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To cite this version:
M. Afsharnaderi, J. Mathon. ANTIFERROMAGNETIC COUPLING OF SURFACE LOCAL MOMENT TO A STRONGLY FERROMAGNETIC SUBSTRATE. Journal de Physique Colloques, 1988, 49 (C8), pp.C8-1641-C8-1642. 10.1051/jphyscol:19888750. jpa-00228993

HAL Id: jpa-00228993
https://hal.archives-ouvertes.fr/jpa-00228993
Submitted on 1 Jan 1988

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ANTIFERROMAGNETIC COUPLING OF SURFACE LOCAL MOMENT TO A STRONGLY FERROMAGNETIC SUBSTRATE

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Abstract. The exchange coupling $J_\perp$ of a surface local moment to a strongly ferromagnetic surface is calculated in RPA using a tight binding model. $J_\perp$ is shown to decrease rapidly with increasing impurity occupancy $n$ and there is a critical $n^*$ for which $J_\perp$ becomes antiferromagnetic. The model is used to discuss Bergmann’s measurements for Fe and Ni impurities on Pd and the observed weakening of exchange for Fe on the surface of FeNiB0.5 glass.

It was shown in [1, 2] that the surface-bulk exchange $J_\perp$ of a ferromagnet can be determined from the measured temperature dependence of the surface magnetisation. It is found [1] that $J_\perp$ in FeNiB0.5 glass depends critically on the chemistry of the surface and is weakened even for bulk-like composition. A very small $J_\perp$ is also found for Fe surface [3]. Another independent evidence for a weakening of $J_\perp$ comes from Bergmann’s measurements [4] for Fe impurities on the surface of Pd. Although Fe in Pd forms a giant moment $\sim 10 \mu_B$, he found no moment on Pd surface. Since the conditions for formation of a surface moment are even more favourable than in the bulk [5], the most likely explanation for the absence of moment is that Fe-Pd exchange is either very weak or even antiferromagnetic.

To gain some insight into the microscopic origin of the observed surface softening of exchange, we have examined the dependence of the surface impurity-substrate exchange $J_\perp$ on the local band structure. To make the calculation tractable, we model the impurity by a single atomic orbital with an intra-atomic Coulomb repulsion $U^i$. The substrate is a strong ferromagnet with the majority band full and with $n$ holes in the minority band. It is described in the tight binding approximation. For a surface impurity in the atop position labelled by $i = a$, the impurity-substrate Hamiltonian is $H = H_i + H_s + H_{i,s}$, where

$$H_i = \sum_{\alpha} c_{i\alpha}^{\dagger} c_{i\alpha} (V + U^i c_{i\alpha}^{\dagger} c_{a,-\alpha}) = \sum_{\alpha} c_{i\alpha}^{\dagger} c_{i\alpha} V (V + U^i),$$

$$H_s = \sum_{i,\sigma} c_{i\sigma}^{\dagger} c_{i\sigma} (V_i + U^i c_{i\sigma}^{\dagger} c_{a,-\sigma}) + \sum_{i,j,\sigma} t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma},$$

$$H_{i,s} = \sum_{\sigma} t (c_{a\sigma}^{\dagger} c_{i\sigma} + c_{i\sigma}^{\dagger} c_{a\sigma}).$$

Here, $c_{i\sigma}^{\dagger}$, $c_{i\sigma}$ are the creation and annihilation operators of a hole of spin $\sigma$ in an atomic orbital at a site $i$, $V$ is the impurity energy level, $V_i$ are the substrate atomic levels, $U$ is the substrate intra-atomic repulsion, $t_0$ is the substrate hopping and $t$ is the impurity-substrate hopping. All five d bands in the substrate are degenerate in this model and s-p band is neglected. The impurity hopping is to a single orbital 0 below the impurity. The energy level $V_0$ of the orbital 0 is allowed to deviate from the level $V_a$ of all the other surface atoms. The level $V_4$ itself is different from the bulk $V_a$ which is taken to be zero.

This model is very similar to that used in [6] to discuss chemisorption on the surface of ferromagnetic iron. We shall apply it to Fe impurities on Ni surface to model an uneven or doped surface of FeNiB0.5 glass and also to investigate the stability of the assumed ferromagnetic ground state of Fe impurities on Pd surface.

The energy required to deviate the impurity spin from its ground-state direction can be calculated by perturbation theory. For small deviations, the effective exchange coupling $J_\perp$ between local moments at the impurity orbital a and the substrate orbital 0 is proportional to the matrix element $\chi_{a0}^+$ of the Hartree-Fock (HF) transverse susceptibility [7]. We shall measure $J_\perp$ relative to the bulk nearest-neighbour exchange $J \propto \chi^{-1}$, where $\chi^{-1}$ is the matrix element of the susceptibility between nearest neighbours in the substrate.

$$\chi_{nm}^{+} = - (1/\pi) \text{Im} \int_{-\infty}^{E_F} G_{nm}(E) G_{nm}^+(E) dE,$$

where $E_F$ is the Fermi energy and $G_{nm}^+$ are the matrix elements of the HF one-electron Green functions between sites $n$, $m$. To obtain $G$, it is necessary to solve first the self-consistent HF ground-state problem. The HF occupations of all the sites which enter the HF potential are themselves determined by the local $G^\sigma$. The calculation of $G^\sigma$ is in two stages. First $G_{nm}^{0\sigma}$ for $H_i + H_s$ is obtained and then the effect of $H_{i,s}$ is included by solving the Dyson equation $G^{\sigma} = G^{0\sigma} + G^{0\sigma} H_{i,s} G^{\sigma}$. It is easy to show [6] that $G_{nn}$ on the impurity orbital is given by

$$G_{nn}^\sigma (E) = (E - V^\sigma - t^2 G_{00}^{0\sigma} (E))^{-1},$$

where $V^\sigma = V + U^i (c_{i\sigma}^{\dagger} c_{a,-\sigma})$ and the local $G_{00}^{0\sigma}$ on the substrate orbital 0 is expressed in terms of the
diagonal element of $G$ in the surface plane, i.e. $G_{\text{surf}}^{\sigma}$

$$G_{\text{surf}}^{\sigma} (E) = G_{\text{surf}}^{\sigma} (E) \left( 1 - (V_0^\sigma - V_0^\sigma) G_{\text{surf}}^{\sigma} (E) \right)^{-1}.$$  

(4)

Here, $V_0^\sigma$ is the spin-dependent HF potential on the orbital 0. The off-diagonal elements of $G$ required in equation (2) are obtained by the same method.

In calculating the ground state, the bulk parameters $E_F$ and $U$ were fixed to give $n = 0.12$ for Ni and 0.07 for Pd (1/5 of the bulk number of holes) and the correct exchange splitting $\Delta$ ($\Delta = 2t_0$ for polarised Pd was assumed, i.e. just strong). The surface potential $V_s$ was chosen to obtain the same surface occupancy as in the bulk. $V_s$ at the orbital 0 was adjusted to keep this atom neutral. Finally, $V$ was chosen to attract the correct number of carriers $n^i = n^i_+ + n^i_-$ to screen the excess impurity charge. This leaves $t$ and $n^i$ as the only free parameters in the problem ($t_0$ determines just the energy scale; all energies are measured in units of $6t_0$).

The whole $(n^i, t)$-plane can be divided into regions with and without impurity bound states [6]. Outside the region of bound states, the impurity-substrate system is a strong ferromagnet. This is because there cannot be delocalised majority hole states in a strongly ferromagnetic substrate. A typical dependence of the impurity-substrate exchange $J_\perp$ on $n^i/n$ in this region is shown in figure 1 for Ni substrate with $\Delta = 6t_0$ and $t = t_0$. (Note that $n^i = n^i_+$ since $n^i_- = 0$). It can be seen that $J_\perp$ decreases rapidly with increasing $n^i$. This suggests that $J_\perp$ might become negative for even larger $n^i$ than those shown in figure 1, thus indicating instability of the ferromagnetic ground state. The total impurity occupancy $n^i \sim 0.8$ required to model Fe impurity ($5 \times 0.8 = 4$ holes/atom) cannot be achieved without creating impurity bound states. In the presence of bound states, equation (2) is not applicable and the ground state must be recalculated. Bound states correspond to poles of Re$G_{\text{surf}}^{\sigma}$ outside the substrate band. It is easy to see from equation (3) that a hole bound state first appears for the minority band. The impurity-substrate system with such a bound state remains strongly ferromagnetic ($n^i_- = 0$) and $n^i_+$ continues to increase with increasing strength of the attractive potential $V_s^i$ on the impurity. This is illustrated in figure 2 for $t = 5$ and $6t_0$ and Pd substrate (hopping to 5-6 neighbours [9]).

The situation changes dramatically when a bound majority hole state first appears. This is indicated by arrows in figure 2. The strongly ferromagnetic state becomes unstable and there are now three selfconsistent solutions for $n^i_+$: non-magnetic, ferromagnetic and antiferromagnetic (impurity moment is antiparallel to the substrate moment). The antiferromagnetic solution has the lowest energy. When it first appears, the impurity moment is close to zero.

We can now discuss Bergmann's measurements. For $n^i$ close to $n$, i.e. for Ni impurities on Pd surface, Ni forms a local moment and its coupling to the moment induced in the substrate is ferromagnetic (Fig. 1), as observed [8]. For $n^i \sim 0.8$ (Fe impurity), the ferromagnetic state becomes unstable and the impurity moment collapses, which explains the absence of Fe moment on Pd reported by Bergmann [4].

Finally, figure 1 demonstrates that the perpendicular exchange of an Fe atom is very much weaker than in the bulk when the number of its magnetic neighbours is reduced. This may happen for a defective or doped surface of FeNiB_{0.5} glass [1].

Fig. 1. – Dependence of the impurity-substrate exchange $J_\perp/J$ on $n^i/n$.