# Atomistic study of thermally-activated magnetization processes in rare earth permanent magnets

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For practical use of magnets, in particular at high temperatures, it is very important to study temperature dependence of magnetic properties [1,2]. We present our trials on this problem for the high-performance $Nd_2Fe_{14}B$ magnets (Fig.1). For this purpose, first we constructed an atomistic Hamiltonian to properly take into account the temperature [3]. With it, we calculated various thermodynamic quantities by methods of statistical physics, e.g., a constrained Monte Carlo method [3] and a stochastic LLG equation [4]. We confirmed that temperature dependences of the magnetization and anisotropy energies well reproduce the corresponding experimental results (Figs.2) [3]. Moreover, microscopic properties, e.g. the domain wall profiles [5], anisotropy of the exchange coupling constant reflecting the crystal structure [6], and also dynamical properties, e.g., the spectrum of FMR (ferromagnetic resonance) [7] were also studied. As a merit of the atomistic model, we can find atom-specific ordering properties [3].

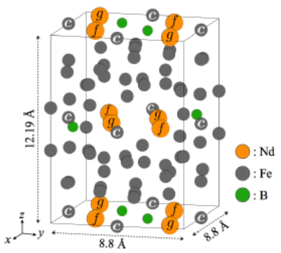


Fig.1 Unit cell of $Nd_2Fe_{14}B$

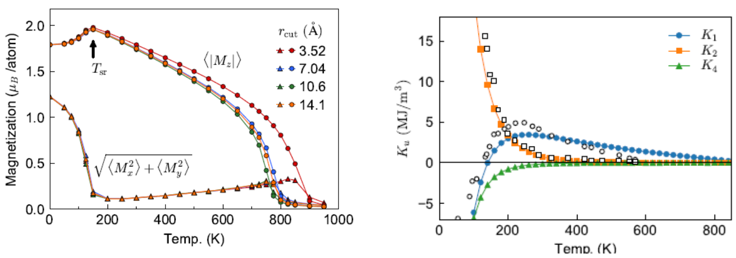


Fig.2 Temperature dependence of magnetization and anisotropy constants [3].

The most important property of magnets is the coercivity. However, in contrast to the above-mentioned thermodynamic quantities, we do not have theoretical formula for the coercivity, and thus so far only little study has been done on quantitative estimation of the coercivity at finite temperatures. We studied this problem in nano-size grains by a method using the free-energy landscape obtained by Wang-Landau method [8], and also by a direct dynamical simulation of the stochastic LLG equation [9]. There, the strength of magnetic field at which the relaxation time of the magnetization reversal is 1second (a definition of coercivity) and its temperature dependence are obtained.

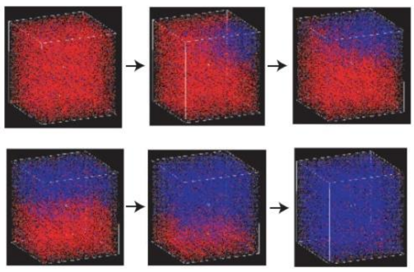

Fig.3 Magnetization reversal in a nano grain [9]

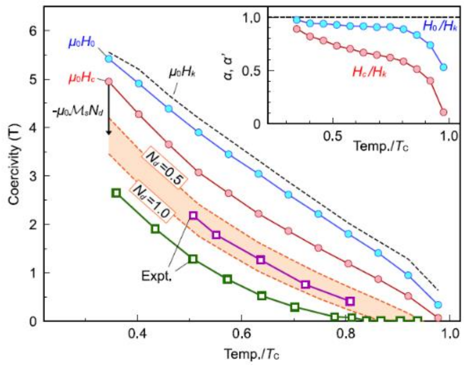


Fig. 4 Temperature dependences of coercivities [8]

It was found that the coercivity at a high temperature (about half of the critical temperature) is around 3T which is the theoretical maximum value although it is significantly reduced from the one at zero temperature. For larger grains, the dipole-dipole interaction plays a role [10] and the multidomain magnetic structure appears [11]. We also discuss a mechanism of coercivity in such cases. Real magnets consist of hard magnet ($Nd_2Fe_{14}B$) grains each of which are covered by grain boundary material. Thus, it is important to study how the boundary phases affect the coercivity [12], which is also presented. Finally, ensemble effects of gains on the coercivity are also reported from a viewpoint of the first-order reversal curves (FORC).


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