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LETTER TO THE EDITOR

The phase diagram of Gd–Y alloys

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Abstract. It is pointed out that some general features of the phase diagram of Gd–Y alloys in the temperature–composition (T, x) plane may be explained by assuming that the system has a three-fold rather than six-fold symmetry. In particular this symmetry may account for the fact that no ferromagnetic phase exists in which $S_\perp \neq 0$ but with $S_z = 0$, where $S_\perp$ and S_z are the components of the magnetisation in the xy plane and z direction, respectively. This analysis also suggests that in the helical phase, characterised by the Fourier components $S_{\perp,q}$, a small modulated structure $S_{z,3q}$ should be induced.

The phase diagram of Gd–Y alloys in the temperature–concentration (T, x) plane has been studied extensively in recent years [1–4]. These alloys seem to have a hexagonal symmetry, derived from the HCP structure of pure Gd [5, 6]. It has been found that the system exhibits a rather complicated phase diagram with three magnetically ordered phases: a ferromagnetic phase (FI) in which the ferromagnetic moment points along the z axis, a canted ferromagnetic phase (FII) in which the magnetic moment lies in some intermediate direction in the xz plane, and a helimagnetic phase, in which the magnetic moments seem to lie in the xy plane (see figure 1). This phase diagram displays certain features which look accidental. For example, at the transition line γ separating the helical and the canted ferromagnetic phases, two distinct processes take place: on the one hand the q-vector characterising the helical structure tends to zero as the line is approached from the helical side. On the other hand, as the transition line is crossed into the ferromagnetic phase, the magnetic moment develops a component along the z axis. There is no *a priori* reason why these changes should occur simultaneously along the same line. In fact, in simple models which are consistent with the hexagonal symmetry assumed for these alloys, this line would split into two lines: one associated with the vanishing of q, and the other with the onset of the rotation of the local magnetic moment out of the xy plane. Another interesting feature of the phase diagram is that while in the helimagnetic phase the magnetic moments seem to lie in the xy plane, both ferromagnetic phases have non-vanishing z components S_z.

In the present Letter we argue that these seemingly accidental features of the phase diagram may simply be accounted for if one assumes that the point symmetry of Gd–Y alloys is D_{3d} rather than D_{6h}. In particular, we show that the commensurate–incommensurate transition associated with the vanishing of the q-vector should be accompanied by a non-zero z component of the magnetisation in the ferromagnetic phase. We also consider the structure of the helical phase. Let $S_{\perp,q}$ be the order

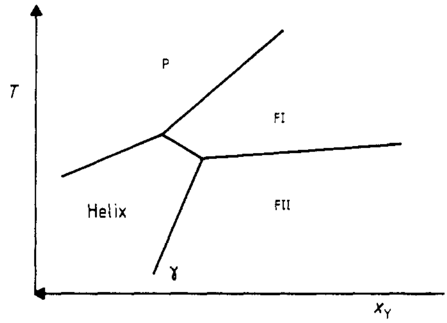

Figure 1. Schematic phase diagram of Gd–Y in the temperature–concentration (T, x) plane, indicating the relative position of the three ordered phases. Here P is the paramagnetic phase, FI is the uniaxial ferromagnetic phase with $S_z \neq 0$ and FII is the canted ferromagnetic phase. The concentration x_Y of the Y atoms increases to the left.

parameter associated with the phase, where $\boldsymbol{S}_\perp = (S_x, S_y)$ is the magnetic moment in the xy plane, and $\boldsymbol{S}_{\perp,q}$ is the Fourier component of $\boldsymbol{S}_\perp$ with wavevector $\boldsymbol{q}$. We show that in systems with three-fold symmetry the order parameter does *not* induce a modulated z component $S_{z,q}$ with the same wavevector as $\boldsymbol{S}_\perp$. However, it is expected that higher harmonics, such as $S_{z,3q}$, should be induced. It would be interesting to test this prediction experimentally, and check whether such a component exists in the helimagnetic phase.

A three-fold symmetry of the Gd–Y alloys may, for example, be a result of a non-uniform distribution of the Y atoms. Pure Gd is composed of the usual $\cdots$ ABAB $\cdots$ type succession of hexagonal planes in HCP structures [5, 6]. If in the Gd–Y alloy, the concentration of the Y atoms in the A-planes is different from that in the B-planes, it would reduce the point symmetry from six-fold to three-fold. Although there is no clear experimental indication that this indeed is the case, we will assume that the point symmetry of this system has a three-fold axis and show that this may account for the interesting features of the phase diagram mentioned above.

Our analysis of the phase diagram is based on a Landau free energy, consistent with the three-fold symmetry. Let $\boldsymbol{S} = (S_x, S_y, S_z)$ be the local magnetisation vector. The Landau free energy associated with the order parameter takes the form

$$F = a(S_x^2 + S_y^2) + bS_z^2 + \alpha[(\mathrm{d}S_x/\mathrm{d}z)^2 + (\mathrm{d}S_y/\mathrm{d}z)^2] + [(\mathrm{d}^2S_x/\mathrm{d}z^2)^2 + (\mathrm{d}^2S_y/\mathrm{d}z^2)^2] + u_1(S_x^2 + S_y^2)^2 + u_2S_z^4 + u_3S_z^2(S_x^2 + S_y^2) + wS_z(S_x^3 - 3S_xS_y^2) \qquad (1)$$

where we have considered terms to order 4 in $\boldsymbol{S}$. The last term [7] in this expression represents a coupling between S_z and $\boldsymbol{S}_\perp \equiv (S_x, S_y)$. This term is compatible with three-fold symmetry, and it vanishes if the symmetry has a six-fold axis along z. As we shall see, this term may account for some of the features of the observed phase diagram of Gd–Y. For simplicity and to ensure stability we consider the phase diagram of this model taking $u_1, u_2, u_3 > 0$ with small w.

The model exhibits three ordered phases. For a, $\alpha > 0$ and $b < 0$ it has a ferromagnetic phase with average magnetisation along z. On the other hand for $a < 0$ and α, $b > 0$, the magnetisation in the xy plane, $\boldsymbol{S}_\perp$, becomes non-zero. However, due to the coupling term w, the components of $\boldsymbol{S}_\perp$ induce a magnetic moment along the z axis, resulting in a canted ferromagnetic phase. Thus the model exhibits two ferromagnetic phases in both of which $S_z \neq 0$. Consider now the regime $\alpha < 0$ and $b > 0$. Here the model produces a helical phase. Considering only terms to fourth order in $\boldsymbol{S}_\perp$ and neglecting for a moment the w-term, one finds that the structure of the helical phase is given by

$$S_x = S\cos(qz) \qquad S_y = S\sin(qz) \qquad (2)$$

where q is the modulus of the wavevector determined by the parameter α. Consider now the coupling term w. Inserting the structure (2) in this term we find that it yields a linear term in S_z of the form

$$wS_zS^3\cos(3qz). \tag{3}$$

This term acts as an ordering field on S_z with modulation vector $3\boldsymbol{q}$. The z component of the magnetisation is thus expected to exhibit a non-vanishing modulated structure with a wavevector $3\boldsymbol{q}$. Note that no modulation of the S_z with the wavevector $\boldsymbol{q}$ is expected in this case. If one considers higher order anisotropic terms in the components of $\boldsymbol{S}_\perp$, such as $v(S_x^3 - 3S_xS_y^2)^2$, the helical structure will deviate from the ideal one given by (2). In this case one expects that the w-term will induce a modulated S_{zq} component with the same wavevector as $\boldsymbol{S}_\perp$. However, if the anisotropic terms are small, this modulation may be too small to be observed.

In conclusion, we find that the simple Landau model (1), compatible with three-fold symmetry, may account for some of the general features of the phase diagram of Gd–Y alloys. The model suggests that in the helical phase, one should find a small modulated z component $S_{z,3q}$ with a modulation vector which is three times that of $\boldsymbol{S}_\perp$. It would be interesting to test this prediction experimentally.

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References

[1] Ito T, Legvold S and Beaudry B J 1981 *Phys. Rev.* B **23** 2409
[2] Bates S, Palmer S B, Sousa J B, McIntyre G J, Fort D, Legvold S, Beaudry B J and Koehler W C 1985 *Phys. Rev. Lett.* **55** 2968
[3] Bates S, Greenough R D, Hetterarchichi D, Hukin D, Palmer S B and Sousa J B 1986 *J. Phys. F: Met. Phys.* **16** 903
[4] Bates S, McIntyre G J, Palmer S B and Sousa J B 1987 *J. Phys. F: Met. Phys.* **17** 1973
[5] Hermann K W 1963 *Iowa State Coll. J. Sci.* **31** 439
[6] Smidt A and Daane A M 1963 *J. Phys. Chem. Solids* **24** 361
[7] Mukamel D 1981 *Phys. Rev. Lett.* **46** 845