Surface spin reorientation in thin Gd films on Fe in an applied magnetic field

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We investigate the magnetic system of a few layers of Gd on bulk Fe in the presence of a magnetic field using mean-field theory and a simple model. At moderate temperatures and low fields the system is in an aligned state where all the Fe spins point along the field direction and, because of the antiferromagnetic coupling of the Fe spins to the Gd spins, all the Gd spins are antiparallel to the field. For higher fields there is a phase transition to a twisted spin state where the Fe and Gd spins near the interface are at an angle with respect to the applied field.

A recent paper[1] has studied the system of a few layers of the rare-earth metal Gd deposited on the transition-metal Fe. In this situation the Fe spins interact ferromagnetically among themselves but couple antiferromagnetically to the Gd spins. There has been some discussion regarding how the Gd spins should couple to each other. Weller *et al.*[2] claim that the first layer of Gd couples antiferromagnetically to the next Gd layer, but that all other layers couple ferromagnetically. In contrast, Taborelli *et al.*[1] have argued that for their system all the Gd-Gd interactions are ferromagnetic. They attribute the difference in results to the difference in the Gd samples. One sample was epitaxially grown while the other was polycrystalline.

The work by Taborelli *et al.* supports their view that all Gd-Gd interactions are ferromagnetic by calculating the magnetization of each layer as a function of the distance of the layer to the interface between the Fe and Gd. They do this within a mean-field theory[3] and find excellent agreement with their experimental results. This gives one some confidence in using the mean-field method with an applied field and looking for surface phase transitions in the presence of the field. We have examined this case and do indeed find a series of surface phase transitions.

In our results we find that for low fields and moderate temperatures the equilibrium configuration is one where all the Fe spins are completely aligned with the field and all the Gd spins are oriented antiparallel to the field. As the field is increased (but with the temperature held constant) there is a phase transition to a twisted spin state. This state is similar in some ways to the spin flop state in an antiferromagnet and is also similar to the configuration found in a domain wall. Such twisted spin states are pervasive in materials with competing interactions[4] and have been studied with continuing interest.

We have also found very striking behavior when one keeps the magnetic field fixed and varies the temperature. The system may start at low temperature in the twisted state, and as the temperature is increased there is a phase transition to the aligned state. As the temperature is further increased the system changes to an aligned configuration where some of the Gd point parallel to the applied field.

The mean-field calculations performed here assume a simple model of a bcc ferromagnet with $S=\frac{5}{2}$ (Fe) which is coupled with $S=\frac{7}{2}$ (Gd). Of course, bulk Gd is not a bcc structure, and furthermore anisotropy fields in Gd, neglected here, play an important role in reorientation transition near $T=235$ K.[5] We note, however, that if we have a polycrystalline material the details of the structure and anisotropy effects are likely to be less important. Our model should give the general features correctly within the limitations of mean-field theory.

The geometry is illustrated schematically in Fig. 1. There are 20 Fe layers and five Gd layers. Layer 1 of Fe is taken to have the properties of bulk Fe, i.e., its moment is that of bulk Fe at the appropriate temperature and it always points in the direction of the applied field, the z direction. The spins in the remaining Fe and Gd layers are free to rotate in the xz plane illustrated in Fig. 1. (The spins are not likely to rotate in the yz plane because this would set up static demagnetizing fields.) The exchange coupling constant between Fe spins is J_1, between Fe and Gd spins is J_I, and between Gd spins is J_2. We consider nearest-neighbor interactions only. In this work we have taken the special case where J_1 and J_I are both fairly strong compared to J_2. This is appropriate for the system under consideration. Our parameters have values $J_1=1$, $J_I=-1$, and $J_2=0.155$. The ratio J_1/J_2 is obtained by comparing the transition temperatures for Fe and Gd.

It is convenient to start by finding the $T=0$ ground state. At $T=0$ the spin configuration may be completely described by a set of angles $\theta_1 \cdots \theta_{25}$ which give the orientation of the spin with respect to the z axis in layers 1 to 25. To find the ground state an initial configuration is chosen and the lowest energy state is found by an iteration method. The spin in layer i sees an effective field H_i, given by the sum of the exchange field and the external field:

$$\mathbf{H}_i = 4(J_{i,i+1}\mathbf{S}_{i+1}+J_{i,i-1}\mathbf{S}_{i-1})+H_0\hat{\mathbf{z}} \ . \tag{1}$$

Here $J_{i,i+1}$ is the exchange coupling constant between layers i and $i+1$, H_0 is the external field, and S_i is the spin in layer i. We rotate this spin so that it points in the direction of the effective field. As has been pointed out,

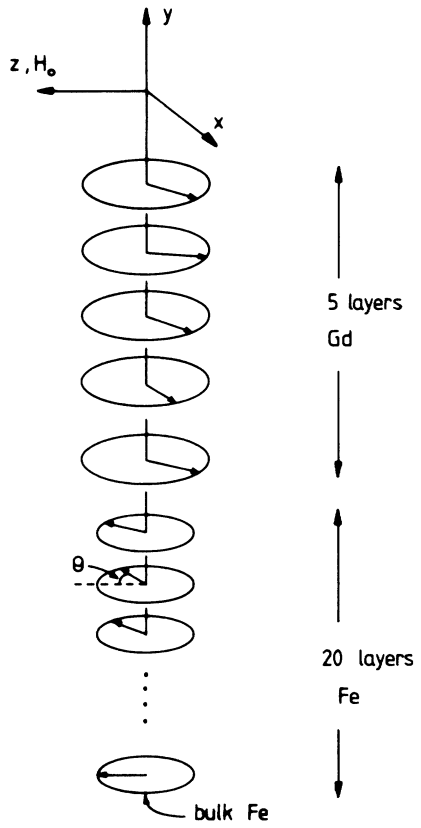

FIG. 1. A schematic illustration of the geometry considered in this paper. The exchange constant for two Fe spins is J_1, for two Gd spins is J_2, and for an Fe spin with a Gd spin is J_I. The spins are free to rotate in the xz plane as is shown. A sample initial configuration is illustrated.

this must lower the energy of the system since

$$E=-\sum_i \mathbf{H}_i\cdot\mathbf{S}_i \ . \tag{2}$$

We then pick a spin in a different layer and rotate it into its effective field. This process is continued until one has a self-consistent state where all spins are aligned with the effective fields produced by the neighboring spins. Since different initial configurations may lead to different self-consistent final states, one must compare the energy of the different stable final states in order to find the ground state.

For finite T, one must specify for each spin both a direction and a thermal averaged magnitude. In the iteration procedure a spin is first rotated into the direction of the effective field and then its thermal averaged magnitude in that direction is calculated through the use of the Brillouin function:

$$\langle S_i\rangle = S_i B_{s_i}(x) \ , \tag{3}$$

where

$$x=(S_i H_i/k_B T) \tag{4}$$

and the Brillouin function is given by

$$B_s(x)=\frac{(2S+1)}{2S}\operatorname{cotanh}\left[\frac{(2S+1)x}{2S}\right] - \frac{1}{2S}\operatorname{cotanh}(x/2S) \ . \tag{5}$$

Here $\langle S_i\rangle$ is the thermal average of the spin in the direction of the effective field. The effective field itself is given by Eq. (1) but with the spins S_{i+1} and S_{i-1} replaced by their thermal averages as well. Again the entire operation is repeated for all spins until a self-consistent configuration results.

Earlier we noted that depending on the initial choice for the spin configuration, different self-consistent states could be found. For finite T one must choose the state with the lowest free energy. The free energy is found from

$$F=-k_B T\ln(Z) \ , \tag{6}$$

where Z is the partition function for the entire system. In the mean-field approximation it is given by

$$Z=\prod_i Z_i \ , \tag{7}$$

where Z_i is the partition for spin i in the self-consistent effective field. Thus

$$Z_i=\frac{\sinh[(2S_i+1)H_i/2k_B T]}{\sinh(H_i/2k_B T)} \ . \tag{8}$$

Using the method outlined above, one can easily construct the H-T phase diagram which is presented in Fig. 2. Several different phases emerge, and typical spin configurations for these phases are shown in Fig. 3. For low fields and moderate temperatures, the ground state is the aligned state where the Fe spins are parallel to the external field and, because of the strong antiferromagnetic coupling of the Gd to the Fe, all the Gd spins are antiparallel to the applied field. With the temperature held constant, but with the field increased, there is a phase transition to

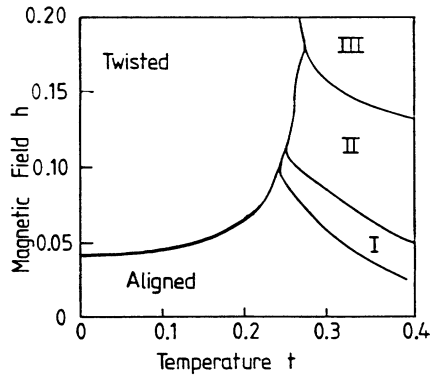

FIG. 2. Phase diagram for the system. The reduced temperature $t=T/T_c$ refers to the critical T_c for Fe. The field is dimensionless units given by $h=H/JS_{\mathrm{Fe}}$. The spin orientations for the various states are shown in Fig. 3.

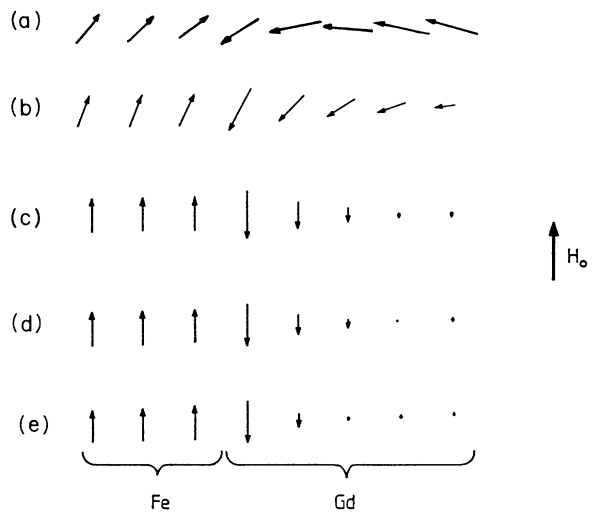

FIG. 3. The spin orientations for the various states. All states are for $h=0.08$ and different values of temperature. (a) The twisted state at $t=0$. (b) The twisted state at $t=0.2$. (c) Aligned state at $t=0.25$. (d) State I at $T=0.3$. (e) State II at $t=0.4$.

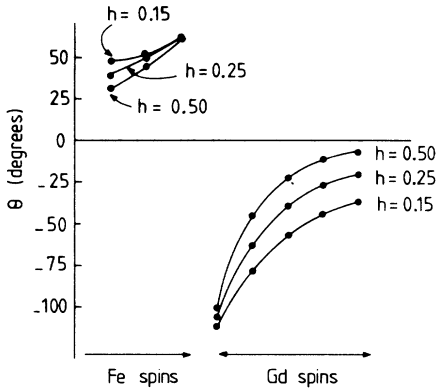

FIG. 4. Angle of orientation for the last few Fe spins and the Gd spins as a function of applied field. As the field is increased the twist becomes tighter. The solid line is a guide to the eye only.

a twisted state which is illustrated in Figs. 3(a) and 3(b). The remaining states shown in the phase diagram, I, II, and III, are ones where some of the Gd spins see such a small field that they have a paramagnetic response to the applied field. In this case, all the spins line up either parallel or antiparallel to the applied field. In state I all Gd spins except those in the outermost layer are antiparallel, in state II all Gd spins except those in the two outermost layers are antiparallel, etc.

The twisted state is particularly striking. As noted earlier, such states often occur due to the presence of competing interactions. Here the two competing energies are the Zeeman energy, which would be minimized if all spins were aligned with the applied field, and the exchange energy, which is minimized if all Gd spins point in the opposite direction to all the Fe spins. A recent example of how a twisted state emerges from the same competition between exchange energy and Zeeman energy is found in superlattices composed of alternating slabs of ferromagnetic and antiferromagnetic materials.[6] A much older example is found in the exchange coupling of a hard magnetic material to a soft magnetic material for use in information storage.[7]

The twisted spin state is similar in many respects to the rotated spins found in a domain wall. For a domain wall there are two fields which govern the properties of the wall—the exchange field and the anisotropy field. An increase in the anisotropy field for example, which gives a preferred direction for the spins, decreases the width of a domain wall. An increase in the strength of the exchange field increases the width of the wall. In the system considered here the external field, which again gives a preferred direction for the spins, plays the same role as the anisotropy field does in a domain wall, i.e., increasing the external field reduces the width over which there is a significant rotation of the spins. We can see this explicitly in Fig. 4 where we plot the angle of spin rotation as function of layer for various magnetic fields at $T=0$. Here the angle is measured from the z direction, the direction of the applied field. We see in this figure that for both the Gd and the Fe spins there is a larger net change in angle as the field is increased and the region of maximum change is more closely confined to the interface. Thus increasing the field makes the twist tighter.

We are now in a position to understand the major features of the phase diagram of Fig. 2. To understand the $T=0$ results, consider a slightly different configuration—a system with five Gd layers and seven Fe layers. An aligned state with the Fe spins parallel to H_0 and the Ge spins antiparallel to H_0 has no net Zeeman energy. Such a system will "flop" into a configuration where both the Gd and Fe spins are mostly perpendicular to the field, but have small components parallel to the applied field as well. (The system is essentially equivalent to an antiferromagnetic in the spin flop state.) Such a "flopped state" is similar to the configuration of spins near the interface when the system is in the twisted state as can be seen in Fig. 3(a). As long as the region over which the twist takes place in the Fe is on the order of seven iron layers or less, adding more Fe layers does not radically change the situation, and the system remains in a twisted state. If the range of the twist in the Fe is larger than about seven layers adding extra layers of Fe tends to force the system into an aligned state. In fact, the phase transition at $T=0$ between the twisted and aligned states occurs when the decay length of the twist in the Fe is between seven and eight layers. Thus at high fields, where the range of the twist is small, the twisted state is stable, and at low fields, where the twisted state would have a very broad range, the aligned state is stable.[8]

Using the above argument, one would expect that the phase transition between the twisted state and the aligned state would occur at a different field if there were a different number of Gd layers. For example, with only three Gd layers one would need about four Fe layers to make a

system with no net Zeeman energy in the aligned state. In this case the transition from the twisted to the aligned state would occur when the range of the twist is on the order of four layers. This clearly requires a larger field, and numerically we find that the transition takes place near $h=0.12$ in this case.

We can now understand the temperature dependence of the phase diagram. Since the rotation of Fe spins costs both Zeeman and exchange energy, the net amount of rotation of the Fe spins (i.e., the value θ_{20}) varies with the amount of Zeeman energy which can be gained by rotating the Gd spins into the direction of the field. As the temperature is increased, the average magnetic moment of the Gd is rapidly reduced compared to the average moment of the Fe spins. As a result, an increase in T reduces the energy gain from the rotation of the Gd spins, and this, in turn, reduces the net rotation of the Fe spins. At some T there is no rotation of the Fe spins, and we have a second-order phase transition into the aligned state. From this argument, we would also expect that as the field is increased, the twisted state should exist over a wider range of temperatures since at higher fields one can gain more Zeeman energy with the Gd spins.

Near $t=0.26$ there is a set of phase transitions from the twisted state to various states where the Gd spins are so weakly exchange coupled that they are nearly paramagnetic. We note that the transition temperature for bulk Gd from the ferromagnetic to the paramagnetic state is at $t=0.275$. The states I, II, and III occur as the magnetic field increases sufficiently to turn over more Gd spins. Since the spins in the outermost Gd layer see the smallest effective exchange field, it is these spins which are turned first. The phase transitions from the twisted phase to the phases where some of the Gd spins behave paramagnetically is second order as one might expect.

In summary, we have obtained the H-T phase diagram for a system of a few layers of Gd on bulk Fe. We find several phases, including a very interesting twisted spin phase. The twisted phase has many similarities with the rotation of spins in a domain wall. As an external magnetic field is increased, the region of the twist becomes more confined to the layers just near the interface.

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[8]Stability is checked numerically. One starts with a configuration arbitrarily close to the configuration of interest. If the program diverges away from the original configuration, that configuration is unstable.