Monte Carlo analysis for finite temperature magnetism of $Nd_2Fe_{14}B$ magnet

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Rare earth permanent magnets, particularly Nd-Fe-B, exhibiting strong magnetic performance are attracting considerable attention because of the rapidly growing interest in electric vehicles. The main focus of research in involving these materials is to increase the coercive field H_c and improve the temperature dependence. Recently, Sasaki et al.1) conducted theoretical studies in the quantitative level on the temperature dependence of magnetic anisotropy for a $Nd_2Fe_{14}B$ bulk system. However, as these theories relied on the mean field approach, they are not enough to include the effects of magnetic inhomogeneities.

Because of the above background, we constructed a realistic classical three-dimensional Heisenberg model using results from first-principles calculations, and investigated the magnetic properties of the $Nd_2Fe_{14}B$ bulk system at finite temperatures. To analyze the finite-temperature magnetic anisotropy, we applied constrained Monte Carlo (C-MC) method2) to the above classical Heisenberg model. The C-MC method fixes the direction of total magnetization, $\boldsymbol{M}$, in any direction for each MC sampling without external magnetic field. This allows us to calculate the angle θ dependencies of magnetization torque and free energy.

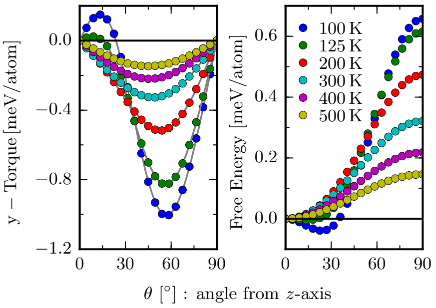

Fig. 1 Angular dependence of torque (left side) and free energy (right side) at each temperature.

Figure 1 shows the y-direction torque and free energy as a function of magnetization angle θ. We can see that for 100 K and 125 K, the torque (free energy) curve attains a local maximum (minimum) at $\theta \neq 0$, which reflect the spin reorientation of $Nd_2Fe_{14}B$. In contrast, above $T \geq 200$ K, the local maximum (minimum) disappears and the torque (free energy) curve approaches $\propto \sin 2\theta$ ($\sin^2\theta$). This behavior implies that the magnetic anisotropy constant K_1^A becomes dominant as the temperature increases.

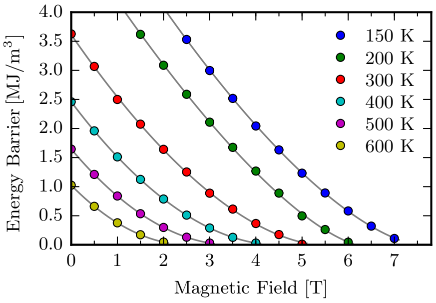

Fig. 2 Height of the energy barrier, $\mathcal{F}_B$, as a function of external magnetic field, H_{ext}, at each temperature.

We also discuss the external magnetic field H_{ext} response of the energy barrier (activation energy) which governs the probability of magnetization reversal via the thermal fluctuation of spins. Figure 2 shows the height of the energy barrier, $\mathcal{F}_B$, when H_{ext} is applied opposite to the z-direction of $\boldsymbol{M}$. The H_{ext} response of $\mathcal{F}_B$ is generally expressed3) by: $\mathcal{F}_B(H_{ext}) = \mathcal{F}_B^0(1 - H_{ext}/H_0)^n$. The exponent n can take various values, such as $n = 2$ for the Stoner–Wohlfarth model and $n = 1$ for the weak domain-wall pinning mechanism.3) The parameters $\mathcal{F}_B^0$, H_0, and n were obtained by fitting $\mathcal{F}_B(H_{ext})$ in Fig. 2. We can find that n takes values of less than 2 in the low-temperature region (below the room temperature, $T_R \sim 300$ K) and approaches 2 as the temperature increases. This reflects the fact that the magnetic anisotropy is mainly governed by the K_1^A term in the high-temperature region.

1) R. Sasaki, D. Miura, and A. Sakuma, Appl. Phys. Express 8, 043004 (2015).
2) P. Asselin, R. F. L. Evans, J. Barker, R. W. Chantrell, R. Yanes, O. Chubykalo-Fesenko, D. Hinzke, and U. Nowak, Phys. Rev. B **82**, 054415 (2010).
3) P. Gaunt, J. Appl. Phys. **59**, 4129 (1986).