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Size and field dependence of the trigger process of the magnetization reversal of $Nd_2Fe_{14}B$ magnet

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Microscopic properties of ordering process of the permanent magnets $Nd_2Fe_{14}B$ at finite temperatures are studied from an atomic view point with a realistic set of material parameters obtained from the first-principle calculations, and anisotropy constants (the crystal-filed parameters up to the 6-th order) by making use of a finite temperature LLG equation[1,2] and Monte Carlo method[3,4]. The structure of the unit cell of this material is depicted in Fig.1(a). The exchange couplings were obtained by the Liechtenstein's formula that has been implemented on the first-principles electronic-structure calculation using the Korringa-Kohn-Rostoker (KKR) Green's function method, Machikaneyama (AkaiKKR) [5]. For the anisotropy of Nd atom (Stevenson factors), we adopted experimental results [6], even though some research for the anisotropy of $Nd_2Fe_{14}B$ have performed using first-principles calculations. With these parameters, the reorientation transition around 140K due to the deviation of the easy axis of magnet from the c-axis was well reproduced (Fig.1(b)). The Curie temperature of ferromagnetic phase (about 600K) also agrees well with the experimental one (Fig.1(b)). Temperature dependence of the anisotropy energy $K(T)$ for this transition was also studied and $K_2(T)$, $K_4(T)$ and $K_6(T)$ are estimated. The ordering nature of types of atoms, i.e., Fe and Nd, were studied individually, and found the anisotropy of Nd decreases rapidly with the temperature. Temperature- and size-dependence of the free-energy barrier of magnetization reverse were also obtained [3,4].

Making use of the same model, temperature dependence of the domain walls along the a-axis and also in c-axis was also studied [5](Fig.1(c)). It was found that the domain wall width increases with the temperature increase. The width of the domain wall along the c-axis (perpendicular to the Nd plane) is shorter than that along the a-axis.

Dynamical properties at finite temperatures of the nucleation and domain wall formation from the nucleation under the field in the opposite direction have been studied by a stochastic LLG simulation. Up to the 10nm cube (12x12x9 unit cell), the nucleation occurs from one of the corners, and it reversed region increases with domain wall propagation. Temperature and size-dependence of the relaxation time in detail. The simulation beyond the time duration larger than 10ns is difficult and some statistical method to estimate the longer relaxation time is introduced.

As to the instability of the uniform mode in large systems, nonuniform instability, e.g., the curling would be important. To study such processes, we need to take into

account the effect of the dipole-dipole interaction. We have introduced a new Monte Carlo method to avoid the simulation of *N*x*N* calculation time, where *N* is the number propagation in 12x12x9 unit cell of spins [7], and report the nonuniform instability. We will also report (T=400K, H=-4T) effects of the dipole-dipole interaction on the domain wall propagation.

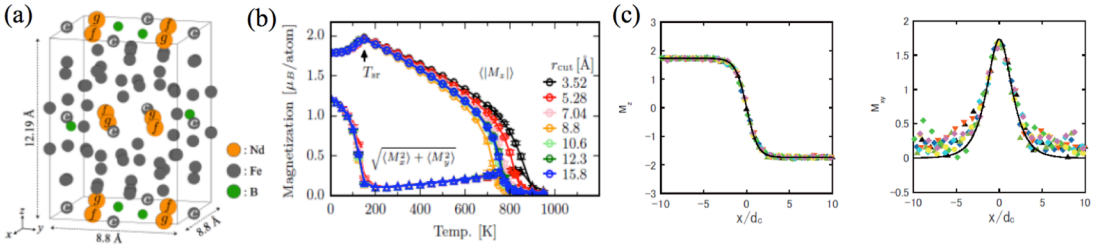

Fig.1: (a) unit cell of $Nd_2Fe_{14}B$, (b) Temperature dependence of the magnetization, (c) Domain walls.

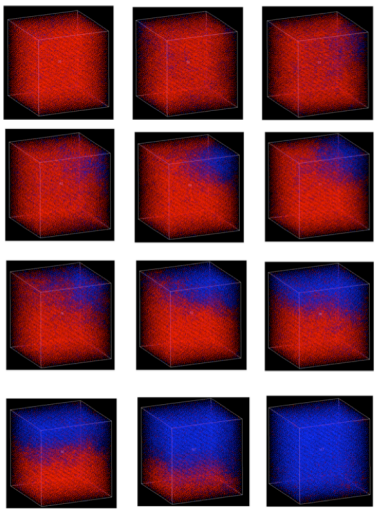

Fig.2: Nucleation and domain wall propagation in 12x12x9 unit cell (T=400K, H=-4T)

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