Simulation analysis for magnetization process of torus ring clusters with different radius

Kenichi Terashima¹*, Kenji Suzuki¹, and Katsuhiko Yamaguchi¹

¹Faculty of Symbiotic Systems Science, Fukushima University

* k_terashima@sss.fukushima-u.ac.jp

Received: March 13, 2015; Accepted: January 12, 2016; Published: August 8, 2016

Abstract. Monte Carlo simulations were performed for magnetization process of torus ring clusters with different radii. Simulation results show characteristic reversal curves which have plateau region in halfway. To investigate the factor that these two curves arise, the change of magnetic spin arrangements in the reversal process were calculated, moreover, closure domain parameters and total energy were analyzed. As a result, it is clear that the two curves are distinguished by a state which is either closure domain state or head-to-head state in halfway of the reversal process. Some clusters with different radii take only one path through closure domain state and the reversal process slightly change. In this paper, the magnetic properties and relations between reversal process and the radii of clusters are discussed.

Keywords: Magnetic hysteresis, Magnetization processes, Monte Carlo methods, Nanoscale devices

1. Introduction

Recently, magnetic torus rings have been attracting a lot of interest from the viewpoint of both experimental and theoretical research because of their stable properties of closure domain (CD) state [1]. A torus ring is nano-scales and minimizes the magnetic energy to form closure domain structure. Therefore, due to its magnetic stability, the torus ring has possibilities to contribute to the development for authentic magnetic devices such as high-density storage and it is important to understand the magnetic properties for magnetic reversal process. Some experimental research has been performed for thin film of Co torus ring with outer diameters of 140-520nm [1, 2]. The experimental results show that hysteresis curve includes plateau region in magnetic reversal process. In addition, simulation analysis has been performed for magnetization process using the Landau-Lifshitz-Gilbert (LLG) equation. The
Simulation results show that hysteresis curves include either CD state or head-to-head state depending on the ring size [2]. The simulation results by LLG equation, however, are not match for experimental ones because experimental hysteresis curves with plateau region look to be superposition of CD state and head-to-head state. Zhu et al. explained that experimental hysteresis curves are statistical results by summation of many rings and each ring has only CD state or head-to-head state. Here, there is a question that one ring shows hysteresis curve include only either CD state or head-to-head state in magnetic reversal process.

In the present study, hysteresis curves of magnetic torus ring clusters with different radii were simulated by Monte Carlo (MC) method. The torus ring clusters were modeled for torus ring with outer diameters of several hundred nano meter. Furthermore, by using the simulation results, the dependence of radius on the properties of the torus rings is numerically investigated.

2. Simulation method

The size of the torus ring clusters was prepared for the simulation. In the preparation of clusters, magnetic sites are disposed on lattice points in simple cubic lattice. The lattice constant was set as 1 for fundamental unit of length in this simulation. The point of origin was taken to the cluster center, and the cluster shape was determined as shown in Fig. 1 (a) by following eq. (1).

\[
\left( \sqrt{x^2 + y^2} \right)^2 + z^2 + r^2 = R^2
\]  

(1)

Here, \(x, y \) and \(z\) are defined by Cartesian coordinate system. \(R\) and \(r\) represent major radius and minor radius. Eight types of clusters for magnetic torus rings were prepared, which has \(R = 8, 10, 15, 20\) and \(r = 3, 5\), respectively. Figure 1 (b) shows the case of torus cluster with \(R = 20, r = 3\). The blue dots represent magnetic sites. The total magnetic site number \(N\) is increased as \(R\) and \(r\) become larger. The spin vector \(S\) were set on magnetic site as magnetic moment and numbered 1 to \(N\).

![Figure 1: (a) Schematic diagram for torus ring cluster and (b) the case of torus ring cluster with \(R = 20, r = 3\).](image)
Using these clusters with different radii above, the simulation was performed by Monte Carlo method. In this simulation, following Hamiltonian was set:

$$H = H_J + H_D + H_B.$$  \hfill (2)

Here, $H_J$, $H_D$ and $H_B$ are defined by follows:

$$H_J = \sum_{nn} J S_i S_j$$  \hfill (3)

$$H_D = D \sum_{all} \frac{S_i S_j}{|r_{ij}|^3} \frac{3}{|r_{ij}|^5}(S_i \cdot r_{ij})(S_j \cdot r_{ij})$$  \hfill (4)

$$H_B = \sum_i B S_i$$  \hfill (5)

Each term of $H_J$, $H_D$ and $H_B$ represent exchange interaction energy, magnetic dipole interaction energy and applied magnetic field energy, respectively. Here, $S_i$ denotes the magnetic moment of $i$-th site and $r_{ij}$ represents the position vector between $i$-th site and $j$-th site. $S_i$ was set as $|S_i| = \sqrt{S_{ix}^2 + S_{iy}^2 + S_{iz}^2} = 1$. Here, $S_{ix}$, $S_{iy}$ and $S_{iz}$ denote $x$, $y$ and $z$-component of $S_i$. In the first term $H_J$, as shown in eq. (3), $J$ stands for an exchange interaction energy constant between $i$-th and $j$-th sites. The “$nn$” in eq. (3) means nearest neighbor and the exchange interaction works between nearest neighbor sites. The constant value $J$ is equivalent for all magnetic moment. In the second term $H_D$, as shown in eq. (4), $D$ stands for a magnetic dipole interaction constant. The magnetic dipole interaction works on all magnetic sites because it is due to magnetic field interspersed in all space. In the third term $H_B$, as shown in eq. (5), $B$ represents applied magnetic field which acts equally on all magnetic sites. The changing of $S_i$ on MC simulation progresses as spin-flips by Metropolis sampling. The random sampling is iterated sufficiently with acceptance probability $e^{\frac{\Delta E}{k_B T}}$ at constant temperature $k_B T$. Here, $k_B$ and $T$ denote Boltzmann constant and absolute temperature, $\Delta E$ is energy difference between the two states that calculated from eq. (2). The random number was generated by Mersenne Twister algorithm. The cycle of the random number is $2^{19937} - 1$. $S_i$ has dimension of magnetic moment. Equation (3) is converted for eq. (6).

$$H_J = \sum_{nn} J |S_i| |n_i| |S_j| n_j$$  \hfill (6)
Here, $\mathbf{n}_i$ represents a unit vector with the direction of $\mathbf{S}_i$. $J|\mathbf{S}_i||\mathbf{S}_j|$ has dimension of energy. Moreover, $J|\mathbf{S}_i||\mathbf{S}_j| = J$ by $|\mathbf{S}_i| = 1$, $J$ has dimension of energy. On the other hand, $\mathbf{B}$ is magnetic field of $x$-direction. Equation (5) can be transformed to the following equation using $\mathbf{B} = |\mathbf{B}|\mathbf{i}$, where $\mathbf{i}$ denotes a unit vector of the $x$-direction for the magnetic field $\mathbf{B}$.

$$H_B = \sum_i \tilde{\mathbf{B}} \cdot \mathbf{n}_i$$  \hspace{1cm} (7)

Here, $\tilde{\mathbf{B}}$ is defined by $\tilde{\mathbf{B}} = |\mathbf{B}|\mathbf{S}_i$, and $\tilde{\mathbf{B}}$ was scaled by $J$. In the same way, all energies $k_B T$, $H_J$, $H_D$ and $H_B$ were scaled by $J$ in the calculation. Therefore, these parameters have no dimension. In this simulation, the parameters were set as $k_B T = 0.1$, $J = 1.0$, $D = 0.1$. In addition, the magnetization $M$ represents summation of $S_{ix}$ for all spins and that is defined by

$$M = \sum_{i=1}^{N} S_{ix}.$$  \hspace{1cm} (8)

The maximum value of $M$ is different by $N$ for each cluster. In the reference [3], the MC method for the magnetic dynamic process is described in detail.

3. Results and discussion

Figure 2 shows simulation results of hysteresis curves for torus ring cluster with $R = 8$, 10, 15, 20 for (a) $r = 3$ and (b) $r = 5$. The magnetic field was applied along to $x$-axis as shown in Fig. 1. The simulation was repeated three times, that is, three loops were obtained for each cluster and Fig. 2 shows either one loop of three loops, respectively. The hysteresis curve for torus ring with $r = 3$, $R = 8$ includes plateau region in demagnetization curve. On the other hand, the curve does not include plateau region in increase magnetization curve. These two magnetic reversal processes are seen in all simulation results of each torus cluster in case of $r = 3$ and which process is chosen seems to be randomly, although there may be some tendency depending on cluster size. In case of $r = 5$, some clusters take curve with plateau region. The reason why the clusters take curve with plateau region in magnetic reversal process is discussed later. In Fig. 2 (a), the coercivity ($H_c$) is increased as $R$ becomes larger. Because the cluster which have larger $R$ has more magnetic sites, amount of exchange interaction energy increases in larger $R$ cluster. However, $H_c$ of a ring with $r = 5$ and $R = 8$ is smaller than one of a ring with $r = 3$ and $R = 8$. This tendency is also seen in other pairs of clusters which have same $R$ and different $r$. As this reason, it is assumed that magnetic domain wall is harder to move in smaller $r$ due to magnetic constrain. Next, the details of reversal process focused on spin arrangement are shown. In the following, the major radius $R$ is fixed as $R = 8$. 


Figure 3 shows snapshots of characteristic state at each point from A to H in demagnetization process with plateau region for the torus ring with $r = 3$. The color of snapshots represents for vector of $S_\theta$. The color of spins in each snapshot shows blue for $S_\theta = -1.0$ and red for $S_\theta = 1.0$. The schematic view of spin arrangement is shown above each snapshot. The torus ring of schematic view is divided for eight regions by magnetic spins direction. The arrows in schematic view represent average value of magnetic spins. The areas of eight regions are changed by applied magnetic field. We can see from this figure that values of $S_\theta$ in regions (iii) and (v) are gradually reduced at the point A and B. At the point C, values of $S_\theta$ in (ii) and (vi) are spread and the spins take clockwise direction. Subsequently, (iii) and (v) are become like domain wall. At the point C to D, (iv) is reduced, according as increasing for (ii) and (vi). Then spin arrangement becomes CD state for clockwise. Sometimes, (i) and (vii) are reduced instead of (iii) and (v). Then spin arrangement becomes CD state for counterclockwise. It is assumed that the probability which rotations are chosen is equal because the clusters are isotropic for the applied magnetic field.

At the point Fig. 3 E, in the region of (viii), some spins of near to origin start to reverse and then small CD structure is generated as shown at the point F. The small CD structure moves to outside of the torus ring as shown at the point G and thus, magnetic reversal process is finished. In the following, the magnetic reversal process is called CD path as shown in Fig. 3.

Figure 4 shows snapshot and schematic view at each point from I to M in demagnetization process without plateau region for the torus ring with $r = 3$ which reverses quickly. In I to J, two regions of (x) and (xiv) are gradually reduced and then, regarding these two regions as domain walls, the spin arrangement takes a state such that upside and downside regions opposite each other (head-to-head state). The magnetization reverses as if the whole rotate.
keeping the head-to-head state as shown in Fig. 4 K to M. In the following, the magnetic reversal process is called rotation path as shown in Fig. 4.

Figure 3: Snapshot at each point from A to H in demagnetization process with plateau region for torus ring with \( r = 3 \). The schematic view of spin arrangement is shown above the each snapshot.
Figure 4: Snapshot at each point from I to M in demagnetization process without plateau region for torus ring with $r = 3$. The schematic view of spin arrangement is shown above the each snapshot.

Figures 5 show Monte Carlo steps (MCS) dependence of numerical value for cluster with (a) $r = 3$, (b) $r = 5$. The total energy $E_{\text{total}}$ is set:
Here, $E_J$, $E_D$ and $E_B$ are the value of energy corresponding to Hamiltonian $H_J$, $H_D$ and $H_B$. The MCS is denoted as time course. The closure domain parameter ($M_\phi$) represents degree of CD state and the value of $M_\phi$ is defined by:

$$M = \frac{1}{N} \sum_i S_i \cdot \frac{\mathbf{r}_{\text{spin}}}{|\mathbf{r}_{\text{spin}}|}. \quad (10)$$

Here, $\mathbf{r}_{\text{spin}}$ is the position vector of $i$-th spin site with respect to the origin which is center of $R$. $N$ is total magnetic site number [4, 5].

In Fig. 5 (a), $M_\phi$ takes high value in reversal process which takes CD path (e.g. $\approx 1 \times 10^5$ MCS) due to forming CD state as it can be seen at point D in Fig. 3. In this reversal process, $H_D$ is decreases when $H_J$ is increased before that CD state is formed, that is, these two energy are trade-off relationship. However, trade-off relationship is broken by forming of CD state. Actually, both of magnetic dipole and exchange interaction energy decrease attending on increasing of $M_\phi$. As the result, $E_{\text{total}}$ also decreases and becomes stable. Because of the above, CD state is stable state and therefore the immobility of the CD state due to the stability makes plateau region in magnetization reversal process of CD path. In the plateau region, the exchange and the magnetic dipole interaction energy are slightly increased to the end of the plateau region and the two energy are drastically increased at the end of the plateau region. At this time, $M_\phi$ decreases drastically and it means that the CD state has been broken. $E_{\text{total}}$ decreases against increasing of the two energy, however, decreasing of magnetic field energy compensated for this gap. On the other hand, in the reversal process with rotation path marked by circle in Fig. 5 (a), $M_\phi$ is slightly increased, however, CD state from I to M is not seen as shown in Fig. 4. This reversal process is completed more quickly than that of CD path. In the case of $r = 5$ as shown in Fig. 5 (b), reversal process take only CD path, however, the process show similar tendency although the shape of $M_\phi$ and energy are blunter than that of (a) $r = 3$. The reason for taking only CD path, it is assumed that few trial times. The rotation path might occur by different random number series and many trials. To make clear the differences between two clusters, $M_\phi$ and $E_{\text{total}}$ are normalized and compared in the next paragraph.
Figure 5: Numerical value in calculation of (a) \( r = 3 \) and (b) \( r = 5 \). The \( x \)-axis is MCS which denotes time course. The reversal process with circle mark in (a) takes rotation path and other reversal processes take CD path.

Figures 6 show dependence of \( M_f \) on the absolute value of the magnetic field for all reversal process in the case of (a) \( r = 3 \) and (b) \( r = 5 \). The line color denotes sequence of reversal process. As mentioned above, in the case of \( r = 3 \), the magnetic reversal process could take both of CD path and rotation path and it is also shown in Fig. 6 (a). It seems that CD path is taken more often than rotation path. On the other hand, in the case of \( r = 5 \), the reversal process seems to take only CD path and some \( M_f \) have plateau region, however, the plateau region is shorter than ones of (a). In addition, \( M_f \) are scattered in some reversal process and the shapes of them are blunt comparing with (a). From the point of view, it is surmised that the case of \( r = 5 \) is more unstable than that of \( r = 3 \) in the reversal process. This conception follow the fact that \( H_c \) in the case of \( r = 5 \) is smaller than one in the case of \( r = 3 \) as shown in Fig. 2.

Figures 7 show normalized \( E_{\text{total}} \) for the torus ring with (a) \( r = 3 \) and (b) \( r = 5 \) in all magnetic reversal process. Here, normalized \( E_{\text{total}} \) means \( E_{\text{total}} \) in Fig. 5 divided by \( N \) for each
cluster. The line color denotes sequence of reversal process. The gaps of normalized $E_{\text{total}}$ between peak and CD state in the cluster with (b) $r = 5$ are smaller than ones in the cluster with (a) $r = 3$. Therefore, the clusters with bigger $r$ reverse more quickly than that with smaller $r$.

Figure 6: Dependence of $M_\delta$ on the absolute value of the magnetic field in the case of (a) $r = 3$ and (b) $r = 5$.

Figure 7: Dependence of normalized $E_{\text{total}}$ on the absolute value of the magnetic field in the case of (a) $r = 3$ and (b) $r = 5$.

Figure 8 shows snapshot of torus ring with $r = 5$ before CD state for the case with $B = -0.06$ at (a) $y$-$z$ plane and (b) $x$-$y$ plane. This reversal process takes CD path. However, this CD path is more complex than that one of torus ring with $r = 3$, that is, a magnetic domain wall could shift even in $z$-axis direction. The reason is that flexibility of $z$-axis is increased as $r$ becomes larger. Therefore, a stability of CD state is changed by torus ring size.

This research has only calculation results. However, the experiment will be tried as future work. Then the results of simulation and experiment will be compared.
4. Conclusion

Some torus rings with different radius were calculated for hysteresis curve by MC method. The results show that one torus ring could take either CD path or rotation path in magnetic reversal process, although some clusters take only CD path in case of large minor radius $r$. The CD path includes CD state and the rotation path includes head-to-head state. Then, the change of spin states for two paths was cleared by detailed confirmation. Moreover, the calculation results were analyzed for closure domain parameter, exchange interaction energy,
magnetic dipole interaction energy and magnetic field energy. Consequently, it is surmised that the case of large minor radius is more unstable than that of small minor radius in the reversal process, because flexibility of thickness direction is increased as minor radius becomes larger. In the future work, the measurement for magnetic property of torus ring will be tried, and the experiment results will be compared to simulation results.

References


