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A Semi-graphical Analysis on the Sublattice Anisotropy of a Two Sublattice System with Uniaxial Anisotropy: Application to $Pr_2Fe_{14}B$

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A method to analyze the anisotropy constants of a two sublattice system with uniaxial anisotropy has been investigated by extending the Sucksmith and Thompson's method to higher order anisotropy terms. Using graphical analysis together with numerical calculation, the sublattice anisotropy constants of a two sublattice system are calculated. Using the method, a set of anisotropy constants for Pr-sublattice of $Pr_2Fe_{14}B$ at 4.2 K has been obtained as K_{1Pr}=5210 J/kg, K_{2Pr}=−7200 J/kg, K_{3Pr}=−770 J/kg, K_{4Pr}=4940 J/kg and K_{5Pr}=700 J/kg for N_{PrFe}=2.2 T/Am²kg^{-1}. The magnetization calculated by an energy minimum method by using the sublattice anisotropy constants well reproduced the experimental results and satisfied the simulation assumptions.

1. Introduction

Rare earth elements and 3*d* transition metals make many types of ferromagnetic compounds. Due to the orbital moment of 4*f* electrons of rare earth elements, the compounds show strong magnetocrystalline anisotropy which is suitable for permanent magnet applications [1, 2].

The magnetocrystalline anisotropy of 4*f*-3*d* compounds has been studied by a fitting method based on the crystalline electric field theory [3-5] or phenomenological anisotropy constants [6-8]. In order to obtain the right set of CEF or anisotropy constants, fitting on magnetization curves as many as possible is desirable. The analytical method, on the other hand, has the merit to obtain the right set of constants from minimum number of experimental curves without trial and error procedure. For example, the present authors [9] previously extended the Sucksmith and Thompson's method [10] to higher order anisotropy and determined the anisotropy constants of $Pr_2Fe_{14}B$ at 290 K based on the rigid coupled magnetization model.

At a low temperature near 4.2 K, due to the strong anisotropy of the 4*f* sublattice, the sublattice moments of some 4*f*-3*d* compounds are not co-linear during magnetization process. The free energy equation describing the two sublattice system is different from a rigid coupled magnetization system (or single magnetic ion system), and the application of Sucksmith and Thompson's method has not been evaluated.

In this paper, we extended the Sucksmith and Thompson's method to higher order anisotropy terms in a two sublattice system and examined the process to analyze the sublattice anisotropy constants of uniaxial anisotropy system. By using a graphical process together with a numerical calculation, we could analyze the sublattice anisotropy constants of a two sublattice system. Application to $Pr_2Fe_{14}B$ at 4.2 K resulted in a good agreement with experiments. The method may be used for the quick and approximate determination of the anisotropy constants prior to the precise fitting process.

2. Analyzing procedures

In order to simplify the calculation, let us consider a tetragonal 4*f*-3*d* compound with uniaxial magnetocrystalline anisotropy of easy magnetization *c*-axis. If the compound is assumed to behave as a two sublattce system of R (4*f*) and T (3*d*) moments, the free energy of the system in a magnetic field $\dot{H}$ is expressed as follows;

$$E = E_{aT} + E_{aR} - (\vec{M}_T \cdot \vec{H} + \vec{M}_R \cdot \vec{H}) + N_{RT} \vec{M}_T \cdot \vec{M}_R \quad (1)$$

Here, E_{aT} and E_{aR} are the magnetocrystalline anisotropy energies of 3*d*- and 4*f*- sublattice, respectively, and N_{RT} is the macroscopic exchange interaction constant [11] between the two sublattices.

If $\dot{H}$ is parallel to crystallographic main axis of [100] or [110], and if the sublattice moments are assumed to rotate on the plane made by *c*-axis and $\dot{H}$, as was proved in a rigid coupled magnetization system [9], the free energy can be expressed as follows;

$$E = K_{1T}\sin^2\theta_T + (K_{2T} \pm K_{3T})\sin^4\theta_T + (K_{4T} \pm K_{5T})$$

$$\sin^6\theta_T + \cdots + K_{1R}\sin^2\theta_R + (K_{2R} \pm K_{3R})\sin^4\theta_R + (K_{4R} \pm K_{5R})\sin^6\theta_R + \cdots - (M_T\sin\theta_T + M_R\sin\theta_R)H + N_{RT}M_TM_R(\sin\theta_T\sin\theta_R + \cos\theta_T\cos\theta_R) \quad (2)$$

Here, the notation θ is the inclination angle of sublattice moments from [001] axis (c-axis), as shown in Fig. 1. The sign of $\pm K_{3T}$, $\pm K_{5T}$, $\pm K_{3R}$ and $\pm K_{5R}$ is positive for $H//[100]$ and negative for $H//[110]$. Since the sublattice magnetization contributed on $\vec{H}$ direction is $m_{T,R}=M_{T,R}\sin\theta_{T,R}$, following equations are obtained from the equilibrium conditions, $\partial E/\partial\theta_T = 0$ and $\partial E/\partial\theta_R = 0$;

$$0 = 2K_{1T}\frac{m_T}{M_T} + 4\left(\frac{m_T}{M_T}\right)^3(K_{2T} \pm K_{3T}) + 6\left(\frac{m_T}{M_T}\right)^5(K_{4T} \pm K_{5T}) + \cdots - M_TH + N_{RT}M_TM_R\left(\frac{m_R}{M_R} - \frac{m_T}{M_T}\frac{\pm\sqrt{1-m_R^2/M_R^2}}{\sqrt{1-m_T^2/M_T^2}}\right) \quad (3)$$

$$0 = 2K_{1R}\frac{m_R}{M_R} + 4\left(\frac{m_R}{M_R}\right)^3(K_{2R} \pm K_{3R}) + 6\left(\frac{m_R}{M_R}\right)^5(K_{4R} \pm K_{5R}) + \cdots - M_RH + N_{RT}M_TM_R\left(\frac{m_T}{M_T} - \frac{m_R}{M_R}\frac{\sqrt{1-m_T^2/M_T^2}}{\pm\sqrt{1-m_R^2/M_R^2}}\right) \quad (4)$$

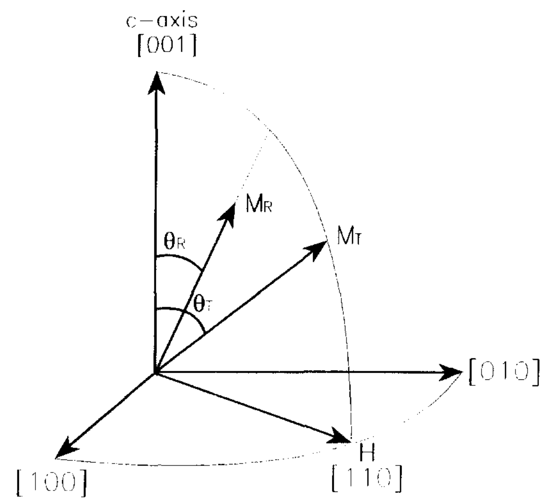

Fig. 1. The relation between the angles θ_R, θ_T and the sublattice magnetizations M_R, M_T in a magnetic field H ($H//[110]$).

Here, the sign of $\pm\sqrt{1-m_R^2/M_R^2}\,(=\cos\theta_R)$ depends on the angle θ_R. It is always positive for a ferromagnetic coupling system and negative for an antiferrocoupling system.

If we know the anisotropy of $3d$-sublattice and N_{RT}, the sublattice magnetizations m_T and $m_R(=m-m_T)$ at a given H can be calculated numerically by equation (3). The $4f$-sublattice anisotropy constants, then, can be determined by graphically from equation (4) according to the following procedures; At first, make a plot of $M_RH - N_{RT}M_TM_R\left(\frac{m_T}{M_T} - \frac{m_R}{M_R}\frac{\sqrt{1-m_T^2/M_T^2}}{\pm\sqrt{1-m_R^2/M_R^2}}\right)$ vs. $2\frac{m_R}{M_R}$. Since high power terms of m_R/M_R are neglected in the low field region, the plot should be linear in the low field region, and K_{1R} can be determined from the slope of the plot. Secondly, apply the value of K_{1R} determined by the above mentioned process into equation (4), and make a plot of $-2K_{1R}\frac{m_R}{M_R} + M_RH - N_{RT}M_TM_R\left(\frac{m_T}{M_T} - \frac{m_R}{M_R}\frac{\sqrt{1-m_T^2/M_T^2}}{\pm\sqrt{1-m_R^2/M_R^2}}\right)$ vs. $4(m_R/M_R)^3$. This plot should show a linear relation again up to a little higher field region in which the terms higher than $(m_R/M_R)^5$ are neglected. Then, the slope of the linear portion corresponds to $K_{2R}\pm K_{3R}$. Repetition of the plot against $(m_R/M_R)^n$ (n=3, 5, 7 ··) will show the value for $K_{(n-1)R}\pm K_{nR}$ as far as the experimental data show linear relation. If experimental data do not show linear relation in high field region, it is due to the leaving of magnetic moments from original rotation plane. The individual constants can then be calculated from the values obtained on the magnetization curves of [100] and [110] directions.

3. Sublattice Anisotropy Constants of $Pr_2Fe_{14}B$ at 4.2 K

$Pr_2Fe_{14}B$ shows uniaxial magnetocrystalline anisotropy at 4.2 K with easy magnetization tetragonal c-axis. Fig. 2 shows the magnetization curves of $Pr_2Fe_{14}B$ at 4.2 K measured (open circles) by Hiroyoshi *et al.* [3] along [001], [100] and [110] directions.

In order to analyze the magnetocrystalline anisotropy from the magnetizations of Fig. 2, we treated the compound as a two sublattice system with Pr and Fe moments and assumed that sublattice moments rotate on the plane made by c-axis and $\vec{H}$. We also assumed the anisotropy of Fe-sublattice as K_{1Fe}=115 J/kg [12-14] obtained from $Y_2Fe_{14}B$, and calculated the sublattice magnetizations for various N_{PrFe} by eq. (3). Fig. 3(a), (b) and (c) are the best plots to determine K_{1Pr}, $(K_{2Pr}\pm K_{3Pr})$ and $(K_{4Pr}\pm K_{5Pr})$, respectively, obtained by applying N_{PrFe}=− 2.2 T/Am^{2}kg $^{-1}$ following the

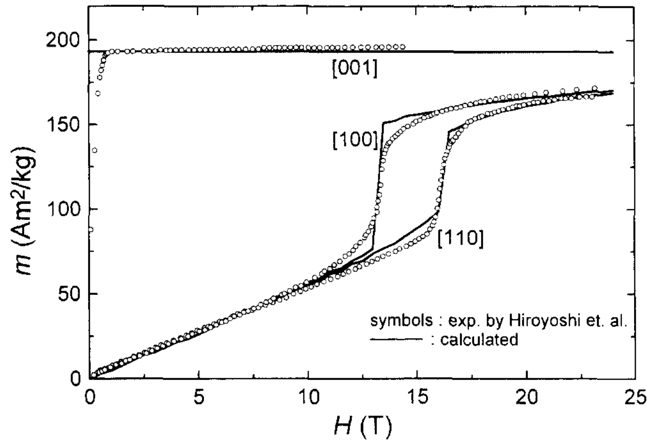

Fig. 2. Magnetization curves of $Pr_2Fe_{14}B$ measured (open circles [3]) and calculated (solid lines) along [001], [100] and [110] at 4.2 K.

Table 1. Parameters and sublattice anisotropy constants of $Pr_2Fe_{14}B$ at 4.2 K

M_{Pr} (Am²/kg)	M_{Fe} (Am²/kg)	N_{PrFe} (T/Am²kg^{-1})	K_{1Pr} (J/kg)	K_{2Pr} (J/kg)	K_{3Pr} (J/kg)	K_{4Pr} (J/kg)	K_{5Pr} (J/kg)
34.9$^+$	158.3$^+$	-2.2	5210	-7200	-770	4940	700

$^+$Calculated from saturation magnetization using the experimental Bohr magnetons [14] of $Pr_2Fe_{14}B$.

procedure explained in section 2. Line up of all the experimental data in Fig (c) implies that the sublattice moments rotate on the plane made by c-axis and H, and consideration up to ($K_{4Pr} \pm K_{5Pr}$) term is enough to analyze the experimental curves.

Table 1 summarizes the applied parameters and the anisotropy constants analyzed by the curves shown in Fig. 3. The solid lines in Fig. 2 are the magnetizations calculated by energy minimum method by applying the set of anisotropy constants. The calculation results fit well to the experiments except for the region around the first order magnetization process. The discrepancy may be due to the simplified model of two sublattice system. The calculation results satisfied the assumption about the rotation of sublattice moments on the plane made by c-axis and H.

4. Conclusion

By extending the Sucksmith and Thompson's method to high order anisotropy terms, a method to determine the sublattice anisotropy constants of a two sublattice system has been suggested. Using the method an anisotropy constant set for Pr-sublattice of $Pr_2Fe_{14}B$ at 4.2 K has been obtained as K_{1Pr}=5210 J/kg, K_{2Pr}=−7200 J/kg, K_{3Pr}=−770 J/kg, K_{4Pr}=4940 J/kg and K_{5Pr}=700 J/kg for N_{PrFe}=−2.2 T/Am²kg^{-1} under the two sublattice model.

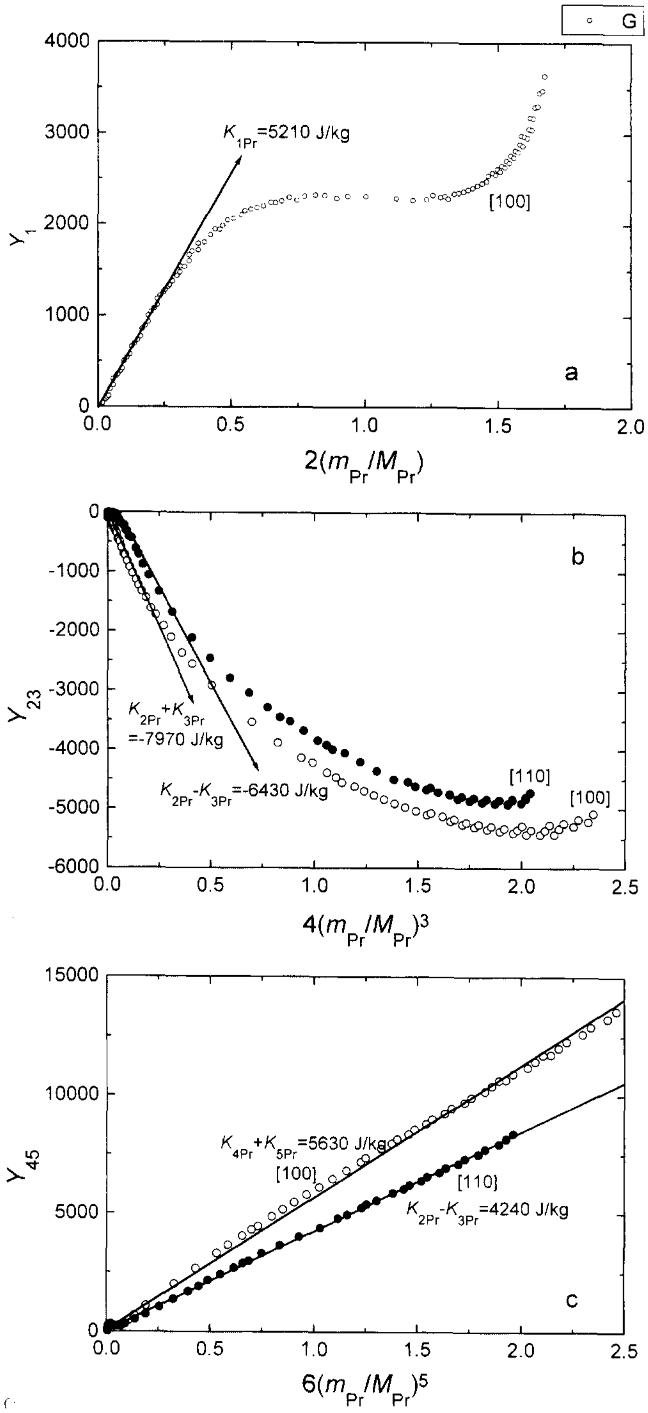

Fig. 3. The plots of (a) $Y_1(=M_{Pr}H-N_{PrFe}M_{Fe}M_{Pr}\left(\frac{m_{Fe}}{M_{Fe}}-\frac{m_{Pr}}{M_{Pr}}\frac{\sqrt{1-m_{Fe}^2/M_{Fe}^2}}{\pm\sqrt{1-m_{Pr}^2/M_{Pr}^2}}\right)$ vs. $2(m_{Pr}/M_{Pr})$, (b) $Y_{23}(=Y_1-2K_{1Pr}(m_{Pr}/M_{Pr}))$ vs. $4(m_{Pr}/M_{Pr})^3$, and (c) $Y_{45}(=Y_{23}-4(m_{Pr}/M_{Pr})^3(K_{2Pr}\pm K_{3Pr}))$ vs. $6(m_{Pr}/M_{Pr})^5$.

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