihara *et al* [10], who investigated the IEC in Fe_NAu_N superlattices for $N = 1$–5 ML by means of Brillouin scattering from spin waves at 300 K and by *ab initio* calculations using full-potential linearized augmented-plane-wave method (FLAPW), assuming an overall fcc structure of the multilayer. For such extremely thin layers, the QW picture cannot be expected to hold; for $N = 1$ the system is equivalent to an intermetallic compound with the $L1_0$ structure. In the experiment, the IEC was found to be ferromagnetic for all N, but its strength exhibits oscillatory behaviour. The IEC was large for even ML and small for odd ML. *Ab initio* calculations of the IEC by Yoshihara *et al* [10] resulted in good agreement with the experimental values, except for $N = 3$ where an antiferromagnetic ground state has been predicted. Yoshihara *et al* considered interface roughness as responsible for this disagreement. Our results agree with the experiments for Au spacer thicknesses with <5 ML except for $N = 4$, possibly for the same reason. The asymmetric behaviour of the IEC found in experiments by Yoshihara *et al*—large for even ML and small for odd ML but still ferromagnetic—is not observed in our case.

Opitz *et al* [11, 12] performed calculations for $Fe_{12}Au_N$ multilayers for $N = 8$–30 ML, using the correct bcc/fcc structure. Their investigations were based on density-functional theory using a scalar-relativistic screened KKR method in the frozen-potential approximation. The calculations were performed at $T = 800$ K, which acted as a technical parameter for accelerating the calculations. Using discrete Fourier analysis they found two ($\lambda_1 = 8.2$ ML and $\lambda_2 = 2.5$ ML) oscillation periods. Table 1 compares our result for the oscillation periods and amplitudes with experimental results and other calculations. For spacers thicker than about 20 ML, our results for the period and phase of the oscillations agree well with the Green-function KKR calculations of Opitz *et al* [11]. For thinner spacers there is considerable disagreement as regards the phase as well, our calculations being in better agreement with experiment. This indicates that the difference between force theorem and total-energy calculations is more important for thinner layers. The calculated strength of the IEC is larger than that determined experimentally, but smaller than our calculated coupling strength. The difference can be attributed to the use of the force theorem, and to the disagreement over the phase noted for the thinner layers—this could contribute to a broadening of the Fourier spectrum and hence to a reduction of the amplitude of the main components. Unfortunately the spectrum (and therefore the quality of the discrete Fourier analysis) is not shown in the article of Opitz *et al* [11]. The analysis of the experimental data taken for Au wedges involves corrections for fluctuations in the growth front, but neglects a possible influence of the roughness of the interface. Therefore Opitz *et al* [11] have attempted to explain the discrepancies between theory and experiment by averaging the theoretical results for N spacer layers with those obtained with $N \pm 1$ layers. The averaging explains the lower amplitude of the short-range oscillations, but tends to obscure the long-range oscillations.

Szunyogh *et al* [14] used scalar-relativistic and fully relativistic Green-function KKR methods and the force theorem as well as total-energy calculations to determine the IEC for all-fcc Fe/Au multilayers with one to three Fe layers and spacer thicknesses of up to 15 ML. Their results demonstrate that the IEC calculated from the force theorem can be larger or smaller than the total-energy results—the difference can be as large as a factor of eight. Their results also show that for such extremely thin magnetic layers, even the sign of the IEC can be changed by adding a further Fe layer. This dependence is more pronounced if the spacer is also very thin. For this reason and because of the use of a different structure of the Fe layers (which is probably legitimate in this limit), their results are not directly comparable with ours.

Costa *et al* [13] studied the IEC in Fe/Au/Fe trilayer structures at several temperatures ($T = 0$, 200 and 400 K) as a function of the spacer thickness. For $T = 0$ K the IEC was estimated for spacer thicknesses ranging from 10 to 50 ML of Au. To calculate the IEC, an empirical tight-binding model with s, p and d orbitals and hopping up to second-nearest neighbours has been used. The calculated couplings showed a short-period oscillatory behaviour with $\lambda_2 = 2.4$ ML for all temperatures. The observed long period is very weak as shown in the Fourier spectrum obtained by Costa *et al* for $T = 0$ K and could not be identified explicitly from the spectrum. Nevertheless, both the long ($\lambda_1 = 9.2$ ML) and the short ($\lambda_2 = 2.4$ ML) oscillation periods were related to extremal spanning vectors of the Au Fermi surface. The observed periods of the IEC are in good agreement with our calculations; nevertheless we would like to point out that in our study a long period was observed.

Stiles [16] calculated the reflection probabilities for Fermi-surface electrons at Fe/Au interfaces to estimate the strength of the oscillatory coupling in Fe/Au multilayers. These calculations revealed that the critical vectors spanning across the Au Fermi surface are compatible with the oscillation periods. The periods extracted from the experimental Fermi surface agree with experimentally measured periods. Stiles found a factor of 1.8 between the coupling strengths of the long and short oscillation periods, which is the same as our prediction. For the short oscillation period he obtained $\lambda_2 = 2.49$ ML, also comparing well with our estimate. The long oscillation period is about $\lambda_1 = 10.3$ ML, which is a little bit larger than our long period.

5. Conclusions

We have performed LSDA + GGA calculations for bcc Fe(100)/fcc Au(100) multilayers, searching for the oscillation periods in the IEC. Comparing with experimental data, we find excellent agreement as regards the sign of the IEC for spacer thicknesses of up to 30 Au ML—without any artificial phase shift. These calculations are the first which treated Fe/Au superlattices with the correct lattice structure fully self-consistently up to 30 ML of Au spacers. Full agreement of the IEC oscillations with experiment has been found. For Au spacer with fewer than about 20 ML, a fully self-consistent calculation of the total-energy differences between ferromagnetically and antiferromagnetically coupled layers is found to be essential. A discrete Fourier analysis of the IEC as a function of a spacer thickness leads to oscillation periods of $\lambda_1 \approx 7$–9 and $\lambda_2 \approx 2.5$ ML, in good agreement with experiment. The ratio of the amplitudes agrees with earlier calculations, but remains smaller than that derived from experiment. The coupling strength is found to be much larger than measured experimentally—as in all previous calculations. We tend to attribute the difference to interdiffusion at the interface, which results in a mesoscopic roughness of the interface, as well as in additional scattering of electrons by defects.

To test the RKKY picture for the oscillatory IEC, an accurate evaluation of the Fermi surface of gold has been performed. The calculated nesting vectors lead to oscillation periods of $\lambda_1 = 8.3$ ML and $\lambda_2 = 2.5$ ML, which are in excellent agreement with the total-energy calculations for FM and AF coupling. Finally, we analysed our electronic spectra for manifestations of QW states. As predicted, the variation of the Au s, p density of states at the Fermi level shows weak oscillations with the same periodicity as the IEC. Thus, our investigation quantitatively verifies that the RKKY and the QW pictures for the IEC are identical. In addition, our calculations offer detailed insight into magnetic profiles of the multilayers and the hybridization of Fe and Au states at the interface.

Acknowledgments

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