Theoretical study on the finite temperature magnetism of rare earth permanent magnets

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1. Introduction

From an industrial viewpoint, magnetic anisotropy is the most important property of ferromagnetic materials. It governs the efficiency of magnetic media in hard disk drive (HDD) devices, permanent magnets in motors and so on. Permanent magnets have strong magnetic anisotropy above room temperature, especially in motors of hybrid and electric vehicles. They are consequently highly desired in terms of addressing energy problem.

In this symposium, we will first overview the general theory for the magnetic anisotropy at finite temperature and show how the magnetic anisotropy constants (MAC) vary as temperature increases.[1] Next, we will discuss on the effects of thermal fluctuation (activation) of magnetization on the reversal (coercive) field, on the basis of magnetic viscosity. Finally, let us show some calculated results for the temperature dependence of MAC of $Nd_2Fe_{14}B$ and mainly discuss the site dependence of the MAC's at around the room temperature. [2,3]

2. Theoretical evaluation of the magnetic anisotropy constants at finite temperature

Suppose that the classical Hamiltonian of a magnetic system having the uniaxial anisotropy is given by

$$H = \kappa_1 \sum_i \sin^2\theta_i + \kappa_2 \sum_i \sin^4\theta_i + H_{ex} \qquad (1)$$

where the first two terms indicate the magnetic anisotropy energy and the last term the exchange energy. Here the constants κ_1 and κ_2 can be expressed through the expansion coefficients of the crystal field energy in terms of the Legendre polynomials $P_l(\cos\theta)$, from which we have $\kappa_1 = -3B_2^0 - 40B_4^0$ and $\kappa_2 = 35B_4^0$ with B_n^0 being the crystal field parameter. The methods to evaluate the temperature dependence of the MAC's are listed as follows:

1) to solve the stochastic LLG (Langevin) equation involving the thermally fluctuated field, and derive the MAC's by the magnetization curves for the applied fields parallel and perpendicular to the easy axis.

2) to calculate the free energy $F(\Theta,T)$ by performing the Monte-Carlo method with the average magnetization direction of Θ, and derive the n-th MAC's $K_n(T)$ by fitting $F(\Theta,T)$ with $K_1(T)\sin^2\Theta + K_2(T)\sin^4\Theta$.

3) to express directly the form of MAC's by means of the first order perturbation theory in terms of the anisotropy terms, which gives

$$K_1(T) = c_2\kappa_1 + (8/7)(c_2 - c_4)\kappa_2,\ \ K_2(T) = c_4\kappa_2, \qquad (2)$$

$$c_2 \equiv (1/2)\langle 3\cos^2\theta - 1\rangle_{H_{ex}} = \langle P_2(\cos\theta)\rangle_{H_{ex}}. \qquad (3a)$$

$$c_4 \equiv (1/8)\langle 35\cos^4\theta - 30\cos^2\theta + 3\rangle_{H_{ex}} = \langle P_4(\cos\theta)\rangle_{H_{ex}} \qquad (3b)$$

Note that $K_1(0) = \kappa_1$ and $K_2(0) = \kappa_2$, since $c_l = 1$ when $T = 0$.

Although the method 1) requires much computational time and resource, it is most realistic to reproduce the magnetization curves. To perform the method 2), it is useful to adopt a new technique proposed recently by Asselin et al.[4] Employing this method, we have successfully reproduced the temperature dependence of MCA's of $Nd_2Fe_{14}B$.[3] The method 3) provides us physically transparent form of the MAC's and is the most convenient way to realize the MAC's if one further adopts the mean field approximation for the exchange term. One can understand from eqs. (2) and (3) that $K_1(T)$ $(T > 0)$ is determined by κ_1 and κ_2, and further by H_{ex} through $\langle P_l(\cos\theta)\rangle_{H_{ex}}$. Additionally, according to the Callen-Callen theory,[5] one should note the relation $\langle P_l(\cos\theta)\rangle_{H_{ex}} \approx \langle\cos\theta\rangle_{H_{ex}}^{l(l+1)/2} = \langle m\rangle_{H_{ex}}^{l(l+1)/2}$ where $\langle m\rangle_{H_{ex}} = M(T)/M(0)$. Recently, we have confirmed by using the methods 2) and 3) that the approximate relation $\langle P_l(\cos\theta)\rangle_{H_{ex}} \approx \langle m\rangle_{H_{ex}}^{l(l+1)/2}$ holds in the wide range of temperature as far as $k_B T < H_{ex}$ is satisfied. Thus, the MAC's can be expressed by using $\langle m\rangle_{H_{ex}} = M(T)/M(0)$ as $K_1(T) = (\kappa_1 + 8/7\kappa_2)\langle m\rangle_{H_{ex}}^3 - 8/7\kappa_2\langle m\rangle_{H_{ex}}^{10}$ and $K_2(T) = \kappa_2\langle m\rangle_{H_{ex}}^{10}$. In Fig. 1, we show the calculated results of the temperature dependence of MAC's of $Nd_2Fe_{14}B$ based on the above expressions. Here, we input the experimental data of $\langle m\rangle_{H_{ex}} = M(T)/M(0)$ and took into accounted for $\sin^6\theta_i$ term in addition to κ_1 and κ_2 terms. One can recognize that the above expressions can work well for the complex compounds like $Nd_2Fe_{14}B$.

In addition, we should emphasis here that $K_n(T)$ $(T > 0)$ is dominated by H_{ex} as well as κ_1 and κ_2, as mentioned above. This implies that the $K_n(T)$ at surfaces or interfaces exhibit larger decrement with temperature than those inside the bulk. Figure 2 shows the temperature dependence of $K_1(T)$ both for H_{ex} = 350 and 175 in units of kelvin.[1] One can see that the $K_1(T)$ values for H_{ex} = 175 [K] is much smaller than those for H_{ex} = 350 [K] as bulk values, when the temperature is above 200 [K], which leads us to consider that the magnetization reversal takes place by a smaller field at the surfaces or interfaces of grains in magnets.

In the symposium, we will discuss the site dependence of the MAE and the effects of thermal activation on the reversal field in Nd-Fe-Bd.

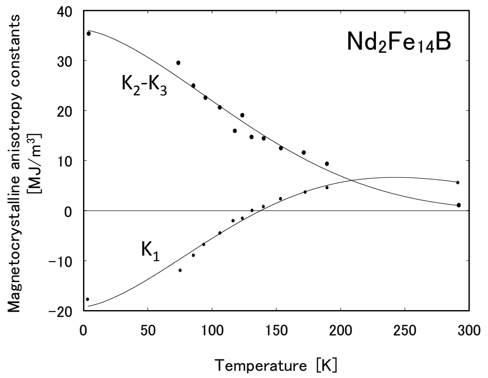

Fig.1 Temperature dependence of K_1 and $K_2 - K_3$ of $Nd_2Fe_{14}B$. The dots are the experimental dada.[6]

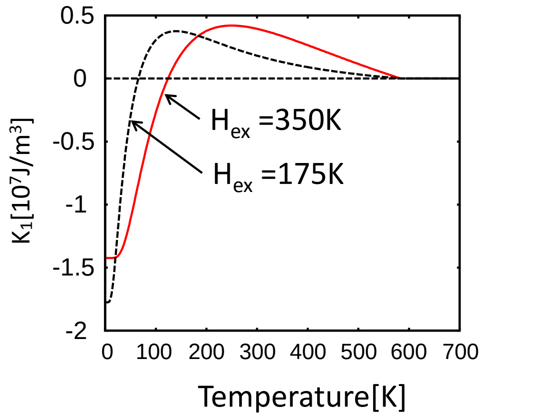

Fig. 2 Temperature dependence of K_1 for the exchange energy H_{ex}=350 and 175 [in units of K] in $Nd_2Fe_{14}B$.

References

1) D. Miura, R. Sasaki, and A. Sakuma, Applied Physics Express, **8**, 113003 (2015).
2) R. Sasaki, D. Miura, and A. Sakuma, Applied Physics Express, **8**, 043004 (2015).
3) Y. Toga, M. Matsumoto, S. Miyashita, H. Akai, S. Doi, T. Miyake, and A. Sakuma, to be submitted.
4) P. Asselin, et al., Phys. Rev. B **82**, 054415 (2010).
5) E. R. Callen and E. Callen, Phys. Rev. **129**, 578 (1966).
6) O. Yamada, et al., J. Magn. Magn. Mater. **54-57**, 585 (1986).