Antiferromagnetic coupling at the surface of a rare-earth metal

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A condition under which the surface and bulk magnetic moments of a rare- earth metal are antiparallel is derived in a simple $s(f)$ model.

Recent experiments involving spin-polarized electrons and the Kerr magneto-optic effect have shown that the moment of the surface atomic layer Gd(0001) is antiparallel to the bulk moment at $T < T_{cv} = 293$ K, where T_{cv} is the bulk Curie temperature.[1,2] Previous descriptions of this effect have used the Ising model, in which it was simply assumed that the exchange integral between a surface atom and the nearest atom of the second layer, J_{12}, was negative.[3] That approach will obviously not reveal the mechanism for the effect. In the present letter we offer a physical interpretation of the experimental data of Refs. 1 and 2 on the basis of a simple $s(f)$ model in which the interaction between the highly localized, rigid $4f$ moments occurs through the s band. We assume that the main reason for the change in the interaction of the $4f$ moments near the surface of a metal, and thus the main reason for the antiferromag-

netic coupling at the surface, is that the susceptibility of the s electrons depends on the index of the atomic layer and on the Fermi level, as the result of an interference of s-electron waves incident on the surface and reflected from it.

The ferromagnetic volume, i.e., the $4f$ moments starting with the second layer, is induced in the linear approximation on the basis of JS (J is the contact exchange interaction of the $4f$ moments with the s electrons, and S is the spin of the $4f$ moment). The moment (per site) of the s electrons at the surface, m_1, is

$$m_1 = \sum_{l=2} m_{1l} = 2JS(g_1(\mu) - \varphi_1(\mu)). \tag{1}$$

Here m_{1l} is the moment of the s electrons in the first layer which is induced by the $4f$ moments of layer l; $g_1(\mu)$ is the unperturbed density of states or the Pauli susceptibility of the s electrons of the first layer; and $\varphi_1(\mu)$ is the unperturbed susceptibility of the s electrons of the first layer if the field is applied to only this layer. The expression for the moment (m_1) of the s electrons at the surface induced by the bulk $4f$ moments can be clarified in the following way. The JS field of the ferromagnetically ordered "up" $4f$ moments is applied to the entire crystal, including the surface. As a result, the s electrons at the surface acquire a moment $m_1^{\uparrow} = 2JSg_1(\mu)$. We then subtract the contribution $2JS\varphi_1(\mu)$, from the local field created by the $4f$ moments of the surface atomic layer alone. It follows from (1) that under the condition

$$\varphi_1(\mu) > g_1(\mu) \tag{2}$$

the moment of the s electrons in the first atomic layer which is induced by the volume is antiparallel to the moment in the volume [$m_v = 2JSg_v(\mu)$, where $g_v(\mu)$ is the density of s-electron states in the interior]. We assume for simplicity that when the surface $4f$ moment flips "down," i.e., upon a surface perturbation $-2JS$, no s-electron surface states of the Tamm type arise, since such states could have only a negligible fraction of the s electrons (because of the small value of J). These states could thus have only a minor effect on the value of φ_1. The moment of the s electrons at the surface thus becomes equal to $m_1^{\downarrow} = 2JS[g_1(\mu) - 2\varphi_1(\mu)]$. The correction to the energy of the system for the difference between the diagonal elements of the interaction of the s electrons and the $4f$ moments in the cases of antiparallel and parallel orientations of the surface and bulk $4f$ moments becomes

$$\Delta E = E^{\downarrow\uparrow} - E^{\uparrow\uparrow} = JSN(m_1^{\downarrow} + m_1^{\uparrow}) = 4J^2S^2N(g_1(\mu) - \varphi_1(\mu)). \tag{3}$$

Here N is the number of sites in the layer. It can be seen from (3) that the satisfaction of condition (2) is advantageous in terms of the energy of the system in the case of an antiparallel orientation. Condition (2) is thus the condition under which the surface and bulk moments of a $4f$ metal are antiparallel. The condition under which the ferromagnetic state is energetically favored in the interior, as in the case of Gd, must of course be satisfied.

Different electronic states make a contribution to $\varphi_1(\mu)$, which is proportional to $\sin^2(\kappa\Delta)$, where Δ is the distance between planes, and κ is the wave number of the transverse mode, because of an interference. The largest contribution comes from states for which the relation $\kappa\Delta \sim \pi/2$ holds. They increase the surface density of

states, $g_1(\mu)$, in comparison with the bulk density of states, $g_v(\mu)$. Consequently, under condition (2), we would simultaneously expect

$$g_1(\mu) \gtrsim g_v(\mu). \tag{4}$$

As a result, the difference between the energies in the ferromagnetic and paramagnetic states of the entire crystal, per surface site, is $E = -J^2S^2g_1(\mu)$. It is smaller than the corresponding figure for the volume, $E_{fm} = -J^2S^2g_v(\mu)$. On the other hand, the energy of the effective interaction of an atom of the first layer with the others, starting with the second layer, is positive in the ferromagnetic state, and is given by $E_{1v} = -\Delta E/(2N)$. Consequently, the fact that $g_1(\mu)$ is larger than $g_v(\mu)$, with allowance for the smaller number of neighbors at the surface, indicates that the effective exchange parameters at the surface are larger than those in the interior. This circumstance was used in Refs. 3–5 for an Ising-model description of the surface magnetism of Gd(0001): $T_{cs} = 315$ K $> T_{cv} = 293$ K.

To verify that condition (2) can be satisfied, we examine the s electrons in the strong-coupling model. Here we can take the boundary of the crystal into account in a systematic way. In this case the Hamiltonian of the s electrons without an interaction can be diagonalized easily by going over from a site representation to a representation of traveling and standing waves. We consider a simple cube with a surface corresponding to the (100) face, for which the condition for the appearance of Tamm states in our case is $|2JS| > |B|$, where B is the amplitude for the jump of an s electron between nearest sites. Under the assumption that this condition does not hold, we can determine the unperturbed local susceptibility:

$$\varphi_1(\mu) = \frac{4}{(L+1)^2}\sum_{q_1q_2}\sin^2\frac{\pi q_1}{L+1}\sin^2\frac{\pi q_2}{L+1}\frac{n_{q_2}-n_{q_1}}{2B(\cos\frac{\pi q_1}{L+1}-\cos\frac{\pi q_2}{L+2})}$$

$$= \frac{-4}{B(L+1)}\sum_q \sin^2\frac{\pi q}{L+1}\cos\frac{\pi q}{L+1}n_q. \tag{5}$$

Here q is the index of the standing-wave mode ($q = 1,2,...,L$), L is the number of layers, and $n_q = 1/N\Sigma_{\vec{k}}n_{\vec{k}q}$, where $\vec{k}$ is the quasimomentum from the 2D Brillouin zone. It is also a straightforward matter to derive an expression for the unknown energy ΔE. When an expansion is carried out up to J^2, this expression is the same as (3), with $\varphi_1(\mu)$ from (5). The densities of states are

$$g_1(\mu) = \frac{2}{L+1}\sum_q \sin^2\frac{\pi q}{L+1}\frac{1}{N}\sum_{\vec{k}}\delta(\mu-\epsilon_{\vec{k}q}),\quad g_v(\mu) = \frac{1}{LN}\sum_{q\vec{k}}\delta(\mu-\epsilon_{\vec{k}q}),$$

$$\epsilon_{\vec{k}q} = 2B(\cos k_x\Delta + \cos k_y\Delta + \cos\frac{\pi q}{L+1}).$$

Figure 1 shows plots of $g_1(\mu)$,$\varphi_1(\mu)$, and $q_v(\mu)$. We see that the antiparallel orientation is energetically favorable under the conditions $1 \lesssim |\mu| \lesssim 2$ and $|\mu| \lesssim 0.6$. Condition (4) does indeed hold. From this figure we find $|E_{1v}/2E| = \varphi_1 - g_1/g_1| \ll 1$. This result

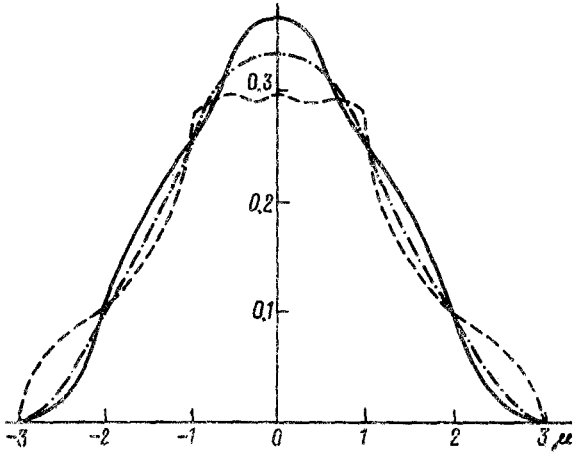

FIG. 1. The bulk density of states g_v (dashed line), the surface density of states g_1 (dot-dashed line), and the local surface susceptibility φ_1 (solid line) versus the position of the Fermi level, μ, in the s band. All quantities are expressed in units of $2|B|$.

indicates that the coupling of the $4f$ moments of the first layer with the bulk moments is weak.

At finite values of JS, a detailed analysis of whether the ferromagnetic state of the volume is energetically favored in comparison with other states is a complicated matter. Such an analysis goes beyond the scope of the present paper. We would, however, like to point out that an antiferromagnetic state of the interior is energetically favorable at values $|\mu| \lesssim 0.6$. In the quadratic approximation in J, the state energy per site is $E_{af} = -J^2S^2\chi(\vec{k}_0)$, where $\vec{k}_0 = \pi/\Delta(1,1,1)$. Since $\chi(\vec{k}_0) = -\int^{\mu}[g_v(\epsilon)/\epsilon]d\epsilon$ diverges logarithmically as $|\mu| \to 0$, we find a disruption of the zone at finite JS and the formation of an antiferromagnetic gap with a width $2|J|S$. At small values of $|\mu|$, we thus have $g_v(\mu) < \chi(\vec{k}_0)$ and therefore $E_{af} < E_{fm}$. It thus appears that an antiparallel orientation of the surface and bulk moments would actually be possible only in the interval $1 \lesssim |\mu| \lesssim 2$.

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