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Ab initio theory of the interlayer exchange coupling in random metallic systems

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Abstract

We present an *ab initio* formulation of the interlayer exchange coupling (IEC) between two magnetic slabs embedded in a non-magnetic spacer wherein the spacer and the magnetic slabs as well as their interfaces may be random. This approach is based on the spin-polarized surface Green function technique within the tight-binding linear muffin-tin orbital method, the Lloyd formulation of the IEC, and the coherent potential approximation using the vertex-cancellation theorem. The periods, amplitudes, and phases are studied in terms of discrete Fourier transformations. Numerical results illustrating the theory are presented.

1. Introduction

The interlayer exchange coupling (IEC) between magnetic layers separated by a non-magnetic non-random spacer has recently been the subject of intensive theoretical studies, particularly on the *ab initio* level [1–3]. The origin of the periods of oscillation of the IEC is now well understood. New theoretical insight can be obtained by addressing the subtle problem of the variation of periods, amplitudes, and phases of the oscillations with the composition of magnetic and spacer alloy layers. Due to unavoidable interdiffusion, substitutional randomness is likely to occur at interfaces between magnetic and spacer layers. Thus, it is important to investigate the influence of disorder on the IEC.

It is the purpose of this paper to perform such a study on an *ab initio* level. We employ the Lloyd formulation of the IEC combined with a spin-polarized surface Green function technique based on the tight-binding linear muffin-tin orbital (TB-LMTO) method [3]. The use of a Green function formulation of the IEC is essential for describing randomness within the coherent potential approximation (CPA) which is known to reproduce compositional trends in random alloys reliably. The calculations are significantly simplified by employing the vertex-cancellation theorem [4].

2. Theory

Our model consists of two, generally different, semi-infinite magnetic subsystems denoted by $\mathcal{L}$ and $\mathcal{R}$, each containing M magnetic layers on the top of a semi-infinite non-magnetic base and separated by a finite spacer slab $\mathcal{C}$ of varying thickness N. A special case is a model of two semi-infinite magnetic slabs sandwiching a finite spacer. Both the magnetic and spacer layers are assumed to be binary alloys of arbitrary composition. We also assume a possible interface roughness or interdiffusion at the interfaces between the magnetic and spacer layers. Further, ϑ is a relative angle between spin directions in the magnetic subsystems $\mathcal{L}$ and $\mathcal{R}$.

The exchange energy $\bar{\mathcal{E}}_x$ is defined as $\bar{\mathcal{E}}_x(\vartheta) = \bar{\Omega}(\vartheta) - \bar{\Omega}(0)$, where the overbar denotes the configurational averaging and Ω is the grand canonical potential. The concept of principal layers as used within the TB-LMTO method leads to a block-tridiagonal form of the structure constants and of the inverse of the Green function [2, 3]. Considering as a perturbation the interlayer coupling at the $\mathcal{L}/C$ and the $\mathcal{C}/R$ interfaces, which is independent of the thickness of the magnetic slabs, and employing the partitioning technique with respect to the trace of the logarithm of the Green function appearing in the expression for the grand canonical potential [2, 3], it is possible to extract directly the term describing the magnetic coupling of interfaces. The resulting expression for the configurationally averaged $\bar{\mathcal{E}}_x(\vartheta)$ is given by the following expression [3, 5]:

$$\bar{\mathcal{E}}_x\vartheta) = \frac{1}{\pi N_\parallel} \operatorname{Im} \sum_{\boldsymbol{k}_\parallel} \int_C \operatorname{tr} \ln\left(1 - \frac{1-\cos(\vartheta)}{2} M(\boldsymbol{k}_\parallel, z)\right) \mathrm{d}z \tag{1}$$

where 'tr' denotes the trace over angular momentum indices, the energy integration is performed over a contour C in the upper half of the complex energy plane starting below the bottom of the valence band and ending at the Fermi energy, the sum runs over $\boldsymbol{k}_\parallel$-vectors in the irreducible surface Brillouin zone, and $N_\parallel$ is the corresponding unit surface area. The quantity $M(\boldsymbol{k}_\parallel, z)$ is defined as[5]

$$M = -\left(1 - S_{10}\bar{\mathcal{G}}^{\uparrow}_{\mathcal{L}} S_{01}\bar{\mathcal{G}}^{\uparrow}_{\mathcal{R}}\right)^{-1} S_{10}\left(\bar{\mathcal{G}}^{\uparrow}_{\mathcal{L}} - \bar{\mathcal{G}}^{\downarrow}_{\mathcal{L}}\right)\left(1 - S_{01}\bar{\mathcal{G}}^{\downarrow}_{\mathcal{R}} S_{10}\bar{\mathcal{G}}^{\downarrow}_{\mathcal{L}}\right)^{-1} S_{01}\left(\bar{\mathcal{G}}^{\uparrow}_{\mathcal{R}} - \bar{\mathcal{G}}^{\downarrow}_{\mathcal{R}}\right) \tag{2}$$

where for simplicity the arguments $\boldsymbol{k}_\parallel$ and z have been omitted. The quantities $S_{01}(\boldsymbol{k}_\parallel)$ and $S_{10}(\boldsymbol{k}_\parallel)$ in equation (2) are the structure constants which couple neighbouring (principal) layers, $\bar{\mathcal{G}}^{\sigma}_{\mathcal{X}}(\boldsymbol{k}_\parallel, z)$, $\mathcal{X} = \mathcal{L}, \mathcal{R}$, is the configurationally averaged surface Green function of the magnetic subsystem and σ denotes the spin index ($\sigma = \uparrow, \downarrow$). It should be noted that in the presence of randomness the expression for the IEC is formally analogous to the case of a non-random spacer [3] in the sense that the surface Green functions which enter equation (2) are replaced by the corresponding configurational averages. The theoretical basis for this simplification—which reduces computational times by almost two orders of magnitude—relies on the 'alloy force theorem' [6] and on the 'vertex-cancellation theorem' [4]. The latter theorem states that the vertex correction to the IEC due to randomness in the system is exactly zero. Strictly speaking, this theorem is valid only in the limit of infinitesimal rotations of the spin-quantization axis, but the numerical studies in [4] verified its validity even for large angles ϑ. This is very much in the spirit of the force theorem. We refer the reader to a recent review paper [7] for more details.

The present approach scales linearly with the thickness of both the magnetic slab and the spacer layer. This makes possible the efficient evaluation of the IEC for a large set of spacer thicknesses which, in turn, allows reliable extraction of periods, amplitudes, and phases from

[5] This form is equivalent to that given in reference [3] after substitution back into equation (1). It factorizes the spin asymmetry and it is directly related to the RKKY-like theories.

calculated data. The theory determines periods, and, in particular, amplitudes and phases of the oscillations from asymptotical expansions, i.e., for large spacer thicknesses. On the other hand, experimental data are usually available for small spacer thicknesses limited to regions with a possible pre-asymptotic behaviour. The advantage of the present approach lies in the possibility of bridging the two regions and thus verifying the theoretical concepts employed in the analysis of experiments.

Periods, amplitudes, and phases of the oscillations are found from a discrete Fourier transform $F(q)$ performed on a large enough set of values of $N^2\bar{\mathcal{E}}_x(N)$. The periods of oscillations p_i are then identified from the positions q_i of pronounced peaks of $|F(q)|$ as $p_i = 2\pi/q_i$, their amplitudes A_i as $A_i = (2/n)|F(q_i)|$, where n is the number of values of $N^2\bar{\mathcal{E}}_x(N)$ used in the Fourier analysis, and the phases φ_i from the relation

$$\varphi_i = \pi/2 - \arctan[\mathrm{Im}\, F(q_i)/\mathrm{Re}\, F(q_i)].$$

Extensive numerical tests for model cases verified the reliability of this approach. In order to exclude pre-asymptotic behaviour, the discrete Fourier transform is performed for values of $N^2\bar{\mathcal{E}}_x(N)$ corresponding typically to $N = 20$–80.

It should be noted that an alternative approach, namely an asymptotic analysis of the IEC as commonly used in model studies [8], can also be generalized to *ab initio* studies as demonstrated recently [9] (see also [7]). Such an approach allows both faster evaluation of corresponding Brillouin-zone integrals and, in particular, separation of contributions of particular spanning vectors of spacer Fermi surfaces.

The effect of temperature on the periods and phases of the oscillations was found to be negligible but can obscure an analysis of the oscillation amplitudes [8, 10]. Hence all calculations are for $T = 0$ K. Throughout this paper we will assume for a simplicity $\vartheta = \pi$.

3. Case studies

For the reference system of fcc-Co/Cu/Co(001) trilayers the following subjects will be discussed:

(i) the effect of interface roughness and interdiffusion on amplitudes of the oscillatory exchange coupling [11];
(ii) the effect of alloying in the spacer on periods and amplitudes of the oscillatory exchange coupling in metallic multilayers [5]; and
(iii) the dependence of amplitudes and phases of the oscillatory coupling on the composition of ferromagnetic layers [12].

For numerical details concerning the evaluation of the IEC we refer the reader to reference [3].

Most of the results discussed in this paper refer to the model of two semi-infinite magnetic slabs sandwiching a finite spacer. For this model the short-period oscillations (SPO) with the period of $p \approx 2.53$ monolayers (MLs) dominate [2, 3] and this simplifies the theoretical analysis. In particular cases, however, the model of two Co(001) slabs each five monolayers thick separated by a spacer will also be considered, for which both the SPO and LPO (long-period oscillations) are present.

3.1. Interface roughness and interdiffusion

We wish to investigate the role of two general cases of imperfections frequently occurring at interfaces of artificially prepared materials like magnetic multilayers, namely:

(i) an interfacial roughness case modelled via randomly distributed large terraces of monolayer heights leading to fluctuations of the spacer thickness in both directions around an ideal interface [13] with the probability r, and
(ii) an interfacial interdiffusion case, in which magnetic and spacer atoms are mixed randomly with the probability x at the system interfaces, i.e., instead of ideally sharp Co/Cu inter-faces we have two buried layers $Co_{1-x}Cu_x/Co_xCu_{1-x}$ at each interface.

The IEC for the interface roughness model defined above can be obtained from the following simple relation:

$$\bar{\mathcal{E}_x}(N) = \sum_n w(N-n)\mathcal{E}_x(n). \tag{3}$$

The deviations of the actual spacer thickness n from its mean value N are specified by the probabilities $w(N-n)$, where $w(0) = (1-2r)^2 + 2r^2$, $w(\pm 1) = 2r(1-2r)$, $w(\pm 2) = r^2$, and $w(m) = 0$ for $|m| > 2$. The convolution-like form of the relation between $\mathcal{E}_x(n)$ and $\bar{\mathcal{E}_x}(N)$ implies that the amplitudes of oscillations with wavenumber q are reduced due to roughness by a factor $\tilde{w}(k) = (1 - 4r\sin^2(k/2))^2$, namely the Fourier transform of the probabilities $w(n)$. An obvious consequence of this result is an efficient suppression of the amplitude of short-period oscillations with period close to $p = 2$ MLs, e.g., as for the case of the SPO for the Co/Cu/Co(001) system. In contrast, the LPO are influenced by interface roughness less efficiently.

The results of calculations for the case of two semi-infinite Co slabs are summarized in table 1. The following conclusions can be drawn:

(i) The effect of interfacial roughness on the coupling strength of the SPO is quite large and the SPO are almost wiped out for $r = 0.25$. It should be noted that the relative suppression of amplitudes of the SPO is not sensitive to the thickness of magnetic slabs (essentially the same relative suppression was found also for the SPO for two Co(001) slabs in fcc-Cu each five monolayers thick [11].
(ii) The effect of interfacial interdiffusion on the coupling strength is even more dramatic. An appreciable suppression of the amplitudes of the SPO is visible already for 2% interdiffusion and amounts to an order of magnitude for 10% interdiffusion.
(iii) The fact that the strong suppression of the amplitude of the SPO does not depend on the Co slab thickness confirms the decisive role of the interface region. We have further addressed this problem by performing calculations with 5% interdiffusion where one of the interfaces was disordered while the other was kept ideal. The relative amplitude for the SPO in the latter case was 0.62, i.e., almost two times larger in comparison with the value 0.36 given in the table.

The present study clearly demonstrates the high sensitivity of the coupling strength with respect to various kinds of interfacial imperfections and the decisive role of interface electron scattering for the exchange oscillatory coupling and, in turn, indirectly also for the giant magnetoresistance in metallic multilayers. The present study also shows that a detailed knowledge of the quality of the system interfaces is needed when comparing theoretical and experimental values of coupling strengths.

3.2. Alloying in spacer layers

The study of the effect of alloying in the spacer represents another powerful experimental and theoretical tool [14–17] for verifying existing models of the IEC by continuously varying the medium between the magnetic layers. We present numerical studies for an fcc-Cu spacer as

Table 1. Relative amplitudes $A(\nu)/A(0)(\nu = r, x)$ of the short-period oscillations for two semi-infinite Co(001) subsystems sandwiching the Cu spacer. The values are given as functions of the interface roughness r and the interface interdiffusion concentration x. The quantity $A(0)$ refers to the ideal Co/Cu interface ($r = 0.0$ or $x = 0.0$).

r	$A(r)/A(0)$	x	$A(x)/A(0)$
0.0	1.0	0.0	1.0
0.05	0.66	0.02	0.69
0.1	0.40	0.05	0.36
0.25	0.01	0.1	0.12

alloyed with Ni or Zn or Au. This choice is motivated by the fact that alloying with Ni or Zn alters the electron concentration and, consequently, modifies the topology of the alloy Fermi surface which is closely related to the coupling periods in terms of Fermi surface spanning vectors [8]. The changes in the coupling periods can then be viewed as a contraction (Ni) or an expansion (Zn) of the alloy Fermi surface. In contrast, alloying of Cu with Au does not alter the electron concentration. In all cases, however, the coupling amplitudes are expected to be influenced by the presence of alloy disorder. Strictly speaking, in random alloys the Fermi surface is not well defined. In particular cases, however, when the alloy Fermi energy lies in the sp part of the spectrum above the d-band complex, alloy broadening is usually weak, therefore causing only little smearing of the Fermi surface. As is obvious from equations (1) and (2), the present Green function formulation does not rely upon the existence of the alloy Fermi surface.

Alloying shifts corresponding peaks of $|F(q)|$ to higher values of q and suppresses their heights as illustrated in figure 1 for the case of five-monolayer-thick Co(001) slabs with an fcc-$Cu_{1-x}Ni_x$ spacer. The results for the concentration dependence of the periods of oscillations for the chosen alloy spacers are summarized in figure 2. For an ideal Cu spacer the SPO and the LPO are 2.53 MLs and 5.05 MLs, respectively. Alloying of Cu with Ni decreases the electron concentration in the alloy and leads to a contraction of the alloy Fermi surface. In terms of the RKKY formulation [8] this leads to an expansion of spanning vectors corresponding to an fcc (001) layer orientation. Both the SPO and the LPO are reduced with increasing Ni concentration but this reduction is more pronounced for the LPO. The present results for the LPO agree qualitatively with the simplified calculations of reference [15] based on an RKKY formulation and approximating the spanning vectors by a linear interpolation between the bulk band structures of Cu and Ni. It is therefore interesting to compare the present results with those performed within the same computational scheme but employing the VCA (virtual-crystal approximation) instead of the CPA. The results for $Cu_{75}Ni_{25}$ are shown in figure 2 as open circles. As one can see, in particular for the LPO the shift of the coupling periods differs in the VCA from that in the CPA.

The opposite behaviour, namely a shift to larger periods and again rather pronounced for the LPO, was found when alloying Cu with Zn, namely the case when the Fermi surface expands. Note that the periods of oscillations for a $Cu_{1-x}Zn_x$ spacer increase faster with x than they decrease in the case of $Cu_{1-x}Ni_x$. Finally, for a $Cu_{1-x}Au_x$ spacer, even for large concentrations of Au (up to 50%), we observe a negligible concentration dependence of the periods of oscillations which is consistent with the composition-independent average electron number in these alloys as well as with available experimental data [16]. From figure 2 it is obvious that the coupling periods obtained for a $Cu_{0.5}Au_{0.5}$ spacer by employing the CPA and the VCA are virtually the same. It was demonstrated quite recently that the study of the IEC with alloyed spacers can be used as an quantitative probe of complex Fermi surfaces such as those which are hosts to electronic topological transitions in transition metal alloys [18].

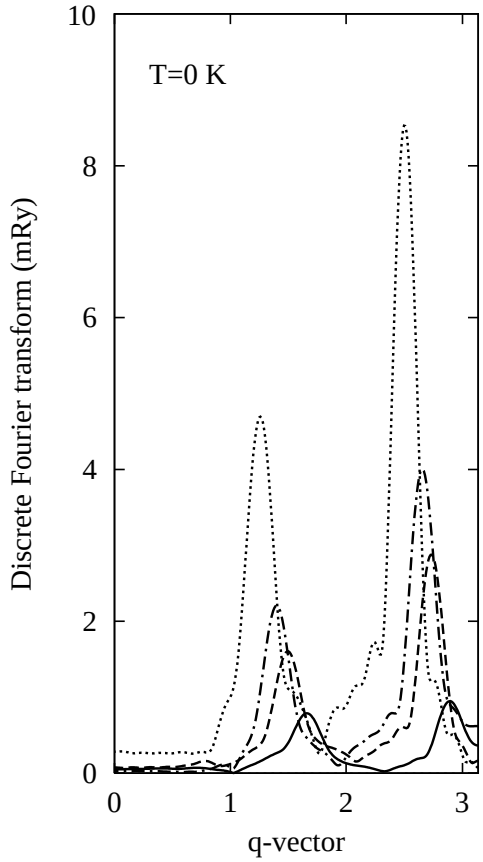

Figure 1. Composition dependence of the absolute values of a discrete Fourier transform of $\bar{\mathcal{E}}_x$ at $T = 0$ K for two Co(001) slabs each five monolayers thick separated by an fcc-$Cu_{1-x}Ni_x$ alloy spacer: (i) $Cu_{0.75}Ni_{0.25}$ (full line); (ii) $Cu_{0.85}Ni_{0.15}$ (dashed line); (iii) $Cu_{0.9}Ni_{0.1}$ (dashed–dotted line); and (iv) an ideal Cu spacer (dotted line).

The dependence of $\bar{\mathcal{E}}_x$ on the spacer thickness N is illustrated in figure 3 for the case of two semi-infinite Co(001) slabs sandwiching $Cu_{0.75}Ni_{0.25}$, $Cu_{0.5}Zn_{0.5}$, and $Cu_{0.5}Au_{0.5}$ alloy spacers. An increase of the coupling period is clearly seen for $Cu_{0.5}Zn_{0.5}$, while the reduction for a $Cu_{0.75}Ni_{0.25}$ spacer is less pronounced. The period of oscillations for a $Cu_{0.5}Au_{0.5}$ alloy spacer remains essentially unchanged. From figure 3 one can also see that the $Cu_{1-x}Ni_x$ and $Cu_{1-x}Au_x$ alloy spacers exhibit an RKKY-like behaviour with the amplitudes being proportional to N^{-2}—however, with values reduced in comparison to those for the ideal Cu spacer. This reduction is particularly pronounced for a $Cu_{0.75}Ni_{0.25}$ spacer (see figure 1). An approximate RKKY-like behaviour with a weak exponential damping $\approx \exp(-0.04N)$ was found for $Cu_{0.5}Zn_{0.5}$.

Detailed understanding of the concentration dependence of amplitudes of oscillations is still lacking. Adopting an RKKY-like picture, the SPO and the LPO periods are connected via so-called stationary points [8] located in different parts of the surface Brillouin zone. Quite probably, the different influence of alloying on the amplitudes of the SPO and the LPO [5] is connected with the anisotropy of electron–impurity scattering at the alloy Fermi level. Such information can be obtained, e.g., from the spectral densities corresponding to stationary points.

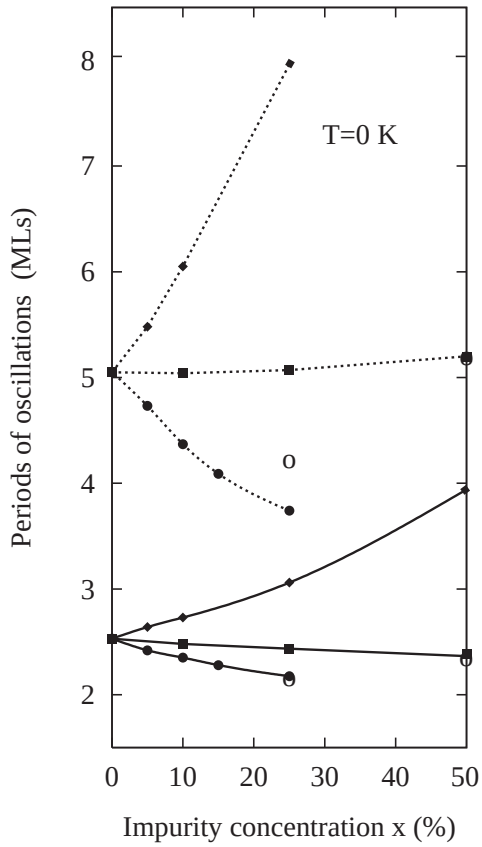

Figure 2. Composition dependence of the coupling periods at $T = 0$ K for two Co(001) slabs each five monolayers (MLs) thick separated by an fcc-$Cu_{1-x}M_x$ alloy spacer: (i) M = Ni (bullets); (ii) M = Au (squares); and (iii) M = Zn (diamonds). The lines serves as a guide for the eye and distinguish between short-period (full lines) and long-period (dotted lines) oscillations. Open circles for $Cu_{0.75}Ni_{0.25}$ and $Cu_{0.5}Au_{0.5}$ represent the approximate virtual-crystal values. The periods are given in MLs.

3.3. Alloying in magnetic layers

Further insight into the physical nature of the IEC can be obtained by studying the variation of the phases of oscillations with respect to the concentration in alloyed magnetic subsystems. A first experimental study of this kind for fcc (001) sputtered Fe–Co–Ni/Cu multilayers [19] was significantly improved by preparing and measuring multiple MBE-grown sandwiches on the same single-crystal substrate [20]. We consider symmetric systems, $A_{1-x}B_x/Cu/A_{1-x}B_x(001)$, as well as asymmetric systems, $A_{1-x}B_x/Cu/M(001)$ and $M'/Cu/M(001)$, where $A_{1-x}B_x = Fe_{1-x}Co_x, Co_{1-x}Ni_x, Fe_{1-x}Ni_x$, and $M, M' =$ Co, Fe, Ni ($M \neq M'$). Alloying Co with Ni (Fe) increases (decreases) the average number of valence electron N_{el} of the ferromagnetic layers. As is well known, by studying Fe–Ni alloys one can make use of the fact that certain compositions have the same N_{el} as in suitably chosen Co–Ni or Fe–Co systems. The role of a particular constituent as well as of N_{el} can thus be investigated. Finally, a study of asymmetric arrangements allows one to verify in detail predictions of an RKKY-like formulation of the IEC [8].

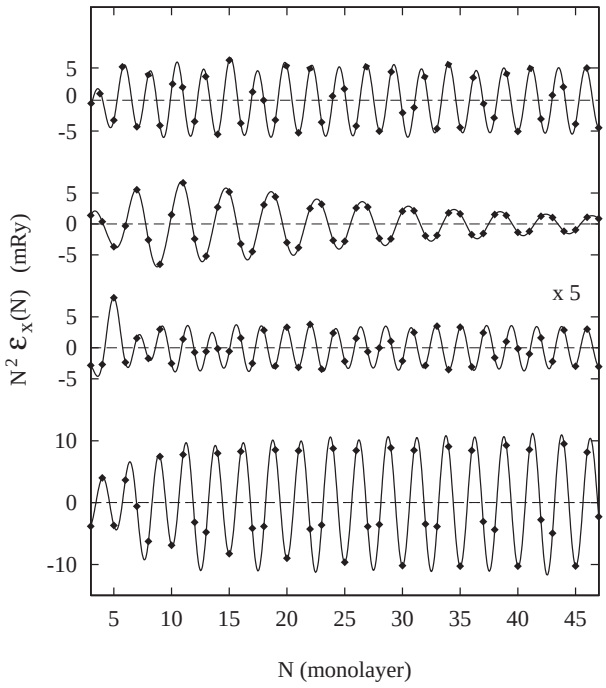

Figure 3. Exchange coupling $N^2\bar{\mathcal{E}}_x(N)$ at $T = 0$ K as a function of the spacer thickness N for two semi-infinite Co(001) subsystems sandwiching a spacer of (from bottom to top) ideal Cu, $Cu_{0.75}Ni_{0.25}$ (multiplied by a factor of 5), $Cu_{0.5}Zn_{0.5}$, and $Cu_{0.5}Au_{0.5}$. Diamonds refer to the calculated values; the full line (Fourier back-transform) serves as a guide to the eye.

In figure 4 two symmetric alloyed magnetic layers, namely $Co_{50}Ni_{50}$ and $Fe_{50}Co_{50}$ layers, are compared with a reference case of ideal Co(001) layers. The results confirm qualitative predictions in terms of an RKKY-like formulation of the IEC: the dominant SPO of 2.53 MLs is unaffected by alloying in the ferromagnetic layers [8]. The suppression of the amplitude of oscillations, pronounced in the $Co_{50}Ni_{50}$ case and rather weak for $Fe_{50}Co_{50}$ layers, is evident. The change of the phase of the oscillations due to alloying in the ferromagnetic layers can also be deduced from figure 4. In both the ideal and the alloyed case, the so-called pre-asymptotic behaviour is limited to the first 10 or 15 layers. This has to be kept in mind when making a detailed comparison with experiment, since experimentally the amplitudes and the phases are determined from the first antiferromagnetic peaks [20] rather than from the asymptotic behaviour as in the present approach.

A summary of the concentration dependence of the phases of the oscillations for Co–Ni, Fe–Co, and Fe–Ni layers is presented in figure 5. The following conclusions can be drawn:

(i) in full agreement with experiments for fcc (001) faces [20], we observe a monotonic change of the phase with N_{el};

(ii) the estimated average phase variations of 0.56, 0.63, and 1.81 π/electron for Fe–Co, Fe–Ni, and Co–Ni layers, respectively, should be compared to 0.65 π/electron found experimentally as an average from Co, $Co_{50}Ni_{50}$, and $Fe_{60}Ni_{40}$ values [20]; and

(iii) for the same N_{el} the phases of the Fe–Ni layers agree very well with corresponding phases of Co–Ni and Fe–Co layers.

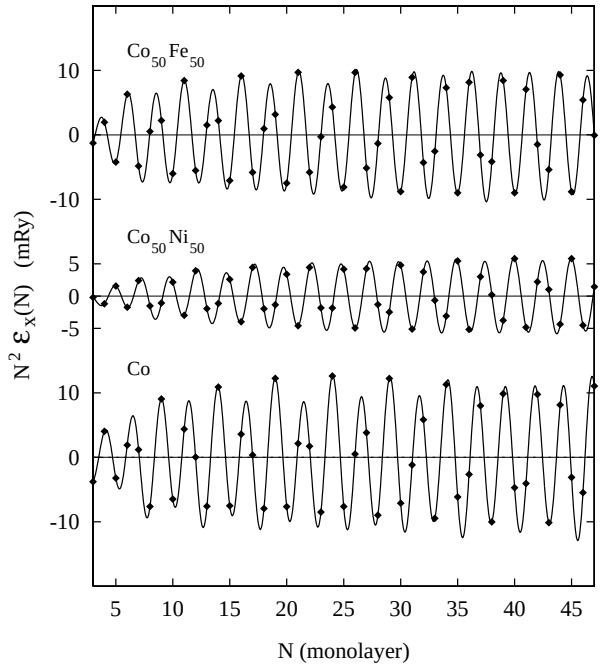

Figure 4. Exchange coupling $N^2\bar{\mathcal{E}}_x(N)$ as a function of the spacer thickness N for three different semi-infinite magnetic slabs separated by an fcc-Cu spacer. Diamonds refer to calculated values; the full lines (Fourier back-transform) serve as a guide to the eye.

The pronounced dependence of the phases on N_{el} and their insensitivity to the specific elements which form the ferromagnetic layers can be explained qualitatively on the basis of a simplified RKKY-like formulation which relates (within a free-electron picture) the amplitudes and phases to the wave vector of the spin-down transmitted wave in the ferromagnet, or, equivalently, to its electron density [8]. It should be noted that the alloys studied are strong ferromagnets with nearly filled spin-up bands. The changes of N_{el} caused by alloying are thus mostly at the cost of filling (emptying) of spin-down bands. Within the free-electron picture the calculated opposite phase shifts for alloyed Co layers with elements having a higher (Ni) or lower (Fe) number of valence electrons as well as the observed insensitivity to the type of the atoms which form the ferromagnetic layers can thus be qualitatively understood. Deviations from the simple RKKY picture reflect the differences between a realistic electronic structure and a free-electron model at the Fermi energy. The assertion of insensitivity of the phases of oscillations to the atom type in the magnetic layers can further be supported by calculations for ternary $\mathrm{Fe}_x\mathrm{Co}_y\mathrm{Ni}_z$ magnetic layers, e.g., for the case $x = y = z = 1/3$ with $N_{el} = 9$. The calculated phase again compares very well with the corresponding one for Co layers with the same N_{el}.

For one dominating period and large enough N, the IEC is given within an RKKY-like description [8] as

$$\mathcal{E}_x(N) \approx \frac{1}{N^2}\,\mathrm{Im}(Z\mathrm{e}^{2\pi\mathrm{i}qN}) \qquad Z = Z_1Z_2 \qquad Z_i = \sqrt{A_i}\mathrm{e}^{\mathrm{i}\varphi_i} \tag{4}$$

where Z_i ($i = 1, 2$) denote complex amplitudes characterizing magnetic subsystems 1 and 2 ($\mathcal{L}$ and $\mathcal{R}$). The wave vectors q are identical, with a relative accuracy 10^{-3} for all systems considered. We have used the values of the amplitudes A^{sym} and the phases φ^{sym} as calculated

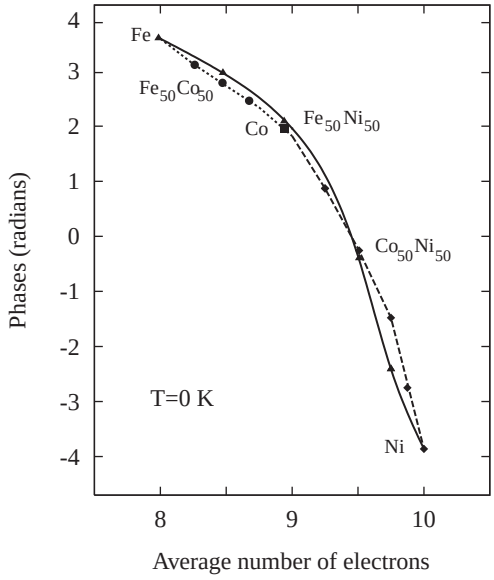

Figure 5. Phases of the exchange coupling in semi-infinite magnetic slabs separated by an fcc-Cu spacer plotted as a function of the average number of valence electrons: (i) Fe–Ni(001) slabs (full line, triangles); (ii) Fe–Co(001) slabs (dotted line, bullets); and (iii) Co–Ni(001) slabs (dashed line, diamonds). The reference case of an ideal Co(001) slab is marked as a square. The lines serve as a guide to the eye.

for symmetric systems M/Cu/M(001) and $A_{1-x}B_x$/Cu/$A_{1-x}B_x$(001) in order to find the complex amplitudes Z_i^{sym} for the individual subsystems $A_{1-x}B_x$ and M as

$$Z_i^{\mathrm{sym}} = \sqrt{A^{\mathrm{sym}}}\exp(\mathrm{i}\varphi^{\mathrm{sym}}/2). \tag{5}$$

Using these Z_i^{sym} in (4) for a wide variety of asymmetric systems $A_{1-x}B_x$/Cu/M(001) and M′/Cu/M(001), we found quite a good agreement with the corresponding *ab initio* values of Z. A least-squares fit applied to all data including symmetric and asymmetric systems yields values of Z_i with a r.m.s. error not exceeding 5%. This result represents perhaps the most complete confirmation of an RKKY-like approach to the IEC for the systems studied as most of the other existing comparisons concentrate just on the periods of oscillations.

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