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Magnetisation processes of the R ions in $R_2Fe_{14}B$ (R = Er and Tm) in a field up to 1000 kOe at 78 K

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Abstract. The experimental magnetisation curves $M(H)$ of $Er_2Fe_{14}B$ and $Tm_2Fe_{14}B$ along the [100], [110] and [001] axes up to 550 kOe measured at 78 K are reproduced well by a calculation based on the single-ion model. The calculation shows that during the magnetisation process in such a high field both the magnetic moment and magnetic anisotropy of the R ion vary strikingly. When the field is applied along the [100] and [110] axes, both the magnetic moment and magnetic anisotropy quench at about 740 and 570 kOe for the Er and Tm ions, respectively. But when the field is applied along the [001] axis, they quench at about 570 kOe for the Tm ion while no quenching occurs for the Er ion.

1. Introduction

Recently, magnetisation curves $M(H)$ up to 550 kOe have been measured on $R_2Fe_{14}B$ (R = Er and Tm) compounds at 78 K by Kido *et al* (1987). As will be shown in a later section, the curves can be reproduced well by a calculation using the values of the crystalline electric field (CEF) parameters A_{nm} and the R–Fe exchange field H_{ex} presented elsewhere by the present authors (Zhao *et al* 1989). The parameters have been evaluated from the temperature dependence of spontaneous magnetisation, magnetisation curves at 4.2 K and at a higher temperature, and the spin reorientation temperature. The calculation reveals that the characteristics of the magnetisation processes of the rare-earth ions in the compounds for high fields at 78 K are quite different from those in the lower fields. The results are presented in the following.

2. Method of calculation

Neglecting the difference between the f and g sites, there are two magnetically inequivalent R sites: R(1) and R(2) located on the diagonals along [110] and $[1\bar{1}0]$ in the lattice cell. The Hamiltonian of the R ion at the i th site in the $\langle 100 \rangle$ coordinate system with z axis along the c axis is expressed as

$$\mathcal{H}(i) = \sum_{n,m} \theta_n A_{nm}(i) O_{nm} - 2(g_J - 1)\mu_B \mathbf{J} \cdot \mathbf{H}_{ex} + g_J \mu_B \mathbf{J} \cdot \mathbf{H} \quad (1)$$

where

$$\begin{aligned} A_{nm}(1) &= (-1)^{m/2} A_{n-m}(1) = (-1)^{m/2} A_{nm}(2) \\ n &= 2, 4, 6 \quad |m| = 0, 2, 4, 6 \quad |m| \leq n \end{aligned} \quad (2)$$

and θ_n and O_{nm} are Stevens coefficient and Racah operator equivalent respectively (Danielson and Lingard 1972). The other symbols have their usual meanings. For a given \mathbf{H} and \mathbf{H}_{ex} , the eigenvalues $E_n(i)$ and eigenfunctions $|i, n\rangle$ are obtained by diagonalising (1) within the ground J multiplet. $\mathbf{H}_{\text{ex}}(T)$ is assumed to be proportional to $\mathbf{M}_{\text{Fe}}(T)$. The equilibrium direction of \mathbf{H}_{ex} , i.e. the polar angles θ_{Fe} and φ_{Fe} of \mathbf{M}_{Fe} , is determined from the minimum of the total free energy of the $\text{R}_2\text{Fe}_{14}\text{B}$ system:

$$F(\mathbf{H}, \mathbf{H}_{\text{ex}}, T) = -kT \sum_i \ln Z(i) + K_{\text{Fe}} \sin^2 \theta_{\text{Fe}} - \mathbf{M}_{\text{Fe}} \cdot \mathbf{H}. \quad (3)$$

Here

$$Z(i) = \sum_n \exp(-E_n(i)/kT) \quad n = 1, 2, \dots, 2J + 1 \quad (4)$$

and K_{Fe} and M_{Fe} are the magnetocrystalline anisotropy constant and spontaneous magnetisation of the Fe sublattice per formula unit. The values of $K_{\text{Fe}}(T/T_C)$ and $M_{\text{Fe}}(T/T_C)/M_{\text{Fe}}(0)$, where T_C is the Curie temperature of the R compound, are taken to be those of $\text{Y}_2\text{Fe}_{14}\text{B}$ (Hirosawa *et al* 1986). The total magnetisation \mathbf{M} of the system is calculated as

$$\mathbf{M} = -\partial F/\partial \mathbf{H} = \sum_i \mathbf{M}_{\text{R}}(i) + \mathbf{M}_{\text{Fe}} \quad (5)$$

$$\mathbf{M}_{\text{R}}(i) = \sum_n -g_J \mu_{\text{B}} \langle i, n | \mathbf{J} | i, n \rangle \exp(-E_n(i)/kT)/Z(i). \quad (6)$$

The values of A_{nm} and $2\mu_{\text{B}}H_{\text{ex}}(0)$ used in the calculation (in units of K) are: $A_{20} = 380, 350, A_{22}/i = \pm 240, \pm 240, A_{40} = -155, -150, A_{44} = -55, -40, A_{60} = -30, -30, A_{62}/i = \pm 22, \pm 20, A_{64} = -75, -50$ and $2\mu_{\text{B}}H_{\text{ex}} = 300, 270$ for the Er and Tm compounds respectively, where $i = \sqrt{-1}$. These parameters have been evaluated from the other experiments (Zhao *et al* 1989).

The effective field acting on the R ion, \mathbf{H}_{eff} , is

$$g_J \mathbf{H}_{\text{eff}} = -2(g_J - 1)\mathbf{H}_{\text{ex}} + g_J \mathbf{H}. \quad (7)$$

3. Results and discussion

Figures 1(a) and 1(b) show the experimental (Kido *et al* 1987) and calculated magnetisation curves $M(H)$ along the [100], [110] and [001] axes for $\text{Er}_2\text{Fe}_{14}\text{B}$ and $\text{Tm}_2\text{Fe}_{14}\text{B}$ at 78 K. The good agreement between the calculations and experiments would support the following results of the related calculations.

Figures 2(a) and (b) display the magnetic field dependences of the magnetic moment M_{R} of Er and Tm ions during the magnetisation processes along the [100], [110] and [001] axes. It can be seen that M_{R} is far from constant. It is remarkable that while a complete quenching of M_{R} occurs for both the Er and Tm ions during the magnetisation processes along the [100] and [110] axes, the quenching happens only for Tm ion during the magnetisation process along the [001] axis. Figure 3 displays the H dependences of the effective field H_{eff} acting on the Er and Tm ions during the magnetisation process along the [001] axis. With increase of H , H_{eff} acting on the Tm ion decreases and becomes zero at about 570 kOe, just where M_{Tm} quenches completely, while H_{eff} acting on the Er

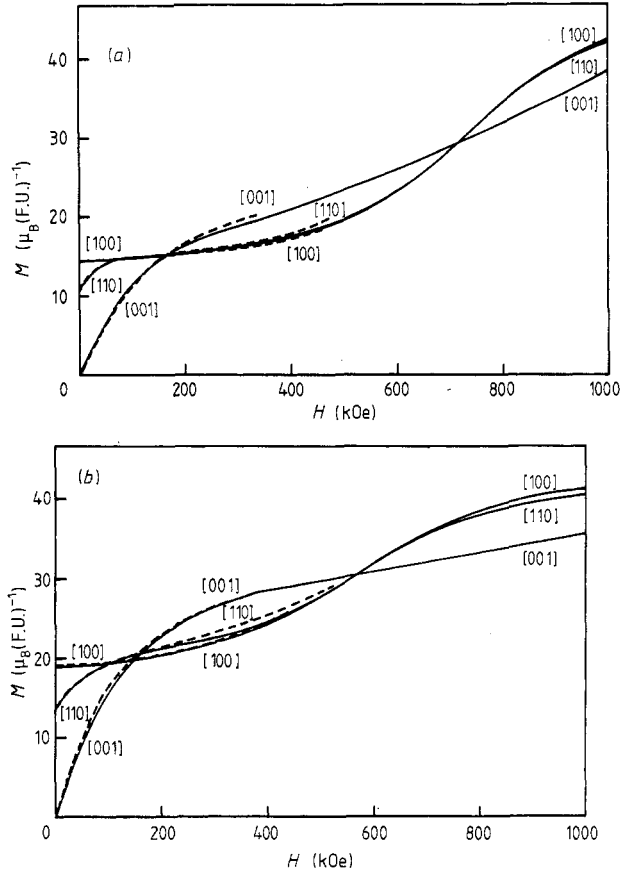


Figure 1. The magnetisation curves of (a) $Er_2Fe_{14}B$ and (b) $Tm_2Fe_{14}B$ along the [100], [110] and [001] axes at 78 K. The broken curve plots the experimental data of Kido *et al* (1987), and the full curve plots the present calculation.

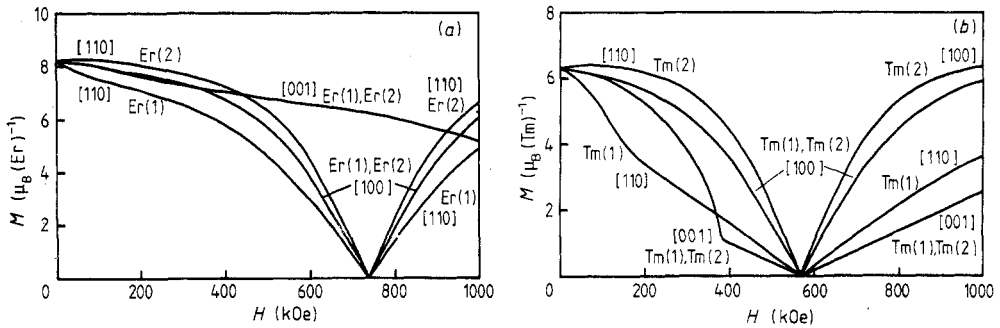


Figure 2. The magnetic moments M_R of (a) the Er and (b) the Tm ions as a function of H during the magnetisation processes along the [100], [110] and [001] axes at 78 K.

ion along with M_{Er} remains fairly large (figure 2). The complete quenching of M_{Tm} at $H_{eff} = 0$ is the result of the symmetry of the CEF part of the Hamiltonian in (1), which belongs to the Abelian point group D_{2h} . It can also be deduced from the symmetrical

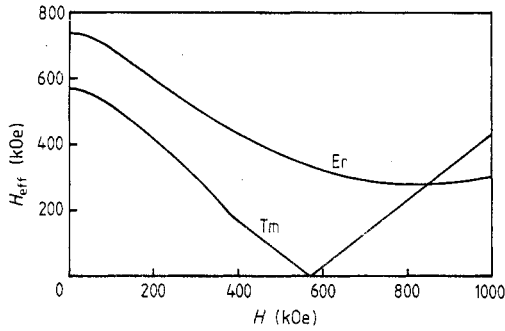


Figure 3. The effective fields H_{eff} acting on the Er and Tm ions as a function of H during the magnetisation process along the [001] axis at 78 K.

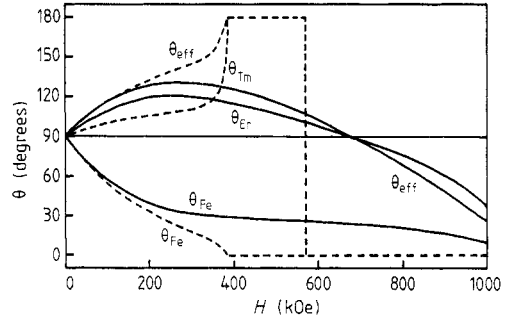


Figure 4. The field dependences of θ_{Fe} , θ_{R} and θ_{eff} for the Er (full curve) and Tm (broken curve) compounds during the magnetisation process along the [001] axis at 78 K.

consideration that an eigenstate of Tm ion is a linear combination of the functions from one of the following four sets of $|J = 6, M\rangle$ functions:

$$\begin{aligned}
 & |6, 0\rangle \quad |6, 2\rangle - |6, -2\rangle \quad |6, 4\rangle + |6, -4\rangle \quad |6, 6\rangle - |6, -6\rangle \\
 & |6, 2\rangle + |6, -2\rangle \quad |6, 4\rangle - |6, -4\rangle \quad |6, 6\rangle + |6, -6\rangle \\
 & |6, 1\rangle - i|6, -1\rangle \quad |6, 3\rangle + i|6, -3\rangle \quad |6, 5\rangle - i|6, -5\rangle \\
 & |6, 1\rangle + i|6, -1\rangle \quad |6, 3\rangle - i|6, -3\rangle \quad |6, 5\rangle + i|6, -5\rangle.
 \end{aligned} \tag{8}$$

It is apparent that the average of the operator \mathbf{J} for each eigenstate vanishes.

Figure 4 shows the magnetic field dependence of the angles θ_{Fe} , θ_{R} and θ_{eff} , made by \mathbf{M}_{Fe} , \mathbf{M}_{R} and \mathbf{H}_{eff} with the [001] axis respectively, for the Er and Tm compounds during the magnetisation process along the [001] axis. For the Er compound, \mathbf{M}_{Fe} , originally parallel to the [100] axis, rotates towards the \mathbf{H} direction monotonically, and \mathbf{M}_{Er} , coupled ferrimagnetically with \mathbf{M}_{Fe} , deviates first opposite to the \mathbf{H} direction for some 30° and then rotates towards the \mathbf{H} direction continuously with increase of the applied field up to 1000 kOe. The processes for the Tm compound are quite different. After behaving similar to the Er compound processes at the lower fields, \mathbf{M}_{Fe} becomes parallel to \mathbf{H} near 380 kOe, and correspondingly both \mathbf{H}_{eff} and \mathbf{M}_{Tm} become antiparallel to \mathbf{H} at the same field. Then, both \mathbf{H}_{eff} and \mathbf{M}_{Tm} , maintaining the collinearity with \mathbf{H} , decrease to zero and then increase along the \mathbf{H} direction. The angle φ_{R} that the projection of \mathbf{M}_{R} onto the (001) plane makes with the $[\bar{1}00]$ axis changes little during the magnetisation process. For example, φ_{Er} changes from 8° at $H = 0$ to 12° at 1000 kOe, and φ_{Tm} from 22° at $H = 0$ to 28° at 380 kOe. Figure 5 shows the stabilisation energies ΔF of the Er and Tm ions as a function of H applied along the [001] axis. ΔF is the difference between the free energies of the R ion with \mathbf{H}_{eff} applied along the [001] and [100] axes. The value of H_{eff} is that corresponding to H applied along the [001] axis (figure 3). In the low applied field range, ΔF , i.e. the axial magnetic anisotropy, is larger for the Tm ion than the Er ion, as is expected from the much higher value of the second-order Stevens coefficient of the former (1.01×10^{-2}) than that of the latter (0.25×10^{-2}). But with increase of H toward 570 kOe where \mathbf{M}_{Tm} quenches, ΔF for the Tm ion decreases to a smaller value than that of the Er ion, and approaches zero. At near 380 kOe the value of H_{eff} , and so of ΔF , for the Tm ion becomes so small that \mathbf{M}_{Fe} and \mathbf{M}_{Tm} are rotated to

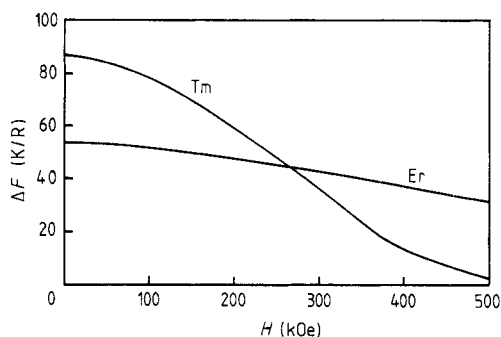


Figure 5. The field dependences of the stabilisation energies ΔF of the Er and Tm ions at 78 K. The field H is applied along the [001] axis.

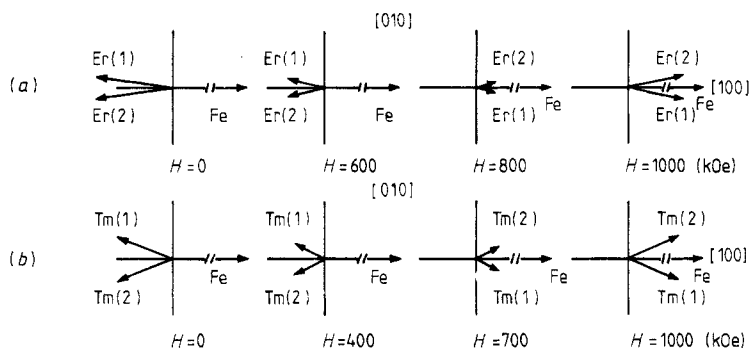


Figure 6. The magnetic structures of (a) $Er_2Fe_{14}B$ and (b) $Tm_2Fe_{14}B$ at different field strengths during the magnetisation process along the [100] axis at 78 K.

be parallel and antiparallel to H by the torques acted by H and H_{ex} respectively (figure 4).

Figure 6 illustrates the variation of the magnetic structures of the Er and Tm compounds during the magnetisation process along the [100] axis. The coupling between M_R and M_{Fe} remains non-collinear in the whole field range, and M_{Er} and M_{Tm} quench at $H = [2(g_J - 1)/g_J]H_{ex}$. During the magnetisation process along the [110] axis, M_R and M_{Fe} coupled ferrimagnetically in the low fields become collinear above 150 and 200 kOe for R = Er and Tm, respectively, with M_{Fe} becoming parallel to H . Maintaining the collinearity, the values of M_{Er} and M_{Tm} decrease to zero at about 740 and 570 kOe, respectively, and then increase along the H direction.

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