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Temperature dependence of the exchange field of $R_2Fe_{14}B$ ($R \equiv$ Sm, Pr, Nd, Gd, Dy, Tb, Er, Ho, Tm, Lu) compounds

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Abstract

Using the two-sublattice molecular field theory (MFT) the temperature dependences of $H_R(T)$ and $H_R(T)/M_{Fe}(T)$ of the intermetallic compounds $R_2Fe_{14}B$ have been analysed, and fitted forms of $H_R(T)$ and $H_R(T)/M_{Fe}(T)$ varying with temperature for each $R_2Fe_{14}B$ compound are presented.

1. Introduction

In order to understand the magnetism of the new permanent magnetic material $Nd_2Fe_{14}B$, the magnetic behaviour of the whole family of iron-rich systems $R_2Fe_{14}B$ was studied [1]. These compounds have the symmetry of the space group $P4_2/mnm$.

For analysing the spin-reorientation phenomena in $R_2Fe_{14}B$ compounds (*e.g.* plane-to-axis or cone-to-axis), the temperature dependence of the exchange field for each compound is needed. Especially for analysing the plane-to-axis transition, we must know the temperature dependence of the exchange field over a large range of temperatures. For analysing the magnetization processes of the rare earth ions in $R_2Fe_{14}B$ in high fields, the values of $H_R(T)/M_{Fe}(T)$ at any temperature should be known.

It has been proved that the two-sublattice molecular field theory (MFT) is very successful in describing the magnetization of R_nFe_m compounds [2–5], and that the results of MFT are consistent with the experimental data. In this investigation, the two-sublattice MFT is used, and analytic forms of $H_R(T)$ and $H_R(T)/M_{Fe}(T)$ are derived by the least-squares method.

2. Analysis

According to the two-sublattice model [2–5], the exchange field and the total effective field of the rare earth and iron sublattices in $R_2Fe_{14}B$ compounds

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can be expressed as follows:

$$H_R(T)=H+d[2n_{RR}M_R(T)+14n_{RFe}M_{Fe}(T)] \quad (1)$$

$$H_{Fe}(T)=H+d[2n_{FeR}M_R(T)+14n_{FeFe}M_{Fe}(T)] \quad (2)$$

The temperature dependence of each sublattice momentum is determined by the Brillouin functions

$$M_R(T)=M_R(0)B_{J_R}[M_R(0)H_R(T)/kT] \quad (3)$$

$$M_{Fe}(T)=M_{Fe}(0)B_{J_{Fe}}[M_{Fe}(0)H_{Fe}(T)/kT] \quad (4)$$

where H is the applied field. $M_R(T)$ and $M_R(0)$ (or $M_{Fe}(T)$ and $M_{Fe}(0)$) are the magnetic moments of the rare earth ion (or iron ion) at temperatures T and zero. The quantity $d=N_A\mu_B\rho/A$ converts the moment per $R_2Fe_{14}B$ molecule in Bohr magnetons to gauss, where ρ is the density of $R_2Fe_{14}B$ in grams per cubic centimetre, N_A is Avogadro's number and A is the $R_2Fe_{14}B$ formula weight. J_R and J_{Fe} are the individual angular momenta of the rare earth and iron respectively. The values of the density ρ, the rare earth gyromagnetic ratio g_J and the total angular momentum J_R used in the MFT calculations, as well as the coefficients n_{FeFe}, n_{RFe} and n_{RR} obtained in refs. 3 and 4, are listed in Table 1.

3. Results and discussion

The exchange field $H_R(T)$ experienced by the rare earth ions is composed of contributions due to R–R and R–T interactions. The strength of $H_R(T)$ will therefore be determined mainly by the R–T interactions. The curves of $H_R(T)$ for nine $R_2Fe_{14}B$ compounds were obtained by MFT calculation and have been plotted in Fig. 1. From these calculations we know that the

TABLE 1

Density ρ, rare earth gyromagnetic ratio g_J and total angular momentum J_R used in the MFT calculations[a]

R	ρ (g cm^{-3})	$M_{Fe}(0)$	$M_R(0)$	n_{FeFe}	n_{RFe}	n_{RR}	R(%)[b]
Pr	7.49	2.229	3.2	4718	80	1400	1.90
Nd	7.58	2.223	3.27	4860	340	1500	3.05
Sm	7.82	2.277	0.714	4827	250	2765	3.40
Gd	8.06	2.279	7.0	4799	3259	−960	3.40
Tb	7.96	2.229	9.0	4578	1322	−1158	6.22
Dy	8.07	2.236	10	4564	1340	−554	3.95
Ho	8.12	2.229	10	4439	700	−591	1.56
Er[c]	8.04	2.210	9.0	4335	240	−800	2.30
Tm[c]	8.09	2.221	7.0	4025	260	−850	1.29

[a] n_{FeFe}, n_{RFe} and n_{RR} are the MFT coefficients.

[b] R denotes the percentage of error, $R=(\Sigma_i|M_{exp}(Ti)-M_{cal}(Ti)|)/M_{exp}(Ti)$.

[c] This work.

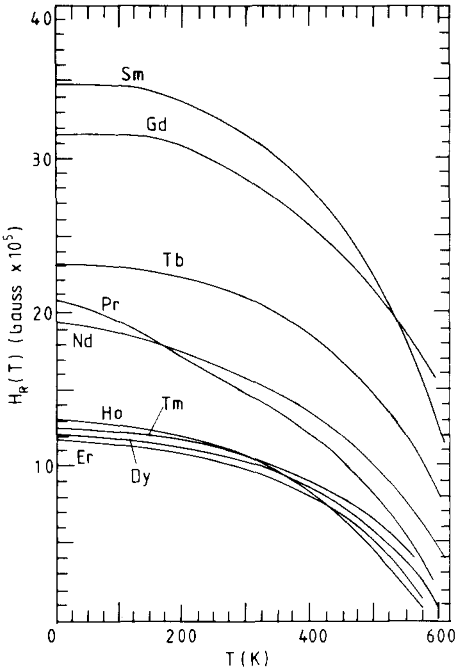

Fig. 1. Temperature dependence of $H_R(T)$ for nine $R_2Fe_{14}B$ compounds.

difference between the exchange fields for holmium, thulium, dysprosium and erbium ions in $R_2Fe_{14}B$ is not large.

Substituting the coefficients n_{FeFe}, n_{RFe} and n_{RR} into eqns. (1) and (2), we can obtain values of $H_R(T)$, which then can be fitted into the analytic form by the least-squares method:

$$H_R(T)/H_R(0) = 1 + a(T/T_c) + b(T/T_c)^2 \qquad (5)$$

or

$$H_R(T)/H_R(0) = 1 + A(T/T_c) + B(T/T_c)^2 + C(T/T_c)^3 \qquad (6)$$

The parameters a, b, A, B and C are listed in Table 2.

The expression $H_R(T) = H_R(0)[1 - \frac{1}{2}(T/T_c)^2]$ has sometimes been used to analyse magnetic properties, such as the spin-reorientation transition from cone to axis in $ErFe_{10}V_2$ and other magnetic materials [6–10]. At low temperatures, the values for this expression are close to that obtained from MFT calculations. However, at high temperatures ($T > 150$ K) there is a larger difference from the values of exchange field obtained from the MFT calculations. Especially for analysing the plane-to-axis reorientation phenomena we must know that values of the exchange field over a large temperature range. Thus we should use eqns. (5) and (6).

In the process of analysing the magnetization processes of rare earth ions in $R_2Fe_{14}B$ in high fields, the ratio of the exchange field and the iron moment at any temperature must be known. In Fig. 2 the curves for $H_R(T)$/

TABLE 2

The coefficients *a*, *b*, *A*, *B* and *C* appearing in eqns. (5) and (6)

R	a $(\times 10^{-4})$	b $(\times 10^{-6})$	A $(\times 10^{-4})$	B $(\times 10^{-6})$	C $(\times 10^{-9})$
Sm	8.062	2.784	1.666	1.223	4.291
Pr	3.304	−1.700	10.25	1.386	3.356
Nd	1.794	2.086	6.442	1.395	3.766
Ho	3.870	2.898	5.430	1.028	4.208
Er	10.91	4.217	5.836	2.718	7.318
Gd	4.711	1.965	0.4839	0.1938	2.338
Dy	9.593	3.733	5.510	2.527	6.642
Tm	11.40	4.351	5.601	2.684	7.412
Tb	5.973	2.484	2.084	0.8648	3.605

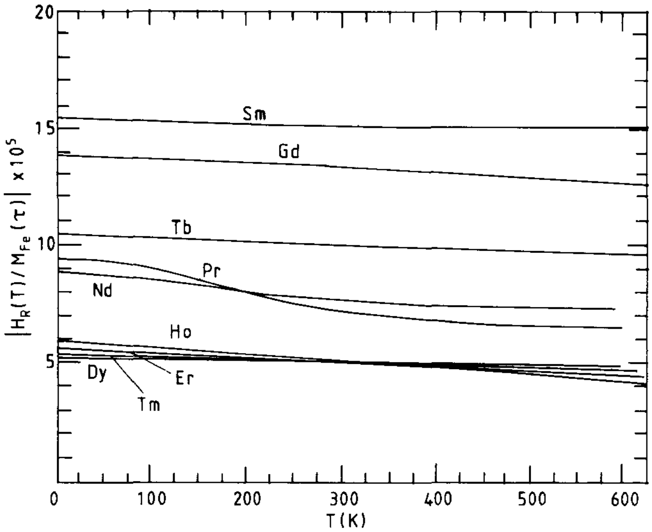

Fig. 2. The curves of $H_R(T)/M_{Fe}(T)$ *vs.* temperature for each of the compounds $R_2Fe_{14}B$.

$M_{Fe}(T)$ varying with temperature for nine $R_2Fe_{14}B$ compounds are presented. The ratio is not a constant but depends on temperature. Except for $Sm_2Fe_{14}B$, the values of $H(T)/M(T)$ of these compounds decrease for $T < T_c$. It is easy to see that these curves are nearly straight lines. In Table 3, we list the coefficients of k appearing in the expression

$$\frac{H_R(T)}{M_{Fe}(T)} = \frac{H_R(0)}{M_{Fe}(0)}(1 + kT) \tag{7}$$

obtained by using the least-squares method. Several authors [11] have assumed that the ratio $H_R(T)/M_{Fe}(T)$ is independent of temperature. For the thulium ions in $R_2Fe_{14}B$, the ratio becomes smaller near T_c. For the dysprosium, thulium and erbium ions in $R_2Fe_{14}B$ the difference in $H_R(T)/M_{Fe}(T)$ between

TABLE 3

The values of $H_R(0)/M_{Fe}(0)$ and k used in eqn. (7)

R	$H_R(0)/M_{Fe}(0)$ ($\times 10^5$)	k ($\times 10^{-4}$)
Sm	15.203	0.1394
Pr	9.2787	−5.3024
Nd	8.6469	−2.6477
Ho	−5.8798	−4.5267
Er	−5.3222	1.9008
Gd	−13.760	0.6333
Dy	−5.3785	1.7115
Tm	−5.4587	1.6986
Tb	−10.428	0.9106

high temperatures and low temperatures is not large, but for the praseodymium and neodymium ions in $R_2Fe_{14}B$ this difference becomes about 20%, and should be taken into consideration when analysing the magnetization processes of the rare earth ions in $R_2Fe_{14}B$.

Acknowledgments

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