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

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Abstract

We study the combined effect of temperature and disorder in the spacer on the interlayer exchange coupling. The temperature dependence is treated on \textit{ab initio} level. We employ 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 representation of integrands by a sum of complex exponentials. Application is made to Co/Cu\textsubscript{100-x}M\textsubscript{x}/Co(001) trilayers (M=Zn, Au, and Ni) with varying thicknesses 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 in the literature. 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 the change of the oscillatory periods (\textit{van Schilfgaarde et al.}, 1995; \textit{Kudrnovský et al.}, 1996). On the other hand, there are very few studies of the temperature-dependence of the IEC (\textit{Bruno}, 1995; \textit{d’Albuquerque e Castro et al.}, 1996), and its systematic study on \textit{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 the temperature on the IEC can be evaluated either analytically or numerically. The analytical approach assumes the limit of large spacer thicknesses, for which all the oscillatory contributions to the energy integral cancel out with exception of those at the Fermi energy. The energy integral is then evaluated by a standard saddle-point method (\textit{Bruno}, 1995). The general functional form of the temperature-dependence of the interlayer exchange coupling
\( \mathcal{E}_x(T) \) in the limit of a single period is then:

\[
\mathcal{E}_x(T) = \mathcal{E}_x(0) t(N, T), \quad t(N, T) = \frac{cNT}{\sinh(cNT)}.
\]

(1)

Here, \( T \) denotes the temperature, \( N \) is the spacer thickness in monolayers, and \( c \) is the constant which depends on the spacer Fermi surface. The term \( \mathcal{E}_x(0) \) exhibits a standard \( N^{-2} \)-dependence (Bruno, 1995), while the scaling temperature factor \( t(N, T) \) depends on \( N \) via \( NT \).

In the preasymptotic regime (small spacer thicknesses) the functional form of \( t(N, T) \) differs from that of Eq. (1), particularly in the case of the 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, not limited to large spacer thicknesses, 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 the left and right magnetic subspaces 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 \( \mathcal{E}_x(T) \) can be written as

\[
\mathcal{E}_x(T) = \text{Im} \ I(T), \quad I(T) = \int_C f(T, z) \Psi(z) \, dz,
\]

(2)

where \( f(T, z) \) is the Fermi-Dirac distribution function and

\[
\Psi(z) = \frac{1}{\pi N ||} \sum_{k ||} \text{tr}_L \ln M(k ||, z)
\]

(3)

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, \( \text{tr}_L \) denotes the trace over angular momentum indices \( L = (\ell m) \), the sum runs over \( k || \)-vectors in the surface Brillouin zone, and \( N || \) is the number of lattice sites in one layer. The quantity \( M(k ||, z) \) is expressed in terms of the screened structure constants which couple neighboring (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 \( z \to \infty, \text{Im}z > 0 \). Let us define a new function \( \Phi(y) = -i \Psi(E_F + iy) \) of a real variable \( y, y \geq 0 \). Then at \( T = 0 \) K,

\[
I(0) = \int_0^{+\infty} \Phi(y) \, dy,
\]

(4)
while at $T > 0$ K,

$$I(T) = 2\pi k_B T \sum_{k=1}^{\infty} \Phi(y_k),$$  \hspace{1cm} (5)

where $k_B$ is the Boltzmann constant and $y_k$ 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 in the form

$$\Phi(y) = \sum_{j=1}^{M} A_j \exp(p_j y),$$  \hspace{1cm} (6)

where $A_j$ are complex amplitudes and $p_j$ 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:

$$I(T) = -2\pi k_B T \sum_{j=1}^{M} \frac{A_j}{\exp(\pi k_B T p_j) - \exp(-\pi k_B T p_j)},$$  \hspace{1cm} (7)

which for $T = 0$ K gives

$$I(0) = -\sum_{j=1}^{M} \frac{A_j}{p_j}.$$  \hspace{1cm} (8)

3 RESULTS AND DISCUSSION

Numerical studies were performed for an ideal fcc(001) layer stack of the spacer (Cu) and magnetic (Co) layers with the experimental lattice spacing of fcc Cu. The spacer layers can contain the impurities (Zn, Ni, and Au) which form the substitutional alloy with 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 the alloying, for $T = 0$, is the change of the periods of oscillations connected with the change of the corresponding spanning vectors of the alloy Fermi surface (Kudrnovský et al., 1996). The 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 complex exponentials (6), we have evaluated the function $\Phi(y)$ at 40 Matsubara energies corresponding to $T = 25$ 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 $k_\parallel$-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 40000 $k_\parallel$-points in the ISBZ for the first Matsubara energies close to the Fermi energy and the number of $k_\parallel$-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.

\begin{equation}
|\varepsilon_x(q,T)|
\end{equation}

\textbf{Cu} \quad \begin{equation}
|\varepsilon_x(q,T)|
\end{equation}

\textbf{Cu}_{85} \textbf{Ni}_{15}

\begin{equation}
|\varepsilon_x(q,T)|
\end{equation}

\textbf{Cu}_{75} \textbf{Zn}_{25}

\begin{equation}
|\varepsilon_x(q,T)|
\end{equation}

\textbf{Cu}_{50} \textbf{Au}_{50}

Figure 1: Absolute values of the discrete Fourier transformations of $N^2\varepsilon_x(N,T)$ with respect to the spacer thickness $N$ as a function of the temperature $T$ and the wave vector $q$ for a trilayer consisting of semiinfinite Co-slabs sandwiching the spacer with indicated compositions.

The calculations were done for spacer thicknesses $N = 1 - 50$ monolayers and for temperatures $T = 0 - 500$ K (in steps 10 K) and by assuming semiinfinite 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 results (see Drchal et al., 1998) for more details). As an illustration, in Fig. 1
we plot the discrete Fourier transformations (Drchal et al., 1996) of $N^2 \mathcal{E}_x(N,T)$ with respect to $N$, $\mathcal{E}_x(q,T)$, as a function of variables $q$ and $T$. The discrete Fourier transformation on a subset $N \in 10-50$ which avoids the preasymptotic region is employed here. The positions of peaks of $q = q_m$ then determine oscillation periods $p = 2\pi/q_m$, while $|\mathcal{E}_x|$ give oscillation amplitudes (Drchal et al., 1996). In particular, one can see how the modification of the Fermi surface due to alloying changes the temperature dependence of the IEC, i.e., the coefficient $c$ in Eq. (1).

The following conclusions can be drawn from numerical results: (i) The non-random case (Cu) exhibits the 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$_{25}$ alloy are shifted towards higher periods ($p \approx 3.05$ MLs), towards smaller periods for Cu$_{85}$Ni$_{15}$ alloy ($p \approx 2.27$ MLs), while they remain almost unchanged for equiconcentration CuAu 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 Fig. 3 in (d’Albuquerque e Castro et al., 1996) for the case of 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 CuNi and CuAu alloy spacers, while additional exponential damping due to disorder was found for the CuZn alloy. This indicates a finite lifetime of states at the Fermi energy for $k_{||}$-vectors corresponding to short-period oscillations for this case and only a weak damping for CuAu and CuNi alloys; (v) Finally, the effect of temperature (the factor $t(N,T)$ in Eq. (1)) is similar for a pure Cu-spacer, CuNi and CuAu alloys, but it is much smaller for the case of CuZn 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, the combined effect of disorder and temperature leads to a relatively smaller (compared to the case $T = 0$ K) suppression of the oscillation amplitude with the temperature.

Acknowledgment
This work is a part of activities of the Center for Computational Material Science 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 of 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 45.422 and GZ 45.420), and the TMR Network ‘Interface Magnetism’ of the European Commission (Contract No. EMRX-CT96-0089).

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