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Letter

Note on the anisotropy fields in tetragonal $RFe_{10}V_2$ compounds

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Abstract

The temperature dependence of the anisotropy field in $RFe_{10}V_2$ (R≡Nd, Sm, Tb, Dy, Ho, Er, Lu and Y) has been studied from cryogenic temperatures up to the corresponding Curie temperatures. It is shown that the R sublattice anisotropy at room temperature is mainly determined by the second-order crystal field contribution, although fourth-order contributions are substantial and gain in weight at lower temperatures. A comparatively large R sublattice contribution is found in $SmFe_{10}V_2$, indicating the participation of higher multiplet levels.

The $RFe_{10}V_2$ compounds crystallize in a relatively simple structure based on the $ThMn_{12}$ type. There is only a single crystallographic R site and the vanadium atoms are restricted to one of the three transition metal sites. Previous investigations have shown that the magnetocrystalline anisotropy is fairly large in some of these compounds at 4.2 K [1, 2]. However, it has proved difficult to explain the easy magnetization direction in terms of an iron sublattice anisotropy favouring an easy *c* axis and an R sublattice anisotropy governed mainly by the second-order crystal field term. For an adequate description of the anisotropic behaviour of these compounds it therefore appears necessary to include higher-order terms. In the present investigation we have studied the temperature dependence of the anisotropy field for most of the compounds in order to determine the extent to which the influence of the higher-order terms is already present at around room temperature.

The samples $RFe_{10}V_2$ were prepared by standard arc melting from elements of at least 99.9% purity. After arc melting, the samples were wrapped in tantalum foil and subsequently annealed at 950 °C for several weeks inside an evacuated silica tube. After annealing, the samples were investigated by

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X-ray diffraction. All the samples that were prepared in this way were found to be approximately single phase, the crystal structure of the $RFe_{10}V_2$ phases corresponding to that of the tetragonal $ThMn_{12}$ structure type. The temperature dependence of the anisotropy field H_A of the various compounds was determined by means of the singular point detection method (SPD) using pulsed fields.

Results of the SPD measurements are shown in Fig. 1. It can be seen that the anisotropy fields of the compounds investigated show a fairly gradual decrease with temperature in the high-temperature regime and vanish at temperatures close to the corresponding Curie temperatures determined previously [1]. The data obtained for $SmFe_{10}V_2$ show a much greater decrease of H_A with temperature, particularly below room temperature. No cusp-shaped SPD signal was observed for $NdFe_{10}V_2$ in the high-temperature range. Since neutron diffraction [2] had shown that the easy magnetization is parallel to the *c* axis at room temperature, these results may be taken as indication that H_A in $NdFe_{10}V_2$ is comparatively weak in the high-temperature range.

The room temperature values of the anisotropy fields can be compared with each other in Table 1. It can be seen that by far the largest value is found in $SmFe_{10}V_2$; the other values being close to or only slightly higher than the anisotropy fields found in the compounds with non-magnetic yttrium or luthenium. Previous measurements of the anisotropy fields of $RFe_{10}V_2$ compounds were made by Solzi *et al.* [3] for R=Y and Er. Their results are in good agreement with our data.

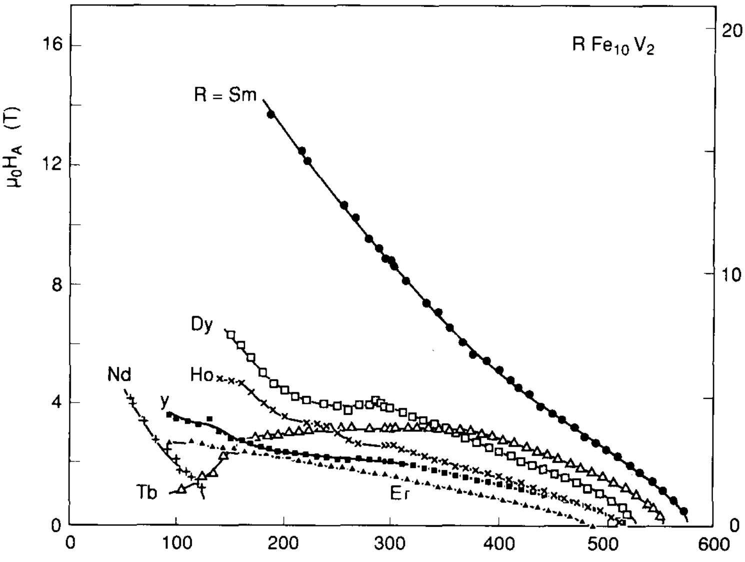

Fig. 1. Temperature dependence of the anisotropy fields in various $RFe_{10}V_2$ compounds derived from SPD measurements.

TABLE 1

Room temperature anisotropy fields (H_A) and magnetic polarization (J) obtained by means of SPD measurements on powder samples[a]

	$\mu_0 H_A$ (T)	J (T)	K_1+2K_2 (MJ m^{-3})	$K_1^R+2K_2^R$ (MJ m^{-3})	m_R (300 K)	$\alpha\langle r^2\rangle\langle O_{20}\rangle$ (×100)	$\beta\langle r^4\rangle\langle O_{40}\rangle$ (×100)
Nd	–	1.1	–	<0	0.40	−1.70	−0.01
Sm	10.5	1.0	4.20	+3.6	0.61	+8.76	+0.20
Tb	3.2	0.47	0.60	−0.0	0.72	−19.72	+4.25
Dy	3.9	0.50	0.78	+0.1	0.64	−13.55	−1.06
Ho	2.2	0.58	0.51	−0.1	0.55	−3.38	−0.25
Er	1.5	0.70	0.42	−0.2	0.44	+1.70	+0.03
Lu	1.7	0.80	0.54	0	0	0	0
Y	2.2	0.82	0.72	0	0	0	0

[a] The values of K_1+2K_2 listed correspond to the total anisotropy, those of $K_1^R+2K_2^R$ only to the R sublattice anisotropy. The values of the reduced R sublattice magnetization m_R at 300 K were used to derive the expectation values of the Stevens operators $\langle O_{nm}\rangle$ at room temperature (see text).

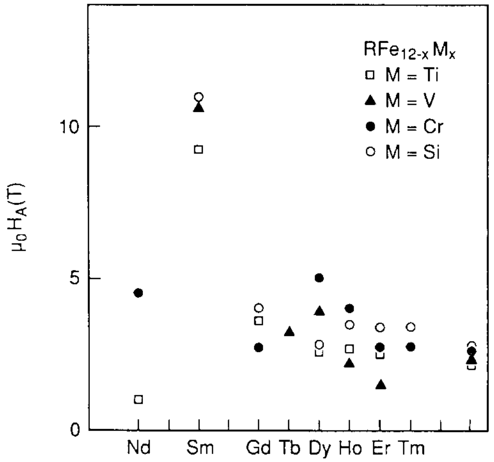

Fig. 2. Comparison of the room temperature anisotropy fields in various $RFe_{12-x}M_x$ compounds of the tetragonal $ThMn_{12}$ structure, using the data obtained in the course of the present investigation and those reported in the literature [3–6].

Our values for the room temperature fields in $RFe_{10}V_2$ compounds are compared in Fig. 2 with the literature data [3–5] of the anisotropy fields in other compounds of the type $RFe_{12-x}M_x$ (M≡Ti, Cr, Si). The trend of H_A in all these materials is approximately the same. Large excess anisotropies with respect to those of the corresponding yttrium compounds are found mainly in the samarium compounds.

The anisotropy field H_A can be expressed in terms of the lowest order anisotropy constants K_n and the magnetic polarization J via the relation

$$K_1+2K_2=\tfrac{1}{2}JH_A \tag{1}$$

Experimental values of the room temperature polarization have been included in Table 1. The values of K_1+2K_2 calculated by means of eqn. (1) can be found in the third column of Table 1. These anisotropy constants are composed of contributions of the iron sublattice (only K_1^{Fe}) and the R sublattice $K_1^{\mathrm{R}}+2K_2^{\mathrm{R}}$. The latter values can be obtained after subtracting the iron sublattice contribution. For the iron sublattice contribution we used the mean value of the data of $\mathrm{LuFe_{10}V_2}$ and $\mathrm{YFe_{10}V_2}$. It can be seen from the values of $K_1^{\mathrm{R}}+2K_2^{\mathrm{R}}$ listed in the table that the R sublattice contribution in $\mathrm{SmFe_{10}V_2}$ is more than an order of magnitude larger than the other $\mathrm{RFe_{10}V_2}$ compounds.

It is interesting to compare the $K_1^{\mathrm{R}}+2K_2^{\mathrm{R}}$ values listed with predictions of crystal-field theory. It is well known that the K_n values can be expressed in terms of the crystal-field parameters A_{nm} and the Stevens operator equivalents O_{nm} (see for instance the review of Li and Coey [6]):

$$K_1=-\tfrac{3}{2}\alpha\langle r^2\rangle \mathrm{A}_{20}\langle \mathrm{O}_{20}\rangle-5\beta\langle r^4\rangle \mathrm{A}_{40}\langle \mathrm{O}_{40}\rangle \tag{2}$$

$$K_2=\tfrac{35}{8}\beta\langle r^2\rangle \mathrm{A}_{40}\langle \mathrm{O}_{40}\rangle \tag{3}$$

where $\langle r^n\rangle$ are expectation values of the Hartree–Fock 4f radii and α and β are the Stevens factors. We have left sixth-order terms out of consideration in eqns. (2) and (3) because they are negligible at room temperature. The reason for this is that the larger the values of n, the more significantly the expectation values $\langle \mathrm{O}_{nm}\rangle$ decrease with temperature. In fact $\langle \mathrm{O}_{nm}\rangle$ decreases with temperature as m_{R}^p, where $m_{\mathrm{R}}=M_{\mathrm{R}}(T)/M_{\mathrm{R}}(\mathrm{O})$ is the reduced R sublattice magnetization and $p=\frac{1}{2}n(n+1)$.

Values of $m_{\mathrm{R}}(T)$ for $T=300$ K are available from a mean-field description obtained previously for the $\mathrm{RFe_{10}V_2}$ compounds [7]. These values have been listed in the fifth column of Table 1. Room temperature values of $\alpha\ \langle r^2\rangle\langle \mathrm{O}_{20}\rangle$ and $\beta\ \langle r^4\rangle\langle \mathrm{O}_{40}\rangle$ were derived by using the values listed for these quantities at 0 K by Li and Coey [6] and scaling them with m_{R}^3 and m_{R}^{10} respectively. These room temperature values are included in Table 1. The m_{R} values of Table 1, or rather m_{R}^{21}, and the $\gamma\ \langle r^6\rangle\langle \mathrm{O}_{60}\rangle$ listed for 0 K by Li and Coey were used to calculate the sixth-order contribution at room temperature. It was checked that these contributions are negligible.

It is generally assumed that the crystal field parameters A_{nm} do not vary much when passing through a series of rare-earth compounds as long as there is no structural change. Attempts were therefore made to fit the experimental $K_1^{\mathrm{R}}+2K_2^{\mathrm{R}}$ values listed in Table 1 by means of eqns. (2) and (3) using R-independent sets of A_{20}, A_{40} values. No such set of A_{20}, A_{40} values could be found; the main difficulty being the extraordinarily large experimental value found for $\mathrm{SmFe_{10}V_2}$ in comparison with the other $\mathrm{RFe_{10}V_2}$ compounds. It has to be concluded, therefore, that there is considerable enhancement of the samarium single-ion anisotropy in $\mathrm{SmFe_{10}V_2}$ arising from a crystal-field and exchange-induced admixture of higher multiplet levels into the ground state multiplet of $\mathrm{Sm^{3+}}$. A similar anisotropy enhancement of samarium relative to the other lanthanides was also observed in compounds of the type $SmFe_{11}Ti$ [6].

Although we are not able to present a set of R independent A_{20}, A_{40} values appropriate for the $RFe_{10}V_2$ compounds, we can derive from our experimental data that there is a significant contribution of the fourth-order terms, even at room temperature. Qualitatively, this can be seen from our experimental data by comparing the data for $TbFe_{10}V_2$ with those of $DyFe_{10}V_2$ and $HoFe_{10}V_2$. As seen from Table 1, the fourth-order term in $TbFe_{10}V_2$ differs in sign from that of the other two compounds. Since the fourth-order contribution decreases more significantly with temperature than the second-order contribution, one expects the opposite trend for $TbFe_{10}V_2$ compared to $DyFe_{10}V_2$ and $HoFe_{10}V_2$. This is indeed seen to be the case in Fig. 1. Similar conclusions regarding a relatively large contribution of higher-order terms to the anisotropy in $RFe_{10}V_2$ compounds had already been reached by Solzi *et al.* [3] when comparing the temperature dependence of the anisotropy fields in $ErFe_{10}V_2$ and $YFe_{10}V_2$.

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