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Analysis of the magnetic properties of R_2Fe_{17} ($R \equiv Gd, Tb, Dy, Ho, Er$ or Tm)

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Abstract. The values of the R–Fe exchange field and the crystalline-electric-field parameters are evaluated by fitting the calculations to the experiments for R_2Fe_{17} ($R \equiv Gd, Tb, Dy, Ho, Er$ or Tm). The experiments include the magnetization curves along the crystal axes at 4.2 K for the Gd, Tb, Dy, Ho and Er compounds, the energy differences between the energy levels for the Ho ion in Ho_2Fe_{17} , and the spin reorientation temperature T_{SR} and the easy-magnetization direction above and below T_{SR} for Tm_2Fe_{17} .

1. Introduction

High-field magnetization curves $M(H)$ of single-crystal R_2Fe_{17} ($R \equiv Gd$ [1], Tb [2], Dy [3], Ho [4] or Er [3, 5]) have been measured at 4.2 K by a number of workers; these curves have been analysed on the basis of the classic two-sublattice model in the same studies. The energy gaps between the energy levels for the Ho ions in Ho_2Fe_{17} have also been measured [6]. For Tm_2Fe_{17} , the $M(H)$ curves are not available yet, but the spin reorientation temperature T_{SR} and the easy-magnetization directions (EMDs) above and below T_{SR} have been measured [7, 8]. This paper evaluates the values of the R–Fe exchange field $H_{ex}(T = 0)$ and the crystalline-electric-field (CEF) parameters A_{nm} by a fit of the calculations with the experimental data.

2. Method of calculation

Rare-earth compounds of the type R_2Fe_{17} crystallize either in the hexagonal Th_2Ni_{17} structure or in the rhombohedral Th_2Zn_{17} structure. There are two rare-earth crystallographic sites in the hexagonal structure, and one site in the rhombohedral structure. Each site splits into two magnetically non-equivalent sites: A and B. The rare-earth ions are assumed to be triply ionized. In the coordinate system with the z and x axes along the c and a axes, the Hamiltonians of the CEF interactions for the rare-earth ions at the A and B sites are closely related, being represented as

$$\begin{aligned} \mathcal{H}_{CEF}(A) &= \sum_{n=2,4,6} A_{n0}C_{n0} + \sum_{n=4,6} A_{n3}(C_{n3} + C_{n-3}) + A_{66}(C_{66} + C_{6-6}) \\ \mathcal{H}_{CEF}(B) &= \sum_{n=2,4,6} A_{n0}C_{n0} - \sum_{n=4,6} A_{n3}(C_{n3} + C_{n-3}) + A_{66}(C_{66} + C_{6-6}) \end{aligned} \quad (1)$$

where

$$C_{nm} = [4\pi/(2n+1)]^{1/2} Y_{nm}(\theta_j, \varphi_j). \quad (2)$$

$Y_{nm}(\theta_j, \varphi_j)$ are the spherical harmonics, and θ_j and φ_j are the polar and azimuthal angles of the position vector r of the j th 4f electron. The signs of the second term on the right-hand side of equation (1) are opposite for $\mathcal{H}_{\text{CEF}}(\text{A})$ and $\mathcal{H}_{\text{CEF}}(\text{B})$, and the contributions of each of them to the total energy of the compound largely cancel each other. If the second terms are neglected, the Hamiltonian of the CEF interaction, averaged over the crystallographic and magnetic non-equivalent sites, therefore, is expressed simply as

$$\mathcal{H}_{\text{CEF}} = \sum_{n=2,4,6} A_{n0} C_{n0} + A_{66} (C_{66} + C_{6-6}). \quad (3)$$

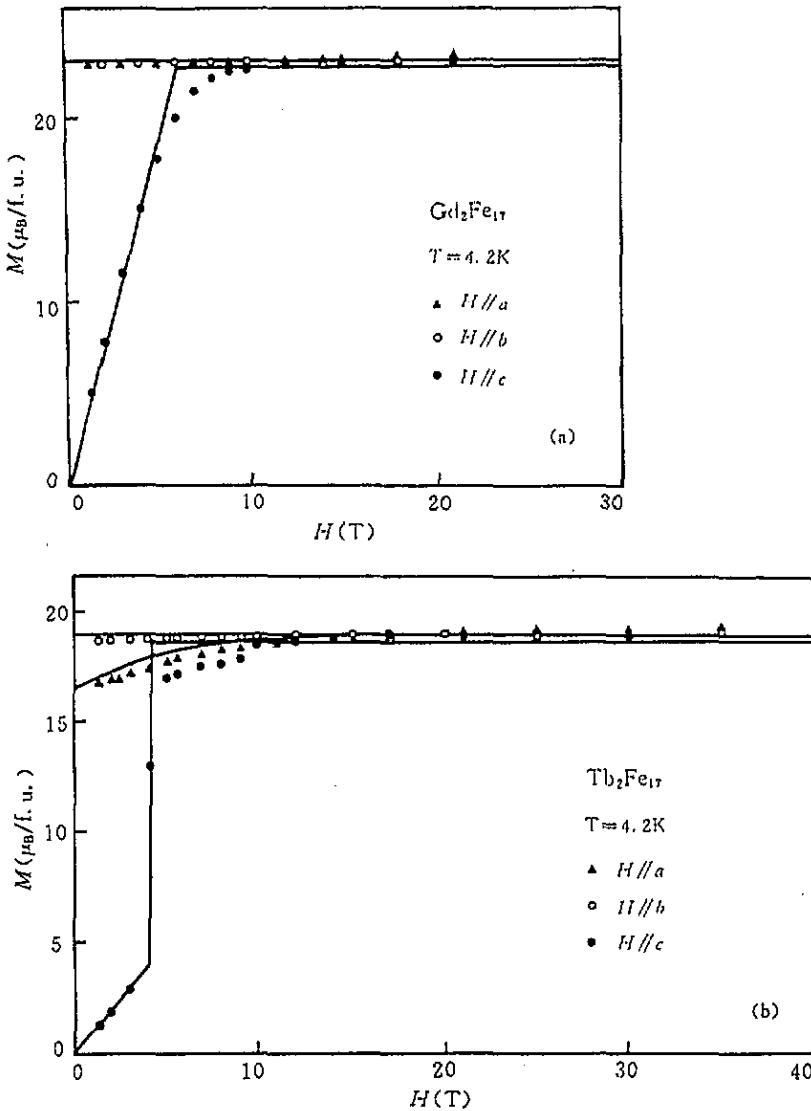


Figure 1. Isotherms at 4.2 K for $R_2\text{Fe}_{17}$ ($R \equiv$ (a) Gd, (b) Tb, (c) Dy and (d) Ho): —, calculations; \blacktriangle , \circ , \bullet , experimental data from [1-4].

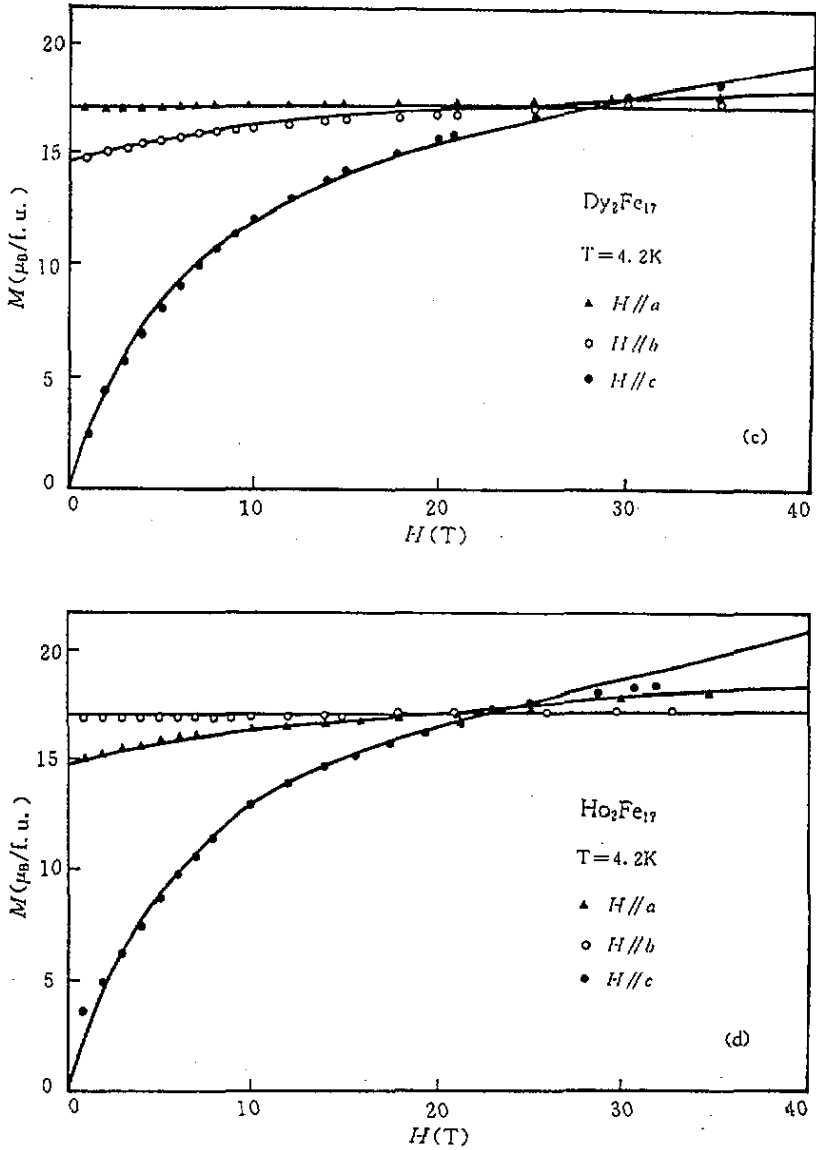


Figure 1. (Continued)

The total Hamiltonian of the rare-earth ion consists of the CEF interaction, the isotropic R-Fe exchange interaction and the Zeeman energy, i.e.

$$\mathcal{H} = \mathcal{H}_{\text{CEF}} + 2\mu_B \mathbf{S} \cdot \mathbf{H}_{\text{ex}} + \mu_B (\mathbf{L} + 2\mathbf{S}) \cdot \mathbf{H}. \quad (4)$$

The R-R exchange interaction, which is believed to be much weaker than the R-Fe exchange interaction, was neglected.

The magnetic moment $M_{\text{Fe}}(T, \theta_{\text{Fe}})$ of the Fe sublattice is anisotropic [9]. The exchange field $\mathbf{H}_{\text{ex}}(T)$ is assumed to be proportional and antiparallel to the magnetic moment $\mathbf{M}_{\text{Fe}}(T, \theta_{\text{Fe}})$ of the Fe sublattice. They are represented as

$$M_{\text{Fe}}(T, \theta_{\text{Fe}}) = M_{\text{Fe}}(T)[1 - p(T) \cos^2 \theta_{\text{Fe}}] \quad (5)$$

$$H_{\text{ex}}(T) = -H_{\text{ex}}(0)M_{\text{Fe}}(T)/M_{\text{Fe}}(0). \quad (6)$$

The relations $M_{\text{Fe}}(T)/M_{\text{Fe}}(0) = [K_{1\text{Fe}}(T)/K_{1\text{Fe}}(0)]^{1/3}$ and $p(T) = \Delta M_{\text{Fe}}(T)/M_{\text{Fe}}(T)$ and $p(0) = 0.008$ were taken from those for Y_2Fe_{17} [9]. The values of $M_{\text{Fe}}(0)$ for each compound were also adjusted around the experimental values for Y_2Fe_{17} ($34.17\mu_{\text{B}}/\text{formula unit (FU)}$) [9] and $35.19\mu_{\text{B}}/\text{FU}$ [10]) for a better fit.

Table 1. The fitted values of $M_{\text{Fe}}(0)$, $2\mu_{\text{B}}H_{\text{ex}}(0)$, A_{20} , A_{40} , A_{60} , A_{66} and the exchange field $2\mu_{\text{B}}H'_{\text{ex}}(0) (= g_J\mu_{\text{B}}M_T n_{\text{RT}}/(g_J - 1))$ for R_2Fe_{17} ($\text{R} \equiv \text{Gd, Tb, Dy, Ho, Er or Tm}$).

R	$M_{\text{Fe}}(0)$ (μ_{B}/FU)	$2\mu_{\text{B}}H_{\text{ex}}(0)$ (K)	A_{20} (K)	A_{40} (K)	A_{60} (K)	A_{66} (K)	$2\mu_{\text{B}}H'_{\text{ex}}(0)$ (K)
Gd	36.9	330					351 [1]
Tb	36.9	300	-15	-190	0	-200	285 [2]
Dy	37.0	285	-85	-180	0	-180	286 [3]
Ho	36.8	270	-80	-170	0	-110	320 [4]
Er	35.4	255	-75	-130	0	-165	255 [1]
Tm ^a	37.9	245	-75	-110	0	-100	

^a The value of A_{66} is estimated from extrapolation of those for the other rare earths.

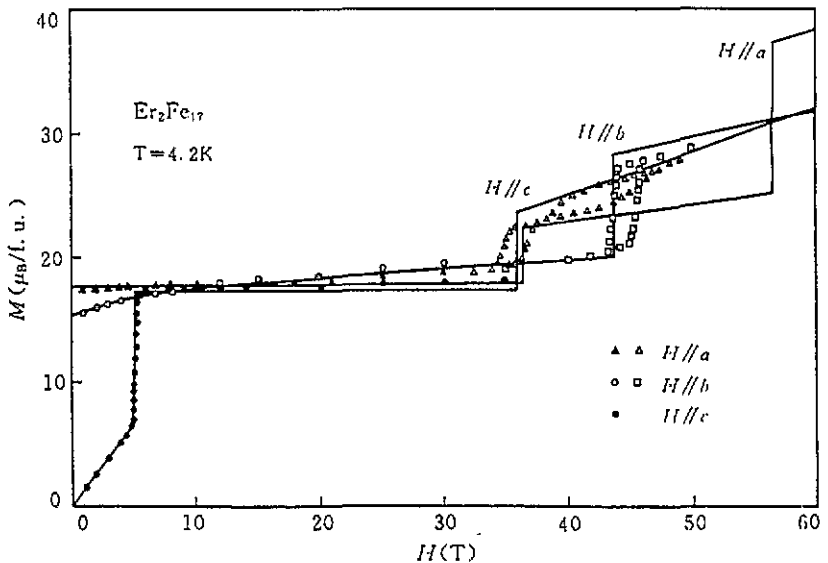


Figure 2. Isotherms at 4.2 K for $\text{Er}_2\text{Fe}_{17}$: —, calculations; \blacktriangle , \circ , \bullet , experimental data from [3]; \triangle , \square , experimental data from [5].

The matrix elements of equation (4) were calculated using the irreducible-tensor-operator technique [11]. For a given applied field \mathbf{H} and a direction of \mathbf{H}_{ex} , the eigenvalues E_i and eigenfunctions $|n_i\rangle$ ($i = 1, 2, \dots, 2J + 1$) are obtained by diagonalizing the

Table 2. The effect of variation in $2\mu_B H_{ex}(0)$ or in A_{nm} by 5 or 10 K from the fitted values on the calculations of $M(H\parallel c, H = 4 \text{ T})$ and FOMR fields H_{cr}^c , H_{cr}^a and H_{cr}^b , all at 4.2 K for Er_2Fe_{17} .

$2\mu_B H_{ex}(0)$ (K)	A_{20} (K)	A_{40} (K)	A_{66} (K)	$M(H\parallel c, H = 4 \text{ T})$ (μ_B/FU)	H_{cr}^c (T)	H_{cr}^a (T)	H_{cr}^b (T)
255	-75	-130	-165	5.23	5.0	36.4	43.7
260	-75	-130	-165	5.17	5.0	37.1	44.5
255	-80	-130	-165	5.25	4.7	36.4	43.7
255	-75	-140	-165	5.19	4.8	36.4	43.7
255	-75	-130	-175	5.20	5.4	36.4	43.7

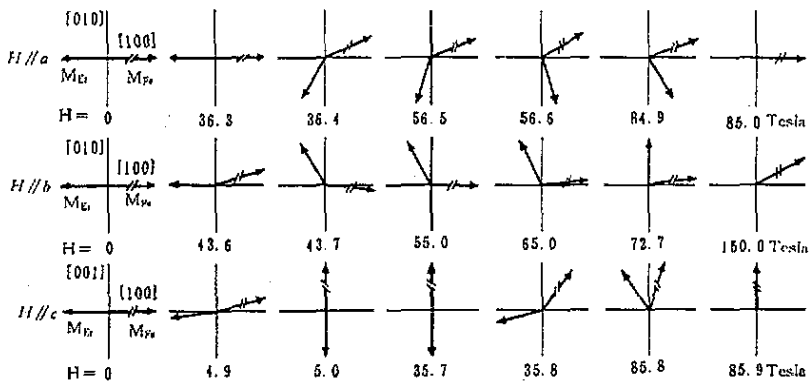


Figure 3. The variation in the directions of M_{Er} and M_{Fe} in Er_2Fe_{17} during the magnetization process along the a axis (upper figures), b axis (middle figures), and c axis (lower figures).

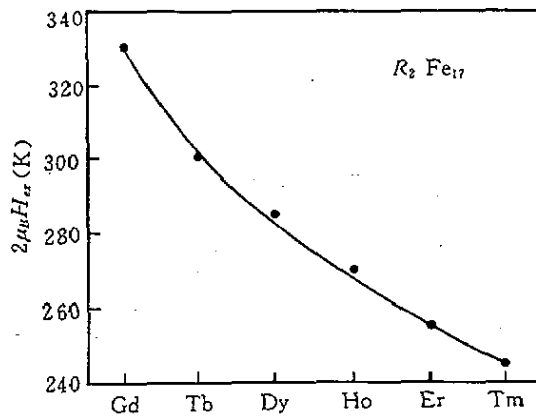


Figure 4. The variation in the exchange field $2\mu_B H_{ex}(0)$ across the R_2Fe_{17} series from $R \equiv Gd$ to Tm .

$(2J + 1) \times (2J + 1)$ matrix of equation (4). The diagonalization was carried out within the ground-state J -multiplet. The free energy for R_2Fe_{17} is given by

$$F(H, H_{\text{ex}}, T) = -2k_B T \ln Z + K_{\text{Fe}}(T) \sin^2 \theta_{\text{Fe}} - M_{\text{Fe}}(T, \theta_{\text{Fe}}) \cdot H \quad (7)$$

where

$$Z = \sum_i \exp\left(-\frac{E_i}{k_B T}\right). \quad (8)$$

$K_{\text{Fe}}(T)$ is the magnetocrystalline anisotropy constant of the Fe sublattice per FU, and the $K_{\text{Fe}}(T)/K_{\text{Fe}}(0)$ -values were taken to be the same as those for Y_2Fe_{17} [9]. The value of $K_{\text{Fe}}(0)$ for all compounds was taken as -47.0 K/FU around the experimental values of Y_2Fe_{17} (-42.8 K/FU [9] and -57.9 K/FU [10, 12]) for a better fit. The equilibrium direction of H_{ex} was determined by minimization of the free energy. The magnetic moment of the rare-earth ion and of R_2Fe_{17} are given by

$$M_{\text{R}}(T) = -\mu_{\text{B}} \langle n_i | L + 2S | n_i \rangle \exp(-E_i/k_B T) / Z \quad (9)$$

$$M(T) = 2M_{\text{R}}(T) + M_{\text{Fe}}(T, \theta_{\text{Fe}}). \quad (10)$$

The magnetization curves and some other magnetic properties were calculated for a set of the parameters of $H_{\text{ex}}(0)$, A_{nm} ($nm = 20, 40, 60$ and 66), $M_{\text{Fe}}(0) \simeq 35\mu_{\text{B}}/\text{FU}$ and $K_{\text{Fe}}(0) \simeq 50$ K/FU for each compound. From a comparison of the calculations with the experimental data, the values of the parameters were adjusted for a better fit for the next calculation. The procedure was repeated until satisfactory agreement was reached. The adjustment of the parameters was guided by knowledge of the different effects of each parameter on the magnetization curves [13, 14].

3. Results and discussion

Table 1 lists the values of the fitted parameters of $M_{\text{Fe}}(0)$, $2\mu_{\text{B}}H_{\text{ex}}(0)$, A_{20} , A_{40} , A_{60} , and A_{66} . The exchange fields $2\mu_{\text{B}}H'_{\text{ex}}(0)$ ($= g_J \mu_{\text{B}} M_{\text{T}} n_{\text{RT}} / (g_J - 1)$, n_{RT} is the intersublattice molecular field coefficient), which are taken from [1–4], are also listed for reference. Figures 1 and 2 show the magnetization curves along the crystal axes at 4.2 K. The full curves represent the calculations and the symbols the experimental data. For $\text{Er}_2\text{Fe}_{17}$, multiple first-order-moment reorientation (FOMR) transitions are observed, and figure 3 shows the variations in the directions of M_{Er} and M_{Fe} near the FOMR fields. Table 2 demonstrates the effect of variation in the value of $2\mu_{\text{B}}H_{\text{ex}}(0)$ or in A_{nm} by 5 or 10 K from the fitted values on the calculations of some magnetic properties, which would provide information about the uncertainty in the values of the fitted parameters. Figure 4 shows the variation in the exchange field $2\mu_{\text{B}}H_{\text{ex}}(0)$ across the R_2Fe_{17} series from $\text{R} \equiv \text{Gd}$ to Tm . The calculated energy gaps between the lowest four energy levels for $\text{Ho}_2\text{Fe}_{17}$ are $E_2 - E_1 = 96.1$ K, $E_3 - E_2 = 58.2$ K and $E_4 - E_3 = 48.8$ K, which are in agreement with the experimental values of 96.3 K, 67.3 K and 55.7 K, respectively [6]. T_{SR} for $\text{Tm}_2\text{Fe}_{17}$ was calculated to be 73 K compared with the experimental value of 72 K [7, 8]. At T_{SR} , the EMD varies between the c axis and b axis.

Acknowledgments

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