SURFACES, VACUUM, AND THEIR APPLICATIONS

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On the relation of roughness and the dipolar interaction

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Abstract. We carried out a calculation to compare the strength of the classical dipolar interaction, relative to RKKY, between two ferromagnetic films separated by a paramagnetic spacer. The classical dipolar coupling, which vanishes if the two interfaces are perfectly continuous and flat, builds up strength as the interface roughness grows for several models of interface topography. Numerical estimates show that, in the presence of interface roughness, the dipole–dipole interaction strength is comparable, and at times even larger, than the RKKY interaction. Thus, for rough interfaces the dipolar interaction is an important ingredient to understand experimental results.

The nature of the interlayer coupling mechanism in ferromagnetic (FM)–paramagnetic (PM) multilayer structures has been intensively studied during the last years. They adopt an oscillating magnetic order and exhibit a significant change in magnetoresistance as a function of the thickness of the spacer [1]. Ruderman–Kittel–Kasuya–Yosida (RKKY), superexchange [2], complete confinement[3], and other quantum effects have been suggested as likely candidates to explain this behavior. In the appropriate limits these different approaches have been shown to be equivalent[4], and yield similar interlayer coupling strengths, which reach a maximum energy of a few tenths of an erg/cm^2, in good agreement with experiments[1]. On the other hand, it is taken for granted that the classical dipolar electromagnetic interaction is of negligible magnitude when compared to these quantum mechanical alternatives[1, 5].

Here we perform a critical comparison of the values of the coupling, evaluating the RKKY and dipolar mechanisms for realistic situations which include structural disorder. With increasing interfacial roughness, the RKKY coupling decreases considerably, while the dipolar coupling grows. For certain models of interface roughness, the lower bound of the dipolar interaction is larger than the RKKY coupling and of the same order of magnitude as the experimentally observed values.

We have carried out calculations of both, the RKKY and the dipolar interaction, for an FM/PM/FM trilayer. In these computations we added the contribution of each one of the atoms that participates in the exchange interaction, assuming a particular interface configuration, with a well defined rough structure correlated with the rough structure of the adjacent interface. This roughness correlation has been adopted in view of experimental results[6], which show that certain deposition conditions lead to the formation of parabolic growth fronts, which are crucial to several physical properties.

The RKKY interaction is computed as described earlier[7] and its magnitude is in agreement with experimental[8] and theoretical [9] results for flat interfaces. The dipolar energy, on the other hand, is calculated directly from first principles, *i.e.* using the textbook expression for the magnetic dipole–dipole interaction[10]. This interaction energy per unit area E_{dip}, between the magnetic moments $\vec{m}_i$ and the magnetic moments $\vec{m}_j$ on the opposite interface across the spacer, is given by

$$E_{dip} = \frac{2}{NA} \sum_{i,j} \frac{\vec{m}_i \cdot \vec{m}_j - 3\,(\vec{m}_i \cdot \hat{n})\,(\vec{m}_j \cdot \hat{n})}{r_{i,j}^3} \equiv I\ \mathrm{sign}(\vec{m}_i \cdot \vec{m}_j)\ ,$$

where $\hat{n}$ denotes a unit vector along the direction that connects the magnetic moments $\vec{m}_i$ and $\vec{m}_j$, A is the area of the two-dimensional unit cell and N the number of atoms in one flat interface (*i.e.* without roughness). The factor of 2 is due to the presence of two atoms per area $A = a^2$, on the 100 planes of the fcc structure. In both cases we write the interaction energy as $E \equiv I\ \mathrm{sign}(\vec{m}_i \cdot \vec{m}_j)$ with I defined as the "interaction coupling strength". With this definition, positive coupling strength, $I > 0$, corresponds to antiferromagnetic order (*i.e.* $\vec{m}_i$ antiparallel to $\vec{m}_j$), whereas $I < 0$ implies ferromagnetic order.

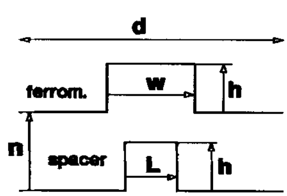

FIGURE 1. Illustration of the spatial parameters that characterize the system: n, h, L, w and d.

The three dimensional system we investigate is illustrated in Fig. 1 and in the insets of the Figs. 2 and 3. It has channels and plateaus along a direction parallel to the interface; the basic module, of length d, which is repeated periodically along the interface is the one shown in the insets. Along the direction orthogonal to the one illustrated, but also parallel to the interface, the system is translationally invariant. Note that the flat atomic planes in the ferromagnet do not contribute to the dipolar interactions. Therefore, only the interface atoms of the ferromagnet were considered. The sums were calculated essentially to infinity (i.e. when the effect was smaller than the computer precision).

The relevant parameters that characterize the interface roughness, illustrated in Fig. 1, are: the repeat unit of the roughness d, the number n of PM spacer layers, the width w of channels and their depth h, the width L of the plateaus and their height, which is also made equal to h. Basically, we have investigated terraced interfacial structures, which seem plausible and consistent with fluctuations of thin film thickness, as experimentally observed and recently reported[6, 11, 12, 13].

The physical parameters we adopted correspond to a Co/Cu/Co trilayer, grown along the 100 face, with an fcc lattice parameter $a = 3.6$ Å, a magnetic moment $|\vec{m}_k| = 1.76\mu_B$ (Bohr magnetons) for Co, $k_F = 1.36$ (Å)$^{-1}$ for the Fermi wavevector and $J = 1$ eV [9, 14] for the exchange interaction between magnetic moments. The magnetic moments are assumed to be parallel to the principal interface and along the 100–direction.

Fig. 2 shows the RKKY and the dipolar magnetic exchange coupling strengths for a terraced surface. The dependence of I as a function of L, with $n = 7$, $h = 5$, $d = 40$ and $w = 20$, is also interesting (see Fig. 3). For these values of the parameters the dipolar strength increases faster, and becomes larger, than the RKKY strength, with growing n. We point out that even for $h = 2$, coupling strengths as large as 0.05 erg/cm^2 are obtained, so this is a non negligible effect even for almost perfect interfaces.

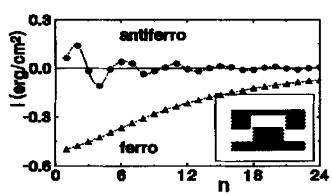

FIGURE 2. Interaction coupling strength I *versus* the number n of PM spacer layers, with $h = 10$, $L = 16$, $w = 20$ and $d = 40$ (in units of $a/2 = 1.8$ Å), for RKKY (circles) and dipolar (triangles) coupling. The inset depicts the structure of the plateaus and channels of the interface for $n = 7$ and illustrates the meaning of h, L, w and d.

With the parameters used here, the implication is that the PM layers have an impurity concentration of FM atoms of $\approx 10\%$ *on the average.* All in all, the RKKY interaction is smeared out due to the variation in the relative orientations of the spins, whereas the dipolar interaction is reinforced by roughness effects.

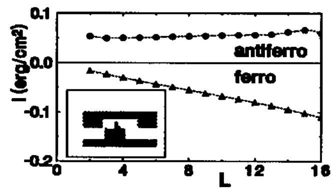

FIGURE 3. Interaction coupling strength I *versus* L, for $n = 7$, $h = 5$, $d = 40$ and $w = 20$, for RKKY (circles) and dipolar (triangles) coupling. The inset, which corresponds to $L = 11$, depicts the structure of the periodic plateaus and valleys of the interface and illustrates the meaning of L, n, h, w and d.

In conclusion, a simple model calculation was carried out to estimate and compare the magnitudes of the dipolar and RKKY interaction strength between magnetic layers separated by a non–magnetic spacer. Special attention was given to the interplay of coupling strength and interface roughness, since surface defects depress the strength of the RKKY interaction, while enhancing the dipolar one.

The results of our computation show that, in the presence of interface roughness, the dipolar interaction energy is of the same order of magnitude as RKKY. These results imply that quantitative structural studies at the atomic level are essential for a meaningful and complete comparison of experiment and theory of magnetic coupling in these systems.

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