PHILOSOPHICAL MAGAZINE B, 1998, VOL. 78, NOS. 5/6, 571–575

# The combined effect of temperature and disorder on interlayer exchange coupling in magnetic multilayers

V. DRCHAL†‡, J. KUDRNOVSKÝ†‡, P. BRUNO§, P. H. DEDERICHS ¶ and P. WEINBERGER‡

†Institute of Physics AS CR, CZ-180 40 Praha 8, Czech Republic
‡Center for Computational Material Science, TU Vienna, Vienna, Austria
§MPI für Mikrostrukturphysik, D-06120 Halle, Germany
¶Forschungszentrum Jülich, D-52425 Jülich, Germany

ABSTRACT

We study the combined effect of temperature and disorder in the spacer on the interlayer exchange coupling. The temperature dependence is treated *ab initio* like by employing the spin-polarized surface Green function technique within the tight-binding linear muffin-tin orbital method and the Lloyd formulation of the IEC. The integrals involving the Fermi–Dirac distribution are calculated using an efficient method based on a representation of integrands by a sum of complex exponentials. Application is made to $Co/Cu_{1-x}M_x/Co(001)$ trilayers (M= Zn, Au, and Ni) with varying thickness of the spacer.

## §1. INTRODUCTION

The oscillatory interlayer exchange coupling (IEC) between magnetic layers separated by a non-magnetic spacer has recently attracted considerable attention. The physical origin of such oscillations is attributed to quantum interferences due to spin-dependent confinement of electrons in the spacer. The periods of the oscillations with respect to the spacer thickness are determined by the spacer Fermi surface, and this conclusion has been confirmed by numerous experiments. In particular, the change of the Fermi surface by alloying thus leads to a change of the oscillatory periods (van Schilfgaarde *et al.* 1995, Kudrnovský *et al.* 1996). On the other hand, there are very few studies of the temperature-dependence of the IEC (Bruno 1995, d'Albuquerque e Castro *et al.* 1996), and its systematic study on an *ab initio* level is missing.

The main mechanism of the temperature dependence of the IEC is connected with thermal excitations of electron–hole pairs across the Fermi level as described by the Fermi–Dirac function. It turns out that other mechanisms (e.g. electron–phonon or electron–magnon interactions) are less important. The effect of temperature on the IEC can be evaluated either analytically or numerically. The analytical approach assumes the limit of large spacer thickness, for which all the oscillatory contributions to the energy integral cancel out with the exception of those at the Fermi energy. The energy integral is then evaluated by a standard saddle-point method (Bruno 1995). The general functional form of the temperature-dependence of the interlayer exchange coupling $\mathscr{E}_x(T)$ in the limit of a single period is then:

$$\mathscr{E}_x(T) = \mathscr{E}_x(0)\, t(N,T), \quad t(N,T) = \frac{cNT}{\sinh(cNT)}. \tag{1}$$

Here, $T$ denotes the temperature, $N$ is the spacer thickness in monolayers, and $c$ is a constant which depends on the spacer Fermi surface. The term $\mathscr{E}_x(0)$ exhibits a standard $N^{-2}$ dependence (Bruno 1995), while the scaling temperature factor $t(N,T)$ depends on $N$ via $NT$. In the pre-asymptotic regime (small spacer thicknesses) the functional form of $t(N,T)$ differs from that of equation (1), particularly in the case of complete but relatively weak confinement due to the rapid variation of the phase of the integrand which enters the evaluation of the IEC (d'Albuquerque e Castro *et al.* 1996).

The second, numerical approach is in principle exact, i.e. not limited to large spacer thickness, however, it may be numerically very demanding, in particular for low temperatures. It is applicable also to disordered systems with randomness in the spacer, magnetic layers, or at interfaces (Bruno *et al.* 1996).

## §2. Formalism

The multilayer system consists of a left and right magnetic subspace separated by a non-magnetic spacer (the trilayer). The spacer may be a random substitutional alloy. We employ the Lloyd formulation of the IEC combined with a spin-polarized surface Green function technique as based on the tight-binding linear muffin-tin orbital (TB-LMTO) method. The exchange coupling energy $\mathscr{E}_x(T)$ can be written as

$$\mathscr{E}_x(T) = \operatorname{Im} I(T), \quad I(T) = \int_C f(T,z)\, \Psi(z)\, \mathrm{d}z, \tag{2}$$

where $f(T,z)$ is the Fermi–Dirac distribution function and

$$\Psi(z) = \frac{1}{\pi N_\parallel} \sum_{\mathbf{k}_\parallel} \operatorname{tr}_L \ln \mathbf{M}(\mathbf{k}_\parallel, z)$$

is a difference of (in the case of disorder, of configurationally averaged) grandcanonical potentials for the antiferromagnetic and ferromagnetic alignments of magnetic slabs (Drchal *et al.* 1996).

The energy integration is performed over a contour $C$ along the real axis and closed by a large semicircle in the upper half of the complex energy plane, $\operatorname{tr}_L$ denotes the trace over angular momentum indices $L = (\ell m)$, the sum runs over $\mathbf{k}_\parallel$ vectors in the surface Brillouin zone, and $N_\parallel$ is the number of lattice sites in one layer. The quantity $\mathbf{M}(\mathbf{k}_\parallel, z)$ is expressed in terms of screened structure constants which couple neighbouring (principal) layers and of the so-called surface Green functions. All details can be found in Drchal *et al.* (1996). We only note that the use of a Green function formulation of the IEC is essential for describing the randomness in the spacer within the coherent potential approximation (CPA) which is known to reproduce compositional trends in random alloys reliably.

The integral in (2) can be recast into a more suitable form using the analytic properties of $\Psi(z)$, namely, (i) $\Psi(z)$ is holomorphic in the upper complex halfplane, and (ii) $z\Psi(z) \to 0$ for $z \to \infty$, $\operatorname{Im} z > 0$. Let us define a new function $\Phi(y) = -\mathrm{i}\Psi(E_\mathrm{F} + \mathrm{i}y)$ of a real variable $y$, $y \geq 0$. Then at $T = 0\,\mathrm{K}$,

$$I(0) = \int_0^{+\infty} \Phi(y)\, \mathrm{d}y,$$

while at $T > 0\,\mathrm{K}$,

$$I(T) = 2\pi k_B T \sum_{k=1}^{\infty} \Phi(y_k),$$

where $k_B$ is the Boltzmann constant, and the $y_k$ are Matsubara energies, $y_k = \pi k_B T(2k - 1)$. In the limit $T \to 0$, $I(T) \to I(0)$ continuously.

We have verified that the function $\Phi(y)$ can be represented with a high accuracy as a sum of a few complex exponentials of the form

$$\Phi(y) = \sum_{j=1}^{M} A_j \exp(p_j y), \tag{3}$$

where the $A_j$ are complex amplitudes and the $p_j$ are complex wave numbers. An efficient method of finding the parameters $A_j$ and $p_j$ is described elsewhere (Drchal *et al.* 1998). The evaluation of $I(T)$ is then straightforward:

$$I(T) = -2\pi k_B T \sum_{j=1}^{M} \frac{A_j}{\exp(\pi k_B T p_j) - \exp(-\pi k_B T p_j)}, \tag{4}$$

which for $T = 0\,\mathrm{K}$ gives

$$I(0) = -\sum_{j=1}^{M} \frac{A_j}{p_j}. \tag{5}$$

## §3. Results and discussion

Numerical studies were performed for an ideal fcc(001) stacking of layers of the spacer (Cu) and magnetic (Co) layers with the experimental lattice spacing of fcc Cu. The spacer layers can contain impurities (Zn, Ni and Au) which form a substitutional alloy with the spacer atoms. Possible lattice and layer relaxations are neglected. Alloying with Ni, Zn or Au alters the electron concentration and, consequently, modifies the Fermi surface, and thus, in turn, also the temperature dependence of the IEC. The most obvious effect of alloying, for $T = 0$, is the change of the periods of the oscillations connected with the change of the corresponding spanning vectors of the alloy Fermi surface (Kudrnovský *et al.* 1996). A more subtle effect of the alloying is connected with damping of electron states and relaxation of symmetry rules due to alloying.

To determine the parameters of the complex exponentials (3), we have evaluated the function $\Phi(y)$ at 40 Matsubara energies corresponding to $T = 25\,\mathrm{K}$. We have verified that the results depend weakly on the actual value of the parameter $T$. Special care was devoted to the Brillouin zone integration. The efficiency of the present approach allows us to perform calculations with a large number of $\mathbf{k}_\parallel$ points in the irreducible part of the surface Brillouin zone (ISBZ). Note also that such calculations have to be done only once and then the evaluation of the IEC for any temperature is an easy task. In particular, we employ typically 40 000 $\mathbf{k}_\parallel$ points in the ISBZ for the first Matsubara energies close to the Fermi energy. The number of $\mathbf{k}_\parallel$ points then progressively decreases for points distant from the real axis. The present calculations agree with the results of conventional calculations (Drchal *et al.* 1996) but they are much more efficient numerically, in particular when calculations for many different temperatures are required.

The calculations were done for spacer thicknesses $N = 1 - 50$ monolayers and for temperatures $T = 0 - 500\,\mathrm{K}$ (in steps 10 K) and by assuming semi-infinite Co slabs. In this case only one period, namely the so-called short period exists, which simplifies the study. There are several possibilities of how to present the results (see Drchal *et al.* (1998) for more details). As an illustration, in figure 1 we plot the discrete Fourier transformations (Drchal *et al.* 1996) of $N^2\mathscr{E}_x(N,T)$ with respect to $N$, $\mathscr{E}_x(q,T)$, as a function of the variables $q$ and $T$. A discrete Fourier transformation on a subset $N \in 10 - 50$ which avoids the pre-asymptotic region is employed here. The positions of peaks, $q = q_m$, then determine the oscillation periods $p = 2\pi/q_m$, while $|\mathscr{E}_x|$ gives the oscillation amplitudes (Drchal *et al.* 1996). In particular, one can see how the modification of the

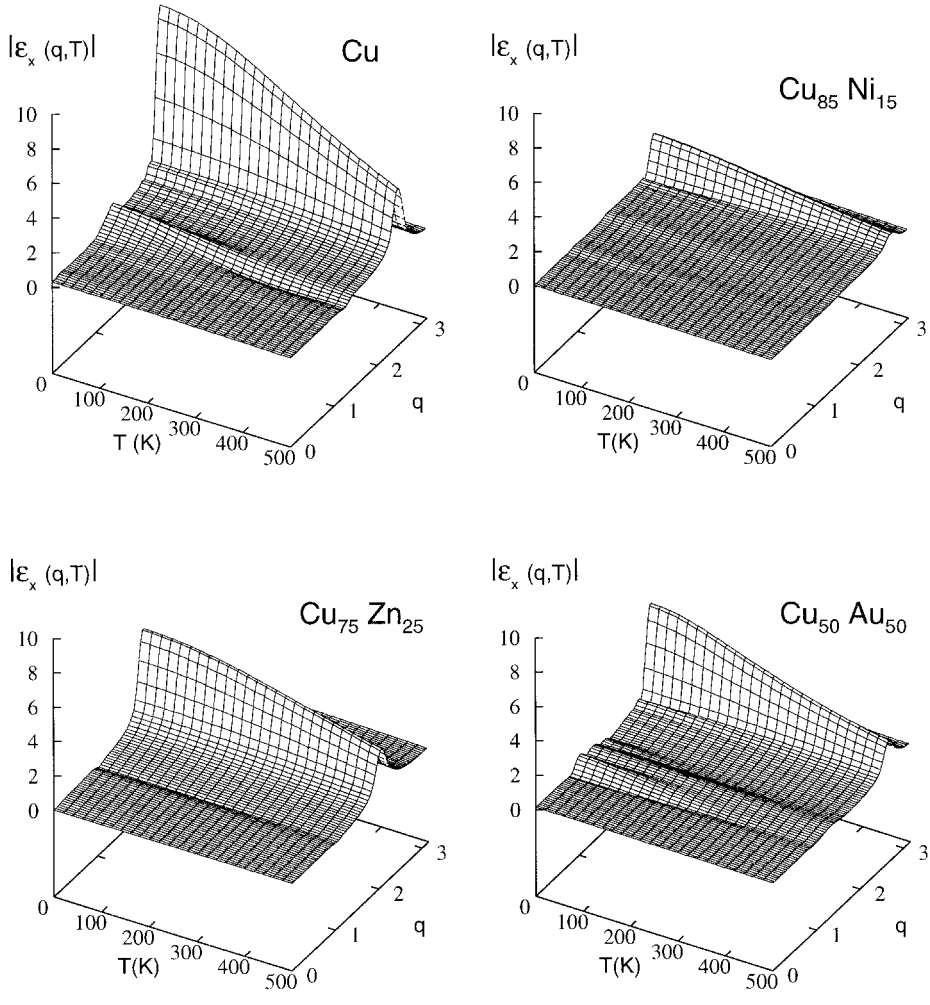


Figure 1. Absolute values of the discrete Fourier transformations of $N^2\mathscr{E}_x(N,T)$ with respect to the spacer thickness $N$ as a function of the temperature $T$ and the wave vector $q$ for a trilayer consisting of semi-infinite Co slabs sandwiching the spacer of indicated composition.

Fermi surface due to alloying changes the temperature dependence of the IEC, i.e. the coefficient $c$ in equation (1).

The following conclusions can be drawn from the present numerical results: (i) the non-random case (Cu) exhibits a period $p \approx 2.53$ MLs (monolayers) or, equivalently, $q_m \approx 2.48$ in accordance with previous calculations (Drchal *et al.* 1996). In accordance with Kudrnovský *et al.* (1996), the periods of oscillations for $Cu_{75}Zn_{25}$ are shifted towards higher periods ($p \approx 3.05$ MLs), towards smaller periods for $Cu_{85}Ni_{15}$ ($p \approx 2.27$ MLs), while they remain almost unchanged for a $Cu_{50}Au_{50}$ alloy spacer ($p \approx 2.36$ MLs). (ii) The periods of oscillations are temperature independent because the electronic structure or, alternatively, spanning vectors are temperature independent. (iii) The amplitudes exhibit a strong temperature dependence in agreement with predictions of model theories (Bruno 1995). In particular, our results agree reasonably well with those of figure 3 of d'Albuquerque e Castro *et al.* (1996), for the case of an ideal Cu spacer. (iv) For alloy spacers at $T = 0$ we mention, in particular, the dependence $N^{-2}$ of the oscillation amplitudes on the spacer thickness $N$ for Cu/Ni and Cu/Au alloy spacers, while additional exponential damping due to disorder was found for a Cu/Zn alloy spacer. This indicates a finite lifetime of states at the Fermi energy for $\mathbf{k}_\parallel$ vectors corresponding to the short-period oscillations for this case and only a weak damping for the Cu/Au and Cu/Ni alloys. (v) Finally, the effect of temperature (the factor $t(N, T)$ in equation (1)) is similar for a pure Cu-spacer, Cu/Ni and Cu/Au alloys, but it is much smaller for the case of Cu/Zn alloys. The effect of temperature, similarly to alloying, is to broaden spanning vectors of the Fermi surface (Bruno 1995). If the damping due to alloying is non-negligible, then as compared to the case $T = 0$ K, the combined effect of disorder and temperature leads to a relatively smaller suppression of the oscillation amplitude with respect to temperature.

## Acknowledgements

This work is part of activities of the Center for Computational Material Science, Prague, sponsored by the Academy of Sciences of the Czech Republic. Financial support for this work was provided by the Grant Agency of the Czech Republic (Project No. 202/97/0598), the Grant Agency ot the Academy Sciences of the Czech Republic (Project A1010829), the Project 'Scientific and Technological Cooperation between Germany and the Czech Republic', the Center for the Computational Materials Science in Vienna (GZ 45.442 and GZ 45.420), and the TMR Network 'Interface Magnetism' of the European Commission (Contract No. EMRX-CT96-0089).

## References

Bruno, P., 1995, *Phys. Rev.* B, **52**, 411.

Bruno, P., Kudrnovský, J., Drchal, V., and Turek, I., 1996, *Phys. Rev. Lett.*, **76**, 4254.

d'Albuquerque e Castro, J., Mathon, J., Villeret, M., and Umerski, A., 1996, *Phys. Rev.* B, **53**, R13306.

Drchal, V., Kudrnovský, J., Bruno, P., and Weinberger, P., 1998 (in preparation).

Drchal, V., Kudrnovský, J., Turek, I., and Weinberger, P., 1996, *Phys. Rev.* B, **53**, 15036.

Kudrnovský, J., Drchal, V., Bruno, P., Turek, I., and Weinberger, P., 1996, *Phys. Rev.* B, **54**, R3738.

van Schilfgaarde, M., Herman, F., Parkin, S. S. P., and Kudrnovský, J., 1995, *Phys. Rev. Lett.*, **74**, 4063.