

# Monte Carlo simulation for magnetic dynamic processes of micromagnetic clusters with local disorder

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## Abstract

Magnetic dynamic processes for micromagnetic clusters with local disorder of crystal structure were simulated by pseudo-non-equilibrium Monte Carlo method. The magnetic field dependence of magnetization showed a little dip at zero magnetic fields. The dip becomes larger as the number of dislocations increase. Simulated Barkhausen noise at the dip was stronger than ordinal-simulated Barkhausen noise around coercivity. The snapshot of spins shows a magnetic fluctuation around dislocations. The result suggests a possibility of a new measurement with high sensitivity, to detect the deformation of micromagnetic clusters.

*Keywords:* Magnetic hysteresis; Barkhausen noise; Magnetic fluctuation; Micromagnetic clusters

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## 1. Introduction

Recently a number of experimental studies have been made on magnetic dynamic processes for micromagnetic clusters such as magnetic nanowire or quantum dots [1–4]. For thin film type magnetic cluster, real-time measurements of magnetic domain wall movements have been tried mainly using magneto-optical Kerr effect [5,6]. On the other hand, other simulations for magnetic clusters like nanowires are dealing with magnetic dynamic process, especially hysteresis loops [7–10]. The information is becoming useful for developing high-density magnetic memories or micromagnetic devices. The influence of local disorder of crystal structure on dynamic magnetic properties, however, has not been considered sufficiently. The local disorder of crystals such as impurity, defects or dislocations is possible to exist even for a well-controlled grown cluster. The rate of disorder will increase as the size of the cluster decreases, and then it will be important to estimate its effect on the magnetic processes.

We have simulated the magnetic dynamic process using pseudo-non-equilibrium Monte Carlo (MC) method [11–14]. In this paper we will present the properties of the magnetic dynamic process for magnetic clusters with local disorder in the crystal structure.

## 2. Numerical method

It is not usual to simulate dynamic magnetic process, because the behavior of a spin system under continuously changing magnetic field has not yet been established. We have been trying to apply MC simulation for the dynamic magnetic process, especially like a Barkhausen noise (BN). The results showed good correspondence with experimental results, especially temperature dependences of BN. Moreover, the results suggested the possibility that closer observation of a magnetic dynamic process, such as BN, provide the information for the state of magnetic materials. The same method is applied in the following for plane type magnetic clusters which include dislocation loops.

In general, MC method deals with the thermal equilibrium state. The conventional process is as below, i.e. (i) at first an initial spin arrangement is set; (ii) then a spin is

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focused in the spin cluster; (iii) next a trial spin-flip is executed for the focused spin; (iv) the local Hamiltonian of the focused spin is calculated for the state before and after spin-flip; (v) each spin state for the focused spin is decided by making a comparison between their energies, including thermal fluctuation effects. One MC step (1 MCS) means scanning up to the total cell a number of times for the process from (ii) to (v). Usually MC steps are repeated until one gets a stable state [15–21].

Now we stopped the repeat before getting a stable state, because of dealing with the magnetic dynamic processes for BN. Under the condition of constant magnetic field, the total spin is in a non-equilibrium state and going to an equilibrium state with progressing MC steps. The magnetic field slightly increases before it comes to the equilibrium state, then the total spin is kept under another non-equilibrium state again, while proceeding to a new equilibrium state. The operation is repeated until the final magnetic field is achieved. Because the change of the magnetic field is minute, it is regarded that a series of steps is an approximately continuous process through a pseudo-non-equilibrium state. Here we introduce an assumption that magnetization intensity ( $M$ ), namely the summation of total spins ( $M = \sum_i s_i$ ;  $s_i$  denotes the  $i$ th spin state), of each MC step can reflect the magnetic dynamic process on the magnetic hysteresis. Therefore, in this study, we differentiate the magnetic process for applied magnetic field ( $dM/d(\text{MCS})$ ) and deal with the discrete components of  $dM/d(\text{MCS})$  as simulated BN. Note that MCS on our simulation varies with time ( $t$ ) on the real system.

Here, a spin system composed of  $31^2 = 961$  cells ( $0 \leq x \leq 30$ ,  $0 \leq y \leq 30$ ) standing for a single square lattice was prepared as a normal spin system. The lattice constant is 1, and this is regarded as a criterion of length. Deformed spin systems were made by introducing one or two dislocation loops on the normal spin system, as shown in Fig. 1.

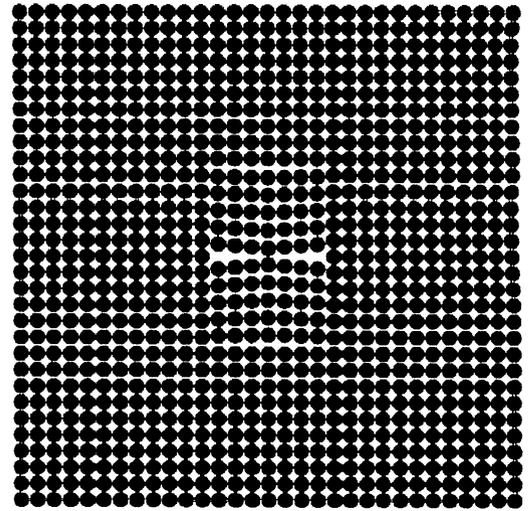
A simple Hamiltonian ( $H$ ) was used for the simulation as shown below:

$$H = - \sum_{ij} J_{ij} S_i S_j + B \sum_i S_i. \quad (1)$$

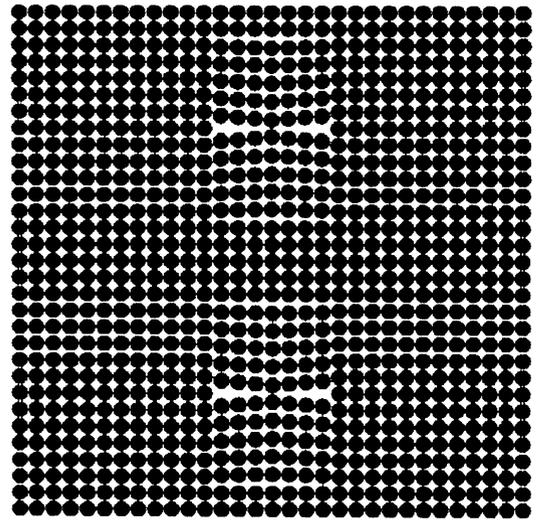
Here  $S_i$  denotes the spin state of  $i$ th cell, and  $J_{ij}$  stands for the effective exchange energy for  $i$ th and  $j$ th spins.  $B$  represents applied magnetic field. For simplicity, magnetic anisotropy and magnetic dipole interaction were neglected. This is justified because the cluster size was set small, and the number of magnetic particles is small. Here, we adopt the physical model of  $J_{ij}$  as a step function  $\theta$ , viz.

$$J_{ij} = \theta(1 - r_{ij}) = \begin{cases} 1 & (r_{ij} \leq 1), \\ 0 & (r_{ij} > 1). \end{cases} \quad (2)$$

$r_{ij}$  denotes the distance between  $i$ th and  $j$ th spins. Although the exchange energy of this model is supposed to be overestimated compared to real magnetic materials, it will be allowed for the purpose to derive intrinsic effect of local



(a)



(b)

Fig. 1. Model of micromagnetic cluster with residual strain including (a) one dislocation loop and (b) two dislocation loops.

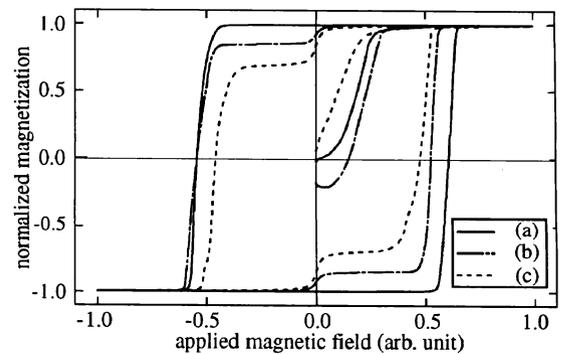


Fig. 2. Magnetic hysteresis curves for magnetic clusters including (a) no dislocation loop, (b) one dislocation loop and (c) two dislocation loops.

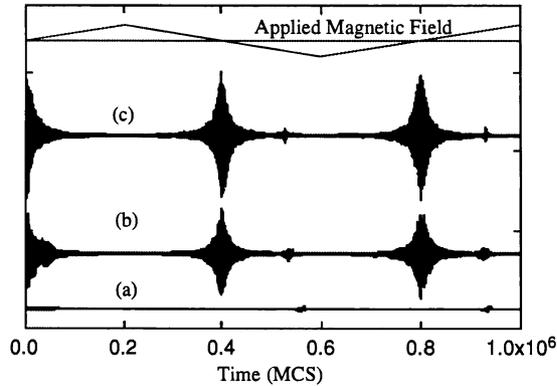


Fig. 3. Simulated Barkhausen noise (BN) for magnetic clusters including (a) no dislocation loop, (b) one dislocation loop and (c) two dislocation loops.

disorder in the crystal structure for dynamic magnetic process. For example, europium oxide (EuO), which is well known as a typical magnetic semiconductor, has a dominant exchange energy  $J_1$  represented as an exponential function of the distance between individual states due to RKKY interaction. That is, the exchange interaction decreases rapidly as the distance increases. When the lattice deformation becomes large, the distribution of  $J_1$  could be regarded as a function similar to Eq. (2).

The simulation was carried out by the use of the super-computer, ORIGIN 2000 in the Institute of Fluid Science, Tohoku University.

### 3. Results and discussion

Fig. 2 shows the calculation results for magnetic field dependence of magnetization (magnetic hysteresis curve) for the magnetic clusters including (a) no dislocation loop, (b) one dislocation loop and (c) two dislocation loops when applied magnetic field ( $B$ ) changes along  $B = 0 \rightarrow +1 \rightarrow 0 \rightarrow -1 \rightarrow 0 \rightarrow +1$ . Magnetization is normalized by the number of sites in the cluster. All hysteresis curves show the saturation magnetic field  $B_S$  around 0.5. The curves for the spin systems with dislocation loops have dips around zero magnetic field, but the dip cannot be seen for the normal spin system. Moreover, the dip depth increases as the number of dislocation loops increases.

Fig. 3 shows simulated BNs under an applied magnetic field of a triangular wave form for (a) no dislocation loop, (b) one dislocation loop, and (c) two dislocation loops. Large BNs are clearly seen in the magnetic field across the zero field when including (b) one dislocation loop and (c) two dislocation loops. The change of magnetization around the zero field is less than the one around coercivity. Small BNs exist around coercivity for all cases. These are supposed to be ordinal BNs which are produced by discontinuous magnetic domain walls movements [22,23].

For investigating the origin of BN around the zero magnetic field, let us follow the change of spins with

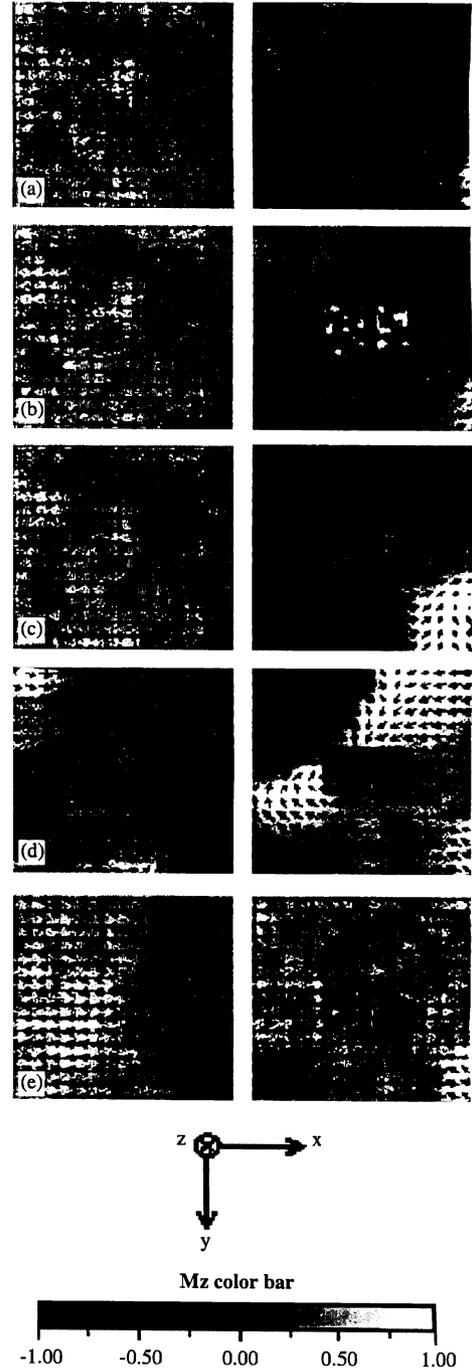


Fig. 4. Snapshots for micromagnetic clusters including no dislocation loop (left side) and one dislocation loop (right side) in a magnetic field changing along (a)  $B = +1 \rightarrow$ , (b)  $B = 0 \rightarrow$ , (c)  $B = -0.3 \rightarrow$ , (d)  $B = -0.4 \rightarrow$ , (e)  $B = -0.6$  in Fig. 2.

triangular waveform magnetic field as time flows. Fig. 4 shows a series of snapshots for micromagnetic clusters including one dislocation loop in magnetic field change along (a)  $B = +1 \rightarrow$ , (b)  $B = 0 \rightarrow$ , (c)  $B = -0.3 \rightarrow$ , (d)  $B = -0.4 \rightarrow$ , (e)  $B = -0.6$  in Fig. 2. We clearly see the furious spin disorders around the dislocation loop when the magnetic field is about zero. Hence, the origin of large

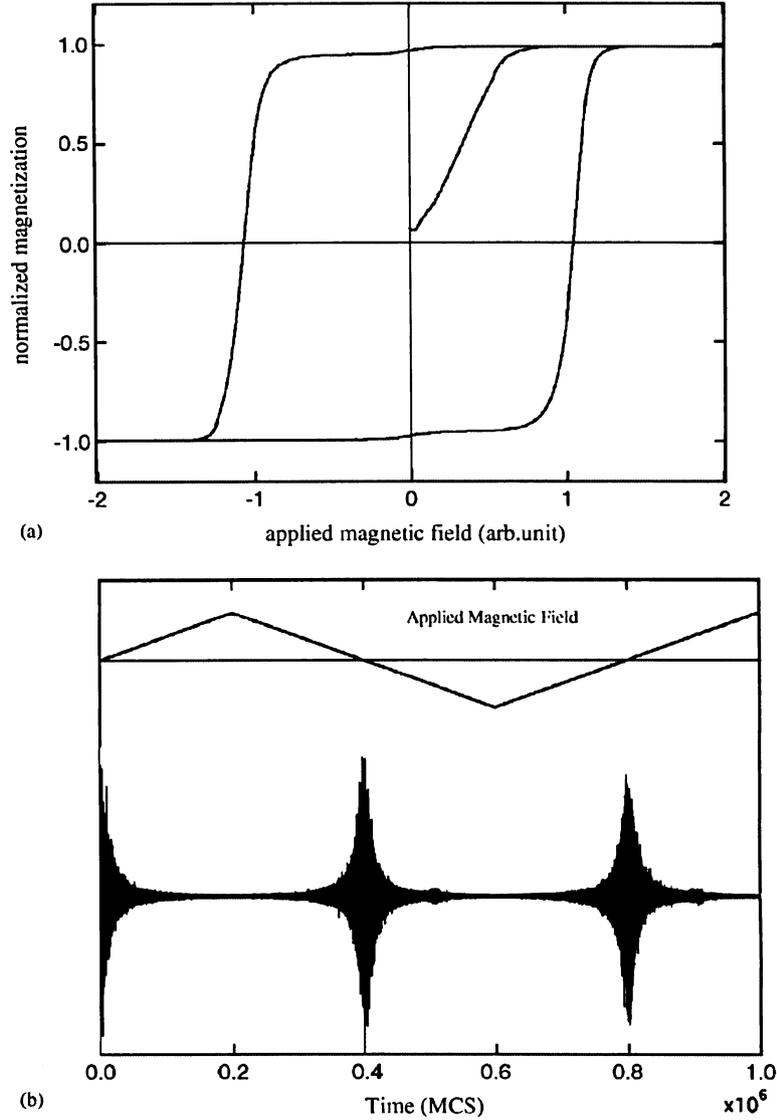


Fig. 5. (a) Magnetic hysteresis curve and (b) simulated BN for a three layer magnetic cluster including one dislocation loop on the intercalation middle layer.

BNs in Fig. 3 will be mainly due to the existence of dislocation. For ordinal magnetic materials, the rate of the area of local disorders in the crystallized magnetic clusters is very small and its effect could not be easily detected. In fact, as shown in Fig. 5(a), the dips around zero magnetic field on the hysteresis curves decrease rapidly when the micromagnetic cluster, including one dislocation loop, viz. a plane represented as Fig. 1(a), is intercalated between double perfect-crystallized planes composed of  $31^2 = 961$  cells ( $0 \leq x \leq 30$ ,  $0 \leq y \leq 30$ ) without any dislocation loops. But the anomalous BN corresponding to the dip does not decrease, as shown in Fig. 5(b), although indicating that the anomalous BN is highly sensitive to such local disorders.

Fig. 6 shows the calculation of the magnetic after-effect under applied magnetic fields changing from  $B = 1$

to  $B = -1$  as a step function of time, as shown below:

$$B(t) = -2\theta(t) - 1 = \begin{cases} 1 & (t \leq 0), \\ -1 & (t > 0). \end{cases} \quad (3)$$

After changing the magnetic field to  $B = -1$ , the magnetization for the cluster without any dislocation loops gradually decreases and finally gets to the opposite saturated magnetization. On the other hand, the magnetization for the magnetic cluster including one dislocation loop has a tiny dip right after the magnetic field was switched. In this case it is also assumed that spin fluctuation exists around the local disorder.

The above results suggest the high fluctuating and stressful state of the spin system including local disorders. Our model for the simulation may include some extreme

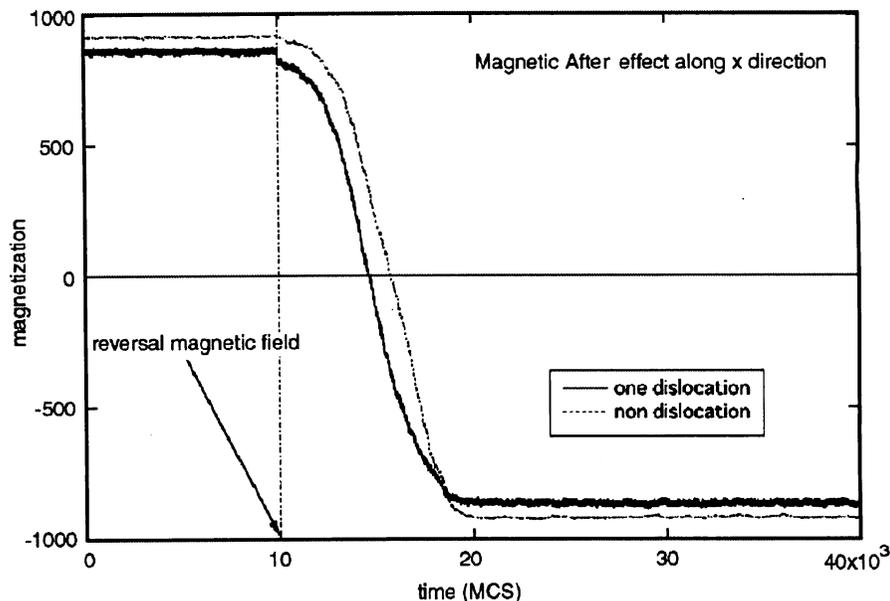


Fig. 6. Calculation of the magnetic after-effect under an applied magnetic field changing from  $B = 1$  to  $B = -1$  as a step function of time for the clusters without any dislocation loops and with one dislocation.

overestimation, especially about the exchange interaction which has a sharp cut-off length. But the tendency will still remain in some degree for the real system. Then we may have a new measurement tool using BN which can detect the local deformation in micromagnetic clusters.

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