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ON THE MAGNETIC ANISOTROPY OF THE $Y_2(Co_{1-x}Fe_x)_{14}B$ COMPOUNDS

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Abstract. – The complex composition dependence of the anisotropy of the 3d sublattice in the $Y_2(Co_{1-x}Fe_x)_{14}B$ compounds at 4.2 K has been analysed by means of the individual site anisotropy model. The cobalt contribution to the magnetocrystalline anisotropy at the site $8j_2$ is found to be of the opposite sign to that given by the iron ion at this site.

1. Introduction

In most R-T intermetallics (R = rare earth, T = transition metal), the 3d ions are known to be situated at several different crystallographic sites, for which sites different contributions to the anisotropy can be expected. In case of the $R_2T_{14}B$ compounds [1, 2], the number of different 3d sites reaches to six. In order to study the 3d anisotropy, compounds in which R is non-magnetic (Y, La or Lu) or magnetically isotropic (Gd) are most suited. Such studies have been carried out in the temperature range from 77 K to 300 K on $Y_2(Co_{1-x}Fe_x)_{14}B$ by Bolzoni *et al.* [3] and on $La_2(Co_{1-x}Fe_x)_{14}B$ by Grössinger *et al.* [4]. In the present contribution, anisotropy measurements are reported for $Y_2(Co_{1-x}Fe_x)_{14}B$ compounds at 4.2 K. The results of this investigation are analysed in terms of the individual site anisotropy model.

2. Experimental

Pseudo-ternary compounds of $Y_2(Co_{1-x}Fe_x)_{14}B$, with $x = 0.0, 0.25, 0.375, 0.5, 0.625, 0.75, 0.875$ and 1.0, were prepared by arc melting and by subsequently annealing the ingots at 950°C for 10 days. The samples are single phase as confirmed by X-ray and thermomagnetic analyses.

The magnetization measurements at 4.2 K have been carried out on aligned powder samples of a cubic shape with one of the sides parallel to the alignment direction. From the magnetization curve along the easy direction (the direction parallel to the alignment field) a value of 0.18 has been derived for the demagnetising factor, which implies a value of 0.41 for the hard directions. The anisotropy constants were de-

termined by fitting the magnetization curve along the hard direction using computer programs that take into account the appropriate distribution of the easy direction of particles around the alignment direction [5]. The value of 99 J/kg obtained for $Y_2Fe_{14}B$ is quite close to a value of 101 J/kg determined for a single-crystalline sample at 4.2 K [6]. The resulting values for the anisotropy constants are collected in table I, together with the values for the saturation magnetisation.

3. Discussion

The most striking feature of the experimental results is the anomalous composition dependence of the anisotropy constant at 4.2 K: a maximum at about $x = 0.75$ and a change in sign around $x = 0.3$, see figure 1. Very similar results have been observed for $La_2(Co_{1-x}Fe_x)_{14}B$ at 4.2 K by Grössinger *et al.* [4]. The same type of anomalous composition dependence of the magnetic anisotropy is also observed in $Y_2(Co, Fe)_{17}$ and has been explained in terms of the individual site anisotropy model as a consequence of the preferential site occupation of the cobalt and iron atoms [7].

The occupancy factors of iron atoms at the site i , f_i, Fe , in $Nd_2(Co_{1-x}Fe_x)_{14}B$ have been determined by Herbst *et al.* [8] by neutron diffraction experiments. Assuming the same f_i, Fe factors for the $Y_2(Co_{1-x}Fe_x)_{14}B$ compounds, the experimentally derived values for $K_1(x)$ in table I have been fitted with the expression:

$$K_1(x) = K_1(0) + \sum n_i f_{i, Fe}(x) \Delta K_1^i \quad (1)$$

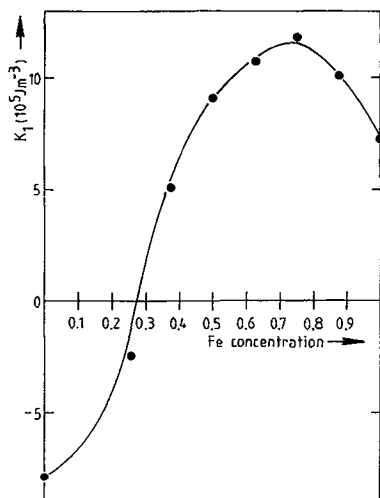
where $K_1(0)$ is the anisotropy constant of $Y_2Co_{14}B$

Table I. – Saturation magnetizations and anisotropy constants K_1 of the $Y_2(Co_{1-x}Fe_x)_{14}B$ compounds at 4.2 K.

x	0.000	0.250	0.375	0.500	0.625	0.750	0.875	1.000
M_s (Am ² /Kg)	106	129	138	150	157	166	172	177
K_1 (10 ⁵ J/m ³)	-8.0	-2.5	4.9	9.0	10.8	11.9	10.2	7.1

Table II. - Values for the difference in the individual site anisotropy $\Delta K_1^i = K_{1, \text{Fe}}^i - K_{1, \text{Co}}^i$ (in 10^5 J/m^3).

Site	16 K ₁	16 K ₂	8 j ₁	8 j ₂	4e	4c
ΔK_1^i	-0.11	0.09	-6.25	4.41	9.41	-1.91
$K_{1, \text{Fe}}^i$				0.10		
$K_{1, \text{Co}}^i$				-4.31		

Fig. 1. - Composition dependence of the anisotropy constant K_1 at 4.2 K for the $\text{Y}_2(\text{Co}_{1-x}\text{Fe}_x)_{14}\text{B}$ compounds. The solid curve represents a fit of equation (1) to the data with values for the parameters ΔK_1^i , as given in table II.

($x = 0$), where n_i is the number of sites i within the unit cell and where $\Delta K_1^i = K_{1, \text{Fe}}^i - K_{1, \text{Co}}^i$ is the difference in the contribution to the anisotropy of the iron and cobalt atoms at the site i . The resulting values for ΔK_1^i are presented in table II. Because of the large number of fitting parameters (six) the followed procedure should be considered as the first approach to determine the individual site anisotropy of the 3d sublattice in the 2:14:B compounds.

Values for the individual site anisotropy constants $K_{1, \text{Fe}}^i$ can now be extracted if the corresponding $K_{1, \text{Co}}^i$ values are known and *vice versa*. A whole set of $K_{1, \text{Fe}}^i$ or $K_{1, \text{Co}}^i$ values is not yet available. However, Burlet *et al.* [9] observed in $\text{Yb}_2\text{Fe}_{14}\text{B}$ a step-wise change in the average hyperfine field value ΔB and in that of the $8j_2$ site, ΔB^{j_2} , upon passing the spin-reorientation temperature at 115 K. This quantity is known to be related to the anisotropy energy at that temperature and can be used to estimate a value for $K_{1, \text{Fe}}^{j_2}$ according to:

$$\frac{K_{1, \text{Fe}}^{j_2}}{K_1(1)} = \frac{\Delta B^{j_2}}{56\Delta B} \quad (2)$$

Using the values of 1.6 T and 0.9 T for ΔB and ΔB^{j_2} , respectively, and taking $K_1(1)$ equal to $10.5 \times 10^5 \text{ J/m}^3$ [3] we calculate a value of $0.1 \times 10^5 \text{ J/m}^3$ for $K_{1, \text{Fe}}^{j_2}$ at 115 K. Taking the same value for this parameter at

4.2 K we obtain a value of $-4.31 \times 10^5 \text{ J/m}^3$ for $K_{1, \text{Co}}^{j_2}$. Although the absolute values for $K_{1, \text{Fe}}^{j_2}$ and $K_{1, \text{Co}}^{j_2}$ are less accurate by this extrapolation from 115 K to 4.2 K, the opposite-sign contribution to the anisotropy of the iron and cobalt atoms at the site $8j_2$ is quite well established. Different signs for the iron and cobalt contributions to the anisotropy is a general feature of the R-T intermetallics and can be understood in terms of different electronic configurations of the iron and cobalt atoms that correspond with opposite signs of the Stevens factors of the iron and cobalt atoms in these compounds.

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