RKKY interactions across yttrium layers in Gd-Y superlattices

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A simple calculation of the RKKY coupling between two Gd arrays in a Gd-Y superlattice is presented. The calculation is valid for Gd arrays consisting of a single atomic layer. The Fourier transform $J(\mathbf{q})$ of the exchange interaction between two Gd layers separated by Y is taken to be that of Gd layers embedded in an Y matrix. Plausible arguments are given in support of this procedure. The coupling is calculated by making use only of the measured $J(\mathbf{q})$ in bulk Gd and of the calculated generalized susceptibilities of Gd and Y. The coupling is found to be of fairly long range and to be consistent in sign with recent neutron scattering measurements of long-range order in Gd-Y superlattices. Numerical calculations on a model, one-dimensional superlattice with two free-electron metals of different electron densities have not provided a useful guide for calculating RKKY interactions in superlattices and further theoretical work is necessary.

The magnetic properties of metallic superlattices, one constituent of which is magnetic, are currently the object of study in several laboratories. In particular, the field and temperature dependence of the magnetization of multilayers of Gd_M Y_N (repeating units of M layers of Gd followed by N layers of Y) have been investigated[1] in this laboratory for values of N as small as 5. One of the intriguing questions that arise is whether the RKKY coupling between two Gd arrays that takes place through the intervening Y layers is significant enough to produce coherence between the magnetizations of successive Gd arrays. An *a priori* theoretical way to answer this question would be to do a self-consistent band-structure calculation of the superlattice, to calculate the *s-f* exchange interaction j_{sf} with this composite band structure and finally to calculate the RKKY interaction across the Y layers. This is a very ambitious program which will not be attempted here; instead we will make a first step toward estimating the magnitude of the coupling, which is based on some observations of the Gd-Y system and on physical intuition.

First, because Gd and Y have very similar lattice parameters, the strain in the superlattice (which is grown normal to the hexagonal planes) will be small and the values of the lattice parameters will be similar to those of bulk Gd or Y.

Second, even for values of M and N as small as 3 and 5, the measured Curie temperatures are found to be close to that of the bulk, and deviations from this value can be understood by assuming that the exchange interactions between Gd ions in an array are *the same* as in bulk Gd, and by taking into account the finiteness of the number of layers in the array and the fact that the RKKY interactions in Gd are of moderately long range.[2] It is as though the propagation of the conduction electrons through the superlattice does not affect the magnitude of the exchange coupling between two Gd ions when they are both in the same array of M layers. It seems reasonable then to assume that the exchange coupling between Gd ions in adjacent arrays, which takes place through the intervening Y layers, is also not affected by the superlattice band structure.

Based on these observations we can now make a simplified calculation of the coupling between two Gd atomic layers separated by N layers of Y (the method is not directly applicable to Gd layers beyond the interface): We compute this coupling as if (a) the two Gd layers are embedded in an infinite Y matrix, and (b) the *s-f* exchange interaction on a Gd ion is the same as it is in bulk Gd. As will be seen below, by making these two assumptions we circumvent the need to do any *a priori* calculations and the coupling across Y layers can be simply calculated by making use of existing measurements of $J(\mathbf{q})_{\mathrm{Gd}}$ in bulk Gd and of published calculations of $\chi(\mathbf{q})_{\mathrm{Gd}}$ and $\chi(\mathbf{q})_{\mathrm{Y}}$, the wave-vector-dependent susceptibilities of Gd and Y. (The subscript on a physical quantity indicates the metal to which it refers.)

A good discussion of indirect exchange interactions in the rare-earth metals, which can be consulted for general background and notation, is given in the review article by Freeman[3]: Briefly, consider $J(\mathbf{q})$, the Fourier transform of the exchange interaction between two localized spins. In the usual approximation of replacing the $\mathbf{k}$ and $\mathbf{k}'$ dependent *s-f* exchange integral $j_{sf}(\mathbf{k},\mathbf{k}')$ by $j_{sf}(\mathbf{q})$ which depends only on $\mathbf{q}=\mathbf{k}'-\mathbf{k}$ the quantity $J(\mathbf{q})_{\mathrm{Gd}}$ is given, to within a numerical factor, by

$$J(\mathbf{q})_{\mathrm{Gd}} = |j_{sf}(\mathbf{q})_{\mathrm{Gd}}{}^2|\chi(\mathbf{q})_{\mathrm{Gd}}. \tag{1}$$

The two assumptions made above amount to the following ansatz for the exchange coupling function $J(\mathbf{q})_{\mathrm{Gd\text{-}Y}}$ of Gd ions in a Y matrix:

$$J(\mathbf{q})_{\mathrm{Gd\text{-}Y}} = |j_{sf}(\mathbf{q})_{\mathrm{Gd}}|^2\chi(\mathbf{q})_{\mathrm{Y}}. \tag{2}$$

Once $J(\mathbf{q})_{\mathrm{Gd\text{-}Y}}$ is known the interplanar coupling is calculated as follows: Since the hexagonal layers are stacked normal to the c axis, only a knowledge of $J(\mathbf{q})$ where $\mathbf{q}$ is along the c axis is needed. Bearing in mind that the hcp structure is made of two interpenetrating simple hexagonal lattices, the distance between adjacent planes is $c/2$ where c is the primitive displacement. The interlayer exchange interaction $J(N)$ between layers that are a distance $(N+1)c/2$ apart (or separated by N layers) is then given by[4]

$$J(N) = \frac{c}{2\pi}\int_0^{2\pi/c} J(q)\cos[(N+1)cq/2]\,dq. \tag{3}$$

The precise meaning of $J(N)$ is that it is the sum of the exchange interactions between each spin of one Gd layer and

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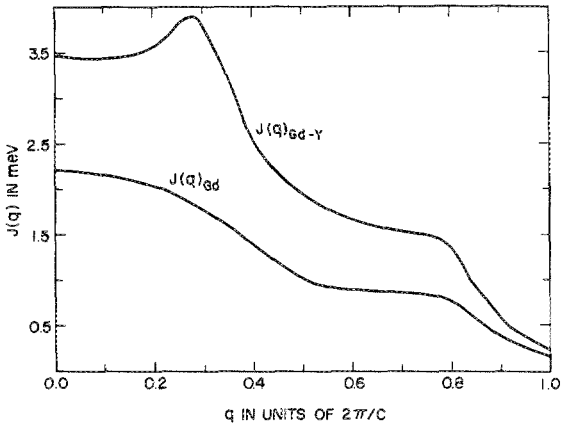

FIG. 1. Functions $J(\mathbf{q})_{\text{Gd-Y}}$ and $J(\mathbf{q})_{\text{Gd}}$ in meV, calculated as described in the text. The wave vector q is normal to the hexagonal plane. The maximum of $J(\mathbf{q})_{\text{Gd-Y}}$ is at $q_{\max} = 0.28 \times 2\pi/c$ as deduced in Ref. 2.

any given spin in the other Gd layer. It is essentially the coupling coefficient between layers considered as sublattices.

We now return to the determination of $J(\mathbf{q})_{\text{Gd-Y}}$. The function $J(\mathbf{q})_{\text{Gd}}$ for $\mathbf{q}$ along the c axis was measured in Ref. 2. The susceptibility functions $\chi(\mathbf{q})$ for Gd and Y were calculated in a paper by Liu *et al.*[5] For Y, a sharp maximum in $\chi(\mathbf{q})$ at $q \simeq 0.4 \times 2\pi/c$ is predicted. Making use of these data, we have numerically calculated $J(\mathbf{q})_{\text{Gd-Y}}$ by simply multiplying $J(\mathbf{q})_{\text{Gd}}$ by the ratio $\chi(\mathbf{q})_{\text{Y}}/\chi(\mathbf{q})_{\text{Gd}}$ which was obtained from the published graphs[5] of these functions. The resulting $J(\mathbf{q})_{\text{Gd-Y}}$ shows a maximum at $q_{\max} = 0.36\pi \times 2\pi/c$, which originates from the maximum of $\chi(\mathbf{q})_{\text{Y}}$. Recent experimental work[6] indicates that the maximum is instead at $q_{\max} = 0.28 \times 2\pi/c$. We have accordingly modified the calculated $J(\mathbf{q})_{\text{Gd-Y}}$ by smoothly shifting the peak to the experimental value. The result is shown in Fig. 1, together with the $J(\mathbf{q})_{\text{Gd}}$ of Ref. 2.

Note that $J(\mathbf{q})_{\text{Gd-Y}}$ is larger than $J(\mathbf{q})_{\text{Gd}}$ for all q values, which leads us to expect larger interactions across Y layers than across the same number of Gd layers. This suggests also that the interactions between Gd ions in a Y matrix are stronger than those in bulk Gd. A recent paper[7] on YGd alloys gives some evidence that this is true. Extrapolation of the straight line of Fig. 2 in Ref. 7 to 100% Gd gives an ordering temperature of 450 °K which is about a factor 1.5 the Curie temperature of bulk Gd. This factor is a rough measure of the relative magnitudes of the exchange couplings that take place via the Y and Gd conduction bands, respectively.

By substituting the function $J(\mathbf{q})_{\text{Gd-Y}}$ in Eq. (3) we have obtained numerically the interlayer interactions $J(N)_{\text{Gd-Y}}$. These are listed in Table I where, for comparison purposes, we have also shown the $J(N)_{\text{Gd}}$ of bulk Gd. The $J(N)_{\text{Gd}}$ are seen to be negligible for $N \geqslant 5$, a fact which presumably is due to the structureless character of $J(\mathbf{q})_{\text{Gd}}$ and the resulting destructive interference in the range function at moderately large N. By contrast, the $J(N)_{\text{Gd-Y}}$ are more than an order of magnitude larger in the range $N = 5$–10, being positive for $N = 5$–7 and negative for $N = 8$–10. In order to exhibit more fully the behavior of the range function for this case, we have calculated, using (3), the Fourier transform of $J(\mathbf{q})_{\text{Gd-Y}}$ for a continuous range of values of the distance z and plotted the result, $J[(z - c/2)/(c/2)]_{\text{Gd-Y}} \equiv j(z)$, in Fig. 2. Notice the well-defined oscillation between $N = 4$ and $N = 11$, with a wavelength of $\lambda \simeq 7(c/2)$. This value of λ corresponds to the position of the maximum ($q_{\max} = 0.28 \times 2\pi/c$) of $J(\mathbf{q})_{\text{Gd-Y}}$. Beyond $N = 11$, destructive interference from the continuum of q values in $J(\mathbf{q})_{\text{Gd-Y}}$ seems to set in and $j(z)$ remains appreciably smaller.

Recent experiments[8] show that for separations of $N = 6$ and 10, successive arrays of Gd order respectively parallel and antiparallel to each other, in agreement with the signs of $j(z)$ calculated in Fig. 2. Our model is thus consistent with experiment.

In the case that the magnetic component of the superlattice is ferromagnetic (such as Gd) and if interactions between Gd arrays that are beyond nearest neighbors are neglected, then the coupling through the intervening Y can only lead to parallel or antiparallel ordering in the superlattice.

However, the RKKY interaction can also lead to long-range coherence between helical configurations of spins, as observed in the work of Salamon *et al.*[9] in Dy-Y multilayers: Consider a Dy array next to an Y array. The exchange field

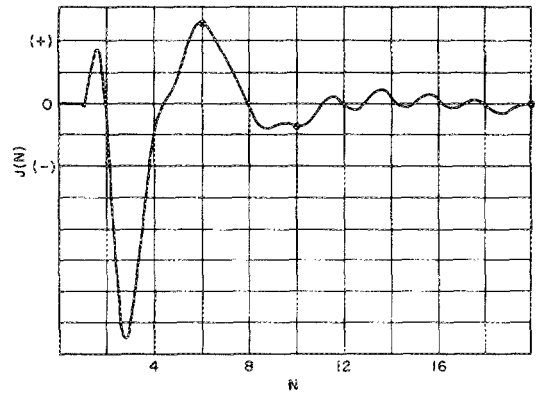

FIG. 2. Range function of the RKKY interaction along the c axis for Gd ions embedded in Y. The abscissa shows the number of Y atomic layers separating the Gd. The ordinate is $J(N)$ [or more accurately, the function $j(z)$ defined in the text, which equals $J(N)$ at $z = (N + 1)c/2$]. One vertical division corresponds to 0.025 meV.

TABLE I. Calculated interlayer interactions in meV. The $J(N)_{\text{Gd-Y}}$ are the interplanar interactions between single Gd layers embedded in an Y matrix. For comparison the $J(N)_{\text{Gd}}$ of bulk Gd are listed in the last column. Our values of $J(N)_{\text{Gd}}$ are half of those listed in Ref. 2 because the latter lists the sum for the two layers on either side of the reference layer.

Number of Y layer (N)	$J(N)_{\text{Gd-Y}}$	$J(N)_{\text{Gd}}$
1	−0.0027	0.0454
2	−0.0253	0.0460
3	−0.1792	−0.0663
4	−0.0197	0.0182
5	0.0245	0.0007
6	0.0646	0.0015
7	0.0324	0.0002
8	−0.0039	−0.0030
9	−0.0183	0.0037
10	−0.0174	0.0014

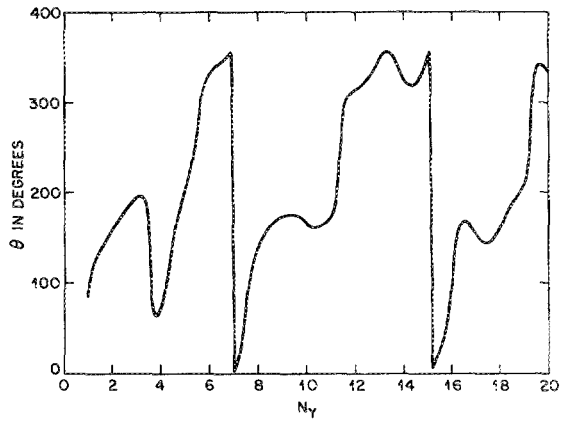

FIG. 3. Turn angle θ of the exchange field seen by a Dy atomic layer separated from the previous Dy array by N_Y atomic layers of Y. The values of θ have physical meaning only at integral values of N_Y. θ, which is continuous, is plotted modulo 2π.

induced at an Y lattice site will be the vector sum of the exchange fields induced by *all* the atomic layers of Dy. Since the directions of the moment in successive Dy layers differ by the pitch angle in Dy, these exchange fields at an Y site will point in correspondingly different directions and also have *different phases*. Because of these phase differences the total exchange field will have the character of an elliptically polarized field as it propagates through the Y medium. The direction of rotation is determined by the helicity of the magnetization in the Dy array. As the exchange field reaches the next Dy array, it acts on this array with this same direction of rotation and thus causes the helicity in this array to be the same as in the preceding Dy array. In this way, the RKKY coupling can lead to long-range coherence of helical orderings in multilayers. We are not prepared to say whether this is the actual explanation of the results of Ref. 9, but only that it offers an alternative explanation for what we believe is still an open question.

We have used our model to compute the magnitude and the angle θ that the exchange field at an Y layer makes with the direction of the moment at the Dy interface. For simplicity, only the RKKY contributions from the two Dy layers closest to the Y were included. The exchange coupling function of Dy,[10] multiplied by the ratio of the susceptibilities of Y and Dy, was used to calculate the exchange fields at the Y sites. Figure 3 shows the angle θ at successive Y layers. It is seen that θ increases by 360° in approximately seven layers, which, as expected, corresponds to the value of q_{max} of the Y susceptibility. The wiggles in the curve result from the interference of the two maxima of $J(q)$ in Dy (Ref. 10) and spoil the simple picture of a smoothly increasing rotation angle, leading possibly even to loss of coherence in the helicity. The magnitude of the exchange field is of order 11 and 4 kG at separations of 9 and 13 layers of Y, respectively. We emphasize that these numbers are obtained with our very simplified model and can be taken only as possible guides.

Since there are no superlattice band-structure calculations that could be used to interpret the present data, we have considered a model, one-dimensional bilayer superlattice whose constituents A, B are two free-electron metals with different electronic densities, n_A and n_B. This difference was imposed by introducing a potential jump V_0 at the interface of A and B. Numerical calculations done with this model have shown that the superlattice wave functions, which are obtained by satisfying the boundary conditions at the potential jump and by imposing periodicity conditions, can have quite unequal mean values of the amplitude squared, $|\Psi_A|^2$ and $|\Psi_B|^2$ in the two constituents. The ratio $Q = |\Psi_A|^2/\Psi_B|^2$ becomes, at moderately large values of V_0, a strong function of the energy of the state. As a result, the RKKY interaction calculated with the eigenfunctions of the superlattice becomes dependent on the value of V_0 in such a way that no useful guide to the experimental results can be obtained.

Actually this free-electron model bears little resemblance to the Gd-Y system in which both constituents have three valence electrons. In addition,[11] band-structure calculations give very closely the same value, 0.34 Ry, for the occupied part of the valence band in both metals. The difference in their $\chi(\mathbf{q})$ arises from a difference in their respective pseudo-potentials and a consequent nesting feature in Y. It is unlikely that substantial transfers of charge occur, upon superlattice formation, between the two metals at specific points of the Brillouin zone, except possibly at $\mathbf{q}$ values close to the nesting region. Clearly more theoretical work is needed in order to understand how the electronic states are affected by superlattice formation.

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