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ANISOTROPY CONSTANTS OF $(Sm_{0.5}RE_{0.5})Fe_{11}Ti$ COMPOUNDS (RE=RARE EARTH)

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Abstract - Using by the x-ray diffractometry(XRD), the thermomagnetic analysis(TMA), a scanning electron microscopy (SEM-EDX), we knew that the $(Sm_{0.5}RE_{0.5})Fe_{11}Ti$ (RE=Ce,Pr,Nd,Sm,Gd,Tb) compounds were formed to tetragonal $ThMn_{12}$-type structure having a uniaxial magnetocrystalline anisotropy with easy magnetization c-axis. The intrinsic magnetic properties of those were determined by fitting the two magnetization curves of experimental and calculation magnetization. The anisotropy constant K_1 of this compounds was in the range of 1.75 - 9.2 MJ/m^3 and approximately one order higher than K_2.. $SmFe_{11}Ti$ had the highest anisotropy of K_1 = 9.2 MJ/m^3, K_2 = 0.4 MJ/m^3 and $\mu_0 H_A$= 19.8 T among the compounds, substitution of any other rare earth elements for Sm decreased magnetocrystalline anisotropy.

I. INTRODUCTION

Since the discovery of $Nd_2Fe_{14}B$ compound[1], novel iron-rich rare earth-transition metal materials as a permanent magnet have been continiously researched. The first attention has been focused $RE(Fe,TM)_{12}$ compounds (RE=rare earth, TM= transition metals) with $ThMn_{12}$-type structure[2,3]. Among them, the $SmFe_{11}Ti$ compound seems to be the most suitable candidate for permanent magnet applications[4] because of having not only high magnetocrystalline anisotropy but also relatively high magnetization and Curie temperature. But there is no anisotropy constants K_1 and K_2 reported in this $ThMn_{12}$-type compounds. Up to now, no systematic study has been reported on the magnetic properties of $(Sm,RE)Fe_{11}Ti$ compounds with the various RE elements except RE=Sm because of difficulty to obtain the single phase. In this article, we report the intrinsic magnetic properties of $(Sm_{0.5}RE_{0.5})Fe_{11}Ti$ compounds (RE=Ce, Pr,Nd,Sm,Gd,Tb) having $ThMn_{12}$-type structure, and effect of rare-earth elements on the magneto-crystalline anisotropy of $ThMn_{12}$-type compounds.

II. EXPERIMENTAL

The alloys of $(Sm_{0.5}RE_{0.5})Fe_{11}Ti$ (RE=Ce,Pr,Nd Sm,Gd,Tb,Dy) were prepared by argon arc melting starting elements with purities of at least 99.9%. An axess amount of Rare earth elements was added to compensate for the loss during melting. The alloys were homogenized at 1000 °C for 4 hours and they were ground into powders smaller than 45 μm in size. X-ray diffraction with Cu-K_α radiation(XRD) was used to identify the structure and easy magnetization direction(EMD) of the alloys, and the phase was examined by a scanning electron microscope(SEM) with energy dispersive x-ray analysis(EDX). The thermo-magnetic analysis(TMA) was performed in order to know the phase and the curie temperature by a vibrating sample magnetometer(VSM) under a constant low field of 80 kA/m (1 kOe). For the measurement of magnetic properties, the powders mixed with paraffin (C_nH_{2n+2}) were aligned and solidificated in a magnetic field of about 1200 kA/m (~15 kOe). The magnetization curves along the parallel and perpendicular to the alignment direction were measured by a superconducting quantum interference device(SQUID) magnetometer. The anisotropy constants (K_1,K_2), magnetization(J_s) were determined by fitting the two magnetization curves to theoretical values.

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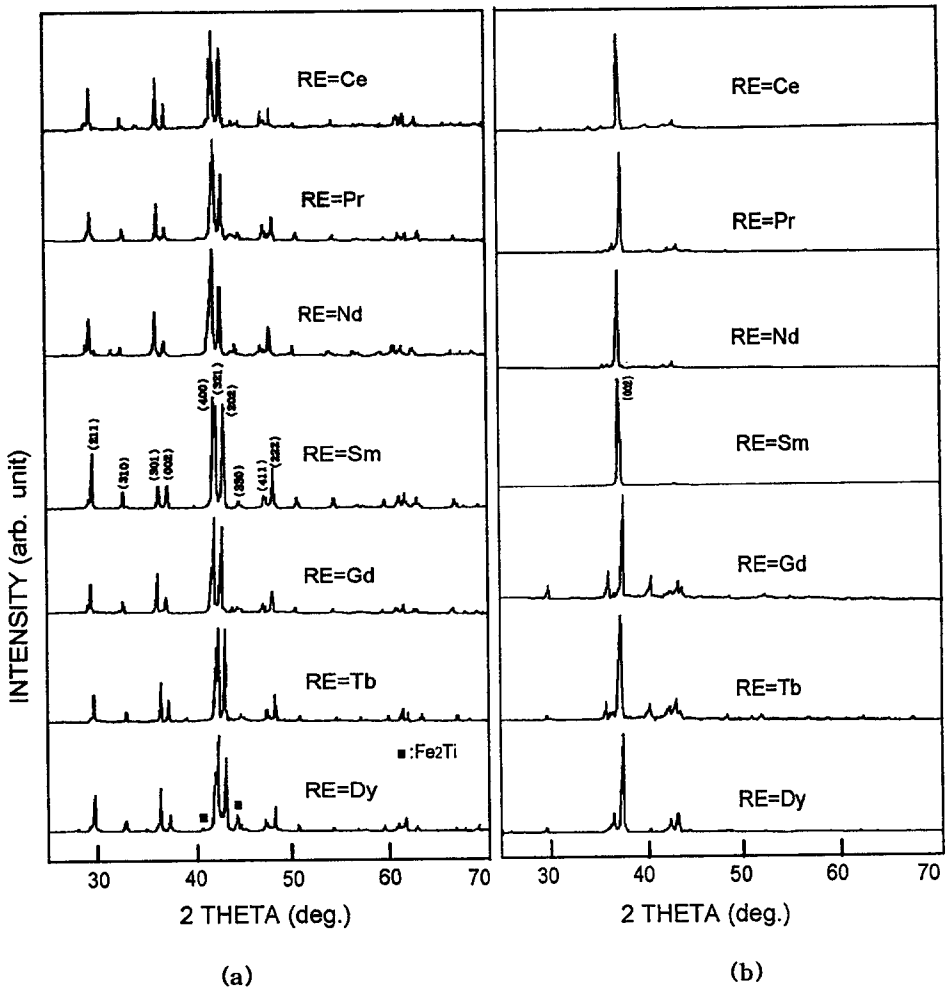

Fig. 1 X-ray diffraction pattern of (a) random and (b) aligned powder of $(Sm_{0.5}RE_{0.5})Fe_{11}Ti$ (RE=Ce,Pr,Nd,Sm,Gd,Tb,Dy) compounds

III. RESULTS AND DISCUSSION

We fabricated the nearly single phased $ThMn_{12}$-type compounds by homogenizing the arc-melted alloys at 1000 °C for 4 hours. Using by XRD, SEM-EDX and TMA, it has been found that the $(Sm_{0.5}RE_{0.5})Fe_{11}Ti$ (RE=Ce,Pr,Nd,Sm,Gd,Tb) specimens consisted of $ThMn_{12}$-type structure with small amount of Fe_2Ti and negligible α-Fe as shown in Fig. 1 (a). Among $(Sm_{0.5}RE_{0.5})Fe_{11}Ti$ (RE=Ce,Pr,Nd,Sm,Gd,Tb,Dy) specimens, the alloy of RE=Dy was estimated to contain about 5 volumetric percent of Fe_2Ti by SEM-EDX analysis. The other alloys were nearly single phase of $ThMn_{12}$-type structure with negligible Fe_2Ti. In order to know the easy magnetization direction(EMD), we examined the x-ray diffraction patterns of the alloy powders aligned in a magnetic field. For our experiments, the plane of diffraction was perpendicular to the aligned direction. As shown in fig. 1(b), a drastic increase of intensity of (002) peak was observed in each of the alloys for comparison with the diffraction patterns of random powder in fig. 1(a). This results suggest that all the $(Sm_{0.5}RE_{0.5})Fe_{11}Ti$ (RE=Ce,PrNd,Sm,Gd,Tb,Dy) compounds uniaxial

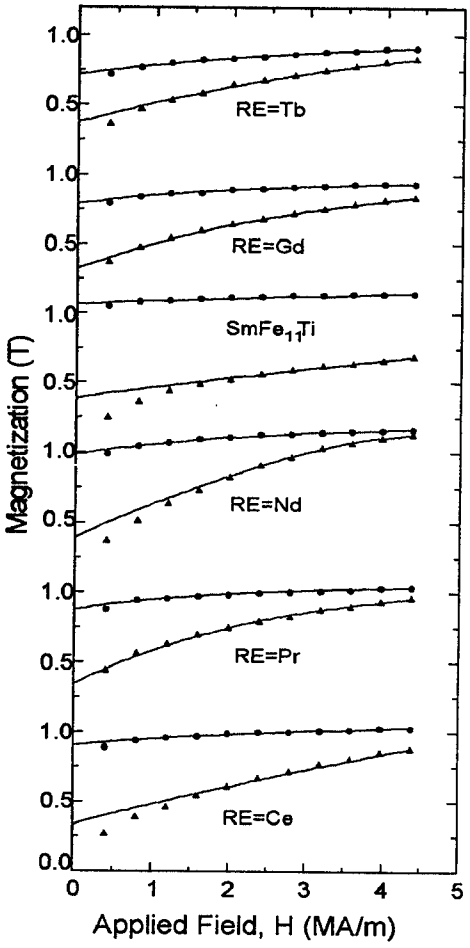

Fig. 2 Magnetization of magnetically aligned $(Sm_{0.5}RE_{0.5})Fe_{11}Ti$ (RE=Ce,Pr,Nd,Sm,Gd,Tb) powders measured parallel(●) and perpendicular(▲) to the alignment direction. The solid line are calculated results based on the fitting method.

anisotropy with c-axis EMD.

$TbFe_{11}Ti$ has in-plane anisotropy at room temperature[5,6]. In this work, $(Sm_{0.5}Tb_{0.5})Fe_{11}Ti$ compound in which the half of Tb was substituted by Sm in $TbFe_{11}Ti$, was found to show uniaxial anisotropy because of the attribution of Sm atoms with the strong uniaxial anisotropy. The lattice constants a_o and c_o calculated from (002) and (321) peaks of random powders were listed in Table 1.

Fig. 2 shows the magnetization curves measured parallel (closed circle) and perpendicular (closed triangle) to the alignment direction. As shown in the fig. 2, all the curves do not meet as high as H=4.4 MA/m (55 kOe), indicating high magnetocrystalline anisotropy of $(Sm_{0.5}RE_{0.5})Fe_{11}Ti$ compounds. The magnetocrystalline aniso-anisotropy constants K_1 and K_2 were determined by the fitting method reported in literratures[7,8].

In order to determine the magnetocrystalline anisotropy constants, we calculated the magnetization of each crystallite by minimizing the total free energy

$$F=K_1\sin^2\theta+K_2\sin^4\theta-M_sH\cos(\delta-\theta) \qquad (1)$$

where θ is the angle between c-axis and magnetization M_s, and δ is the angle between c-axis and applied magnetic field H as shown fig. 3. In calculation, the c-axis of crystallites is assumed to distribute as Gaussian function around

Table 1 Physical and intrinsic magnetic properties of $(Sm_{0.5}RE_{0.5})Fe_{11}Ti$ compounds.

Compounds	E.M.D	Lattice const. a_o[nm]	c_o[nm]	Density [g/cm^3]	Js [T]	K_1 [MJ/m^3]	K_2 [MJ/m^3]	ϕ_o [°]	μ_oH_A [T]	T_c [°K]
$SmFe_{11}Ti$	c axis	0.854	0.478	7.57	1.27	9.20	0.40	24.9	19.8	587
$Sm_{0.5}Ce_{0.5}Fe_{11}Ti$	c axis	0.855	0.479	7.63	1.10	3.40	-0.35	25.2	6.2	552
$Sm_{0.5}Pr_{0.5}Fe_{11}Ti$	c axis	0.855	0.479	7.62	1.07	1.75	0.50	26.3	6.5	561
$Sm_{0.5}Nd_{0.5}Fe_{11}Ti$	c axis	0.858	0.479	7.60	1.21	2.35	-0.14	26.6	4.3	568
$Sm_{0.5}Gd_{0.5}Fe_{11}Ti$	c axis	0.855	0.479	7.62	0.98	2.02	0.48	27.5	7.6	608
$Sm_{0.5}Tb_{0.5}Fe_{11}Ti$	c axis	0.852	0.478	7.72	0.98	2.44	0.16	34.4	7.1	588
$Sm_{0.5}Dy_{0.5}Fe_{11}Ti$	c axis	0.852	0.477	7.71	---	---	---	---	---	568

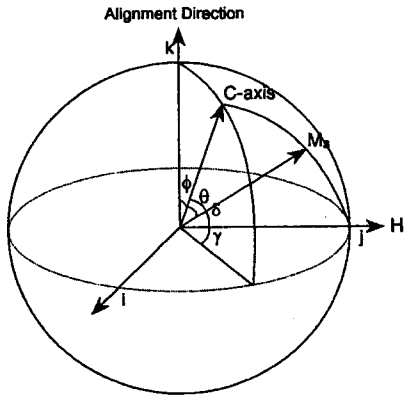

Fig. 3 Schematic representation of the angle θ, δ and ϕ of single particle.

the alignment direction, that is

$$f(\phi)=\exp(-\phi^2/2\phi_0^2)/\int\exp(-\phi^2/2\phi_0^2)d\omega \qquad (2)$$

where ϕ is the angle between c-axis and alignment direction, and ϕ_0 is the width of the Gaussian distribution which represents the degree of alignment. Finally, we calculated the magnetization as follows;

$$M=\int M_s \cdot H/H f(\phi)d\omega \qquad (3)$$

The solid curves in fig. 2 are the calculation results reproducing the experimental results satisfactorily except the low applied fields. Since the homogeneous rotation of magnetization was presumed, the experimental data above 2 MA/m (2.5 T) were used for the caculation. The values of J_s, K_1, K_2 and ϕ_0 derived from the fitting process of the measurement curves and the calculation data are listed in Table 1. The anisotropy constant K_1 was in the range of 1.75 - 9.2 MJ/m^3 and approximately one order higher than K_2. Among the compounds, $SmFe_{11}Ti$ had the highest anisotropy constants of K_1 = 9.2 MJ/m^3 and K_2 = 0.4 MJ/m^3. Substitution of any other rare earth elements for Sm decreased magnetocrystalline anisotropy. The anisotropy field, $\mu_0 H_A$, calculated from K_1, K_2 and J_s showed the highest value of 19.8 T for $SmFe_{11}Ti$ as shown in Table 1. The $(Sm_{0.5}RE_{0.5})Fe_{11}Ti$ (RE=Ce,Pr,Nd,Gd,Tb) compounds showed 20-40 % of the anisotropy field of $SmFe_{11}Ti$.

IV. CONCLUSION

$(Sm_{0.5}RE_{0.5})Fe_{11}Ti$ (RE=Ce,Pr,Nd,Sm,Gd,Tb,Dy) compounds had tetragonal $ThMn_{12}$-type structure and uniaxial anisotropy with easy magnetization c-axis. The anisotropy constant K_1 was in the range of 1.75 - 9.2 MJ/m^3 and approximately one order higher than K_2. Among the compounds, $SmFe_{11}Ti$ had the highest anisotropy of K_1 = 9.2 MJ/m^3, K_2 = 0.4 MJ/m^3 and $\mu_0 H_A$= 19.8 T. Substitution of any other rare earth elements for Sm decreased magnetocrystalline anisotropy.

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