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STRUCTURAL AND MAGNETIC PROPERTIES OF $R(\text{Ti, Fe})_{12}$

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Abstract. – The crystallographic and intrinsic magnetic properties of $R(\text{Ti, Fe})_{12}$, where R represents Nd, Sm, Gd, Te, Dy, Ho, Er and Y, have been investigated by X-ray diffraction and magnetic measurements. They crystallize in the ThMn_{12} structure type. A variety of magnetocrystalline anisotropy including easy axis, easy plane and spin reorientation has been found. The Curie temperatures and saturation magnetizations at 1.5 K are reported.

Introduction

SmTiFe_{11} has been found to have strong uniaxial anisotropy and a relatively high Curie temperature, both of which are comparable to those of $\text{Nd}_2\text{Fe}_{14}\text{B}$ [1-3]. In general, rare earth atoms play an important role for determining the magnetocrystalline anisotropy in 4f-3d intermetallic compounds. In this paper, a systematic study has been made to investigate the structural and magnetic properties of RTiFe_{11} , where R represents rare earth elements.

Experiments

The samples were prepared by arc-melting of 99.9 % pure primary materials in a purified argon atmosphere. X-ray diffraction experiment, electron microscope observations and thermomagnetic analyses were used to identify the single phase. Magnetization curves at 1.5 K and room temperature were measured on aligned samples with a field of up to 70 kOe. Magnetic measurements, as well as X-ray diffraction experiments performed on powdered samples aligned in a field of about 10 kOe at room temperature were made to determine the easy magnetization direction. Curie temperature were measured by using a vibrating-specimen magnetometer in a temperature range between 300 K and 1100 K.

Results and discussions

1. CRYSTALLOGRAPHIC STRUCTURE. – All of the samples prepared were proved to be the single tetragonal phase, except a second phase coexist in NdTiFe_{11} . Lattice constants, unit cell volume V and density ρ_x are listed in table I. It is obvious that when R moves from Nd to Er, the lattice constants and the volume of unit cell V decrease, while the X-ray density ρ_x increases.

2. THE CURIE TEMPERATURES. – The Curie temperature T_c of RTiFe_{11} are listed in table I. T_c of YTiFe_{11} can be referred to the Fe-Fe interactions in this structure. However, the Curie temperature of YTiFe_{11} is

Table I. – Crystallographic and magnetic properties of RTiFe_{11} : a , c : lattice constants. V : volume of the unit cell. ρ_x : X-ray density. T_c : Curie temperature. α_J : the Stevens factor.

RTiFe_{11}	a (Å)	c (Å)	V (Å ³)	ρ_x (g/cm ³)	T_c (K)	α_J
R = Y	8.5028	4.7946	346.6	7.199	540	0
Nd	8.5740	4.9074	360.8	7.426	570	–
Sm	8.5572	4.7994	351.4	7.681	600	+
Gd	8.5476	4.7988	350.6	7.765	610	0
Tb	8.5372	4.8078	350.4	7.785	580	–
Dy	8.5212	4.7990	348.4	7.863	560	–
Ho	8.5056	4.7986	347.2	7.916	543	–
Er	8.4951	4.7948	346.0	7.964	530	+

a little higher than that of ErTiFe_{11} , as was observed in other RFe compounds [4]. T_c reaches a maximum at GdTiFe_{11} . The R-Fe coupling strength varies as $(g-1)^2 J(J+1)$ in the heavy rare earth compounds, while an enhancement of the R-Fe interaction is observed in Nd and Sm compounds. This is in agreement with the argument of Belorizky *et al.* [5].

However the Curie temperatures of these compounds are still very low compared with that of the pure metal iron. In the RTiFe_{11} compounds, iron atoms are distributed on three crystallographically non-equivalent sites which are designated as Fe(8i), Fe(8j) and Fe(8f). The interatomic distance between two Fe atoms on 8f sites is 2.382 Å, and that on 8i sites is 2.390 Å [6]. With such short distances, reduced magnetic interactions, or even negative interactions, are possible. Proper substitutions for iron atoms for improving the Curie temperature in these compounds should be hopeful and some of the work has been done [7].

3. SATURATION MAGNETIC MOMENT. – The values of saturation magnetization measured at 1.5 K in an applied field of 70 kOe are listed in table II. The Fe moment M_{Fe} is obtained from YTiFe_{11} . The deduced R moments M_{R} are shown in table II. A plus sign in front of these numbers means that M_{Fe} and M_{R} are parallel, and a minus sign means that they are antiparallel. For

Table II. - Saturation magnetization (σ_s) of several RTiFe₁₁ compounds measured with a field of up to 70 kOe at 1.5 K. M_s , M_{Fe} and M_R represent the total saturation moment per formula unit, the Fe moment and the R moment.

RTiFe ₁₁	σ_s (emu/g)	M_s (μ_B /f.u.)	M_{Fe} (μ_B /Fe)	M_R (μ_B /R)	gJ
R = Y	138.019	18.568	1.7	0	0
Nd	147.277	21.273	1.7	2.7	3.3
Sm	131.356	19.118	1.7	0.6	0.7
Gd	84.907	12.462	1.7	-6.1	7.0
Tb	65.513	9.635	1.7	-8.9	9.0
Dy	63.368	9.360	1.7	-9.2	10.0
Ho	64.681	9.582	1.7	-9.0	10.0
Er	66.667	9.904	1.7	-8.7	9.0

free 3⁺ ions one expects the M_R values to be equal to $gJ\mu_B$ per R atom. Comparison of the M_R values with the values of gJ in table II shows that there is a good agreement.

4. MAGNETOCRYSTALLINE ANISOTROPY. - By analysing the magnetization curves and the X-ray diffraction pattern of aligned powder samples, a variety of magnetocrystalline anisotropy of RTiFe₁₁ is observed.

The *c*-axis is the easy axis for R = Y, Sm, Gd and Ho.

A spin reorientation occurs with varying temperature for R = Nd, Dy, Tb and Er. Figure 1 shows the variation magnetizations as a function of temperature for DyTiFe₁₁ and ErTiFe₁₁ at a field of 5 kOe; spin reorientation temperature corresponds to 175 K and 60 K, respectively.

GdTiFe₁₁ is found to have a large uniaxial anisotropy with $K_1 = 1.606 \times 10^7$ erg/cm³ at 1.5 K, indicating the strong uniaxial magnetocrystalline anisotropy for the Fe sublattice in the RTiFe₁₁

compounds. For R sublattice in a given series of isotopic compounds it is reasonable to assume that in the compounds for which α_J of the R ions has the same sign, the corresponding anisotropy constants value K_1 should have the same sign and the anisotropy properties should be the same, where α_J is the second-order Stevens constant which is included in table I.

NdTiFe₁₁ and DyTiFe₁₁ have an easy axis at room temperature. The easy magnetization direction deviates from the *c*-axis at low temperature. These spin reorientation results from the competition between R and Fe sublattices. At room temperature, the anisotropy contribution from Fe sublattice is dominant, and at low temperature, the contribution from Dy and Nd sublattices changes the easy direction in these compounds. In contrast, the anisotropy contribution of Fe sublattice in HoTiFe₁₁ is dominant for the whole observed temperature range. TbTiFe₁₁ and ErTiFe₁₁ exist an easy axis at room temperature. They both change their easy directions at low temperature. The detailed calculations explaining the spin reorientation in these compounds will be published elsewhere.

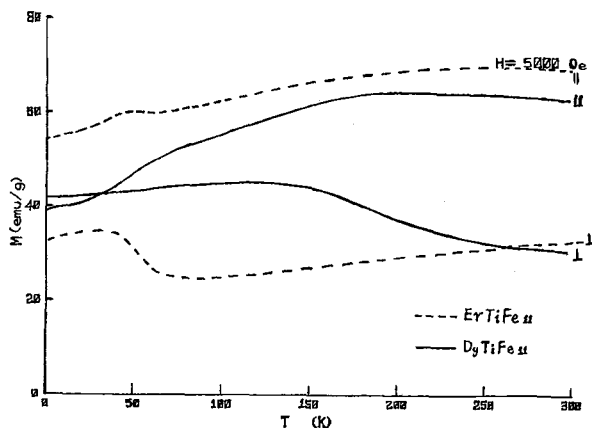


Fig. 1. - Temperature dependence of magnetization of DyTiFe₁₁ and ErTiFe₁₁ aligned samples measured with a field of 5 kOe parallel and perpendicular to the aligned direction.

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