Monte Carlo Simulation for Magnetic Domain Wall Displacement with Conventional Crystal Anisotropy

K. Yamaguchi, K. Suzuki, O. Nittono and T. Takagi

I. Introduction

Magnetic anisotropy is important to understand for magnetic domain structure and magnetic domain wall displacement (DWD) behavior. Usually anisotropy energy in Hamiltonian is phenomenologically introduced as macroscopic field with anisotropy constants such as K_1 and K_2. Inhomogeneous materials, e.g. crystals including defects and residual stress, however, have local disorders of atomic periodical array, and spins around such region will be affected by different anisotropic fields with the macroscopic one.

On the single-ion model of magnetic anisotropy, the easy axis direction of each individual spin is influenced by a crystal field of surrounding ligands through the spin-orbit interaction and, as a result macroscopic anisotropy is introduced for homogeneous materials. Then introducing local disorders will naturally be reflected in a local anisotropy. In this paper Monte Carlo method using a model of conventional crystal anisotropy is proposed based on the single-ion model and the method is applied for the bcc iron to show the usefulness.

II. Method and Results

A following Hamiltonian was used for the simulation:

$$H = -J\sum_{near}\mathbf{S}_i\cdot\mathbf{S}_j + D\sum_{all}\left(\frac{\mathbf{S}_i\cdot\mathbf{S}_j}{|\mathbf{r}_{ij}|^3} - \frac{3}{|\mathbf{r}_{ij}|^5}(\mathbf{S}_i\cdot\mathbf{r}_{ij})(\mathbf{S}_j\cdot\mathbf{r}_{ij})\right) + A\sum_{near}\left(\frac{1}{|\mathbf{r}_{ij}-a\mathbf{S}_i|} - \frac{1}{|\mathbf{r}_{ij}|}\right) + B\sum_i\mathbf{S}_i . \quad (1)$$

Here the first, the second and the last summations show exchange interaction energy, magnetic dipole interaction energy and applied magnetic field energy, respectively. $\mathbf{S}_i$ denotes the spin vector of i-th cell with $|\mathbf{S}_i| = 1.0$ and $|\mathbf{r}_{ij}|$ represents the distance between i-th spin and j-th spin. The third summation is originally introduced as conventional anisotropy energy derived from the crystal field, when $\mathbf{S}_i$ is directed toward a ligand, the energy increases. Below the parameters set to J=1.0, D=0.1, A=10 and a=0.3, respectively.

A spin system of bcc structure with the lattice constant L=1 was formed into a cylindrical cluster with a diameter of 29 L and 3 L thickness. First, the temperature dependence was calculated and 4 divided magnetic domains were produced with 90 degree DW at the lowest temperature as shown in Fig.1. Almost the spins align toward the x-axis [100] and the y-axis [010]. The peripheral spins turn to outside, that is no ligands direction, due to a little magnetic dipole interaction for the small cluster.

K. Yamaguchi, K. Suzuki and O. Nittono are with Faculty of Symbiotic Systems Science, Fukushima University, E-mail: yama@sss.fukushima-u.ac.jp
T. Takagi is with Institute of Fluid Science, Tohoku Universtiy.

Figure 2 shows a B-H curve for the cluster applied the magnetic field along the [100], [010] and [110] directions with representative schematic view of spin snapshots. The anisotropy property corresponds qualitatively to bcc iron's one. The magnetization process along the [110] direction shows DWD region and rotation magnetization region.

Next, square formed bcc cluster with a side length of 29 L was prepared and then the lattice constant along the [010] direction, L_y, was extended from L_y =1.0 to L_y =1.1. Figure 3 shows B-H curve applied the magnetic field along the [100] and [010] directions for the cluster which has initial state with 4 magnetic domains like Fig.1. It is clearly seen uni-axial anisotropy is produced for L_y =1.1. Spins along the y-axis are extremely decreased under weak magnetic fields. With increasing magnetic field along the [100] direction, 180 degree DW is moving toward upper. Contrastively, with increasing the field along the [010] direction, a wedge of the small domain along the [010] direction is driven into the DW and double 90 degree DW spread out toward upper and lower.

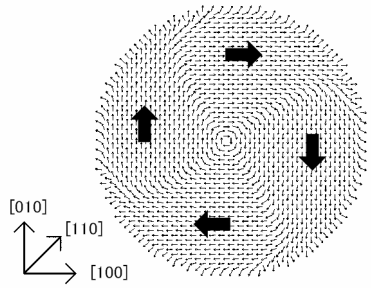

Fig.1. Spin snapshot for a cylindrical bcc cluster at the lowest temperature.

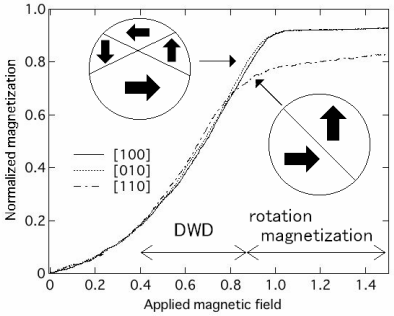

Fig.2. B-H curve along [100], [010] and [110] for the cluster of Fig.1.

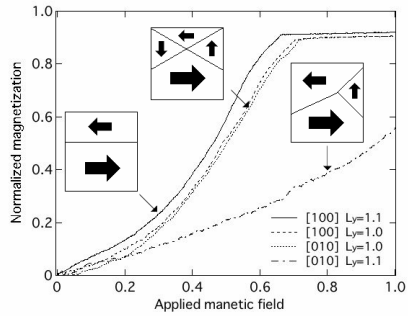

Fig.3. B-H curve for a square cluster with L_y=1.0 and L_y=1.1.