Large-Scale Micromagnetic Simulation of Reversal Processes in Nd-Fe-B Magnets

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Introduction:

Nd-Fe-B sintered magnets which have high maximum energy product and coercivity are widely used in electric motors and generators. To improve their properties, theoretical elucidation of the reversal process is demanded. In particular, the relationship between coercivity and their microscopic structures is an important topic for the improvement both from the scientific and technological points of view [1, 2]. To understand coercivity mechanism, theoretical studies based on micromagnetics have been performed to analyze the reversal process in Nd-Fe-B magnets. However, the edge length of numerical mesh element has to be smaller than the exchange length (1.7nm in Nd-Fe-B phase) in order to avoid “artificial pinning” in the simulation. Typically, grain size of sintered Nd-Fe-B magnets is from 100nm to 10μm. To simulate the pinning and nucleation process in the realistic grain structures, therefore, the number of finite elements involved in the numerical calculations exceeds a huge value of the order of millions. In this study, large-scale micromagnetic simulation is performed on K computer [3]. The effects of microstructure on the coercivity are numerically investigated.

Calculation methods:

We consider the following micromagnetic energy E_{tot} to analyze the magnetization in the simplified microstructure of Nd-Fe-B magnets,

$$E_{tot} = E_{Zeeman} + E_{exc} + E_{ani} + E_d , \tag{1}$$

where, E_{Zeeman}, E_{exc} , E_{ani} and E_d are Zeeman energy, exchange energy, anisotropy energy and magneto-static energy, respectively. The magnetization dynamics of the reversal processes are simulated by calculating the Landau-Lifshitz-Gilbert (LLG) equation,

$$(1+\alpha^2)\frac{\partial \boldsymbol{m}}{\partial t} = -\gamma\left(\boldsymbol{m}\times\boldsymbol{H}_{eff}\right) - \gamma\alpha\boldsymbol{m}\times\left(\boldsymbol{m}\times\boldsymbol{H}_{eff}\right), \tag{2}$$

where, m, γ and α are the normalized magnetization vector, the gyro-magnetic ratio, and the Gilbert damping factor. The effective field $\boldsymbol{H}_{eff}$ is derived from partial derivative of magnetization energies. The spatial distribution of the magnetization vector is numerically divided to the elements of the unstructured mesh which is commonly used in finite element method. To handle the domain wall motion and nucleation of the reverse domains, we used a small mesh size(1nm) and adapted the domain decomposition method by using METIS library, which divided the entire model in the small region and each region was calculated by the separate CPUs [4].

Simulations:

The simulation model is shown in Fig.1. This model is composed of 27 grains whose diameter is 50 nm. The grains are three-dimensionally aligned and the width of grain boundary is 2 nm. The total number of mesh model is about 5 million. We here label the state of a magnetic vector which points to positive y-direction “up”, and the opposite state “down”. As shown in Fig.1, all the initial magnetic vectors are down except for those in the grain of the front side of the top layer, which are initially in the up state. The simulated reversal process in the case of the alignment α=1 is shown in Fig.2. Due to the inclusion of the soft magnetic layers in the grain boundaries, the reversal domain easily propagates into neighboring grains. The simulation result at the alignment α=0.5 is also shown in Fig.3.

This result shows that the grain boundaries pin the domain wall of initial reverse domain and the nucleation occurs at another grains. The reversal mechanism depends on the microstructure and material parameters of the grain boundaries. In the presentation, the parameter dependences of the reversal processes and coercivity will be reported in detail.

Acknowledgment

This research used computational resources of the K computer provided by the RIKEN Advanced Institute for Computational Science through the HPCI System Research project (Project ID: hp120086).

References

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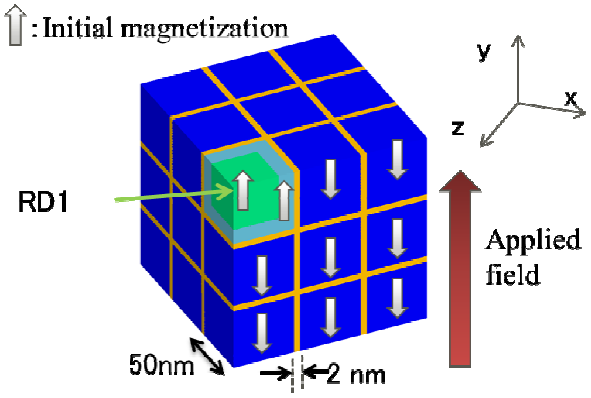

Fig. 1 Simulation Model of multi-grain structure

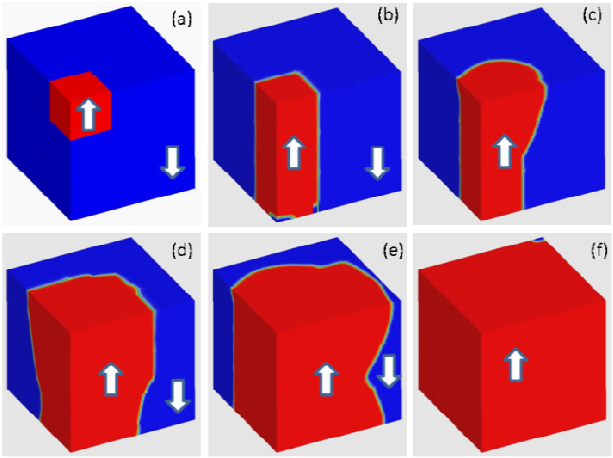

Fig. 2 Contour plot of m_z in the case of alignment parameter α=1.

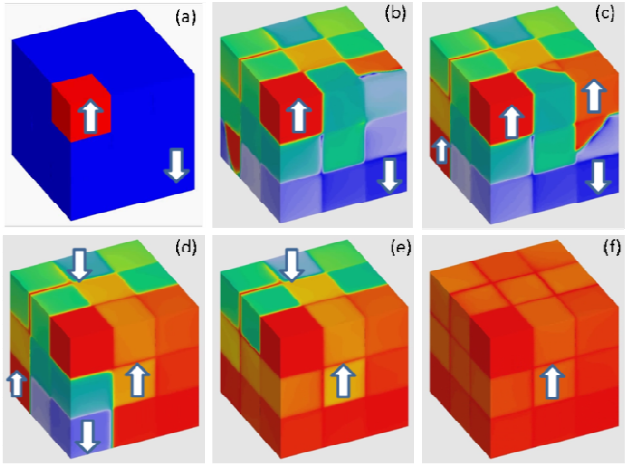

Fig. 3 Contour plot of m_z in the case of alignment parameter α=0.5