Recovery Process from the Reversed Magnetization Simulated with a Square Lattice

Tomoaki Senoo,a Toshihide Sumi,a Masafumi Horio,a Arata Tsukamoto,b Iwao Matsuda,a,†

a The Institute for Solid State Physics, the University of Tokyo, 5-1-5 Kashiwanoha, Kashiwa, Chiba 277-8581, Japan
b College of Science and Technology, Nihon University, 7-24-1 Narashino-dai, Funabashi, Chiba 274-8501, Japan
† Corresponding author: imatsuda@issp.u-tokyo.ac.jp

Received: 29 January, 2022; Accepted: 30 May, 2022; J-STAGE Advance Publication: 28 July, 2022; Published: 28 July, 2022

Control of magnetism has been an attracting issue due to its scientific interests and technological application. In such research, theoretical simulation plays an important role. We performed a Landau-Lifshitz-Gilbert simulation on the recovery process of a ferromagnet from a magnetization reversed state in a square lattice system. During the process, there can be a situation that the magnetization reversal state is enhanced or completed transiently, which may be observed experimentally.

Keywords Simulation; Magnetic domain; Landau-Lifshitz-Gilbert equation; Magnetization dynamics; Femtomagnetism

I. INTRODUCTION

Magnetization controls in materials have been one of the hot topics in condensed matter physics and have also been a key technology to develop our devices today [1–10]. Responses to external triggers and recoveries in a material have led to varieties of functionalities, but, at the same time, the dynamic events are complicated and dependent on many parameters. Theoretical simulations have been important approaches to reproduce the temporal evolutions and to understand their mechanism. It has been thus challenging to conduct simulations with the universal or omniscient model. On the other hand, it has also been found useful to develop a simple model that can be applied appropriately to real cases.

Recently, interests have grown in all-optical controls of magnetization in ferrimagnetic materials that induce femtomagnetism. The non-equilibrium events have shown varieties of dynamic phenomena, i.e., ultrafast demagnetization or magnetization switching. Theoretical simulations have been useful to unveil such spin dynamics and also to predict the following recovery process, trigged by the unique initial states. These ultrafast magnetic states are expected to be technically applicable in future opto-electric devices or fast magnetic memories.

In the present paper, we made a simulation on recovery process of the optically induced magnetization by adopting a simple square lattice to consider magnetic interactions in various types of effective fields. The size of the model system was in the nanometer scale and the dynamic event was considered in the femtosecond–picosecond timescale. The temporal evolution was acquired as a solution of the Landau-Lifshitz-Gilbert equation (LLG eq.) with five terms for the effective magnetic field; external term, anisotropic term, exchange term, demagnetization term, and Dzyaloshinski-Moriya Interaction (DMI) term. Time-dependent changes during the recovery process were obtained at different initial conditions. We discovered that there is a situation that the magnetization reversal state is enhanced or completed transiently. A possible experiment to detect the intriguing event is discussed.

II. SIMULATION

The present simulation considers a case when there is a transient magnetic domain, surrounded by the original state, as shown in Figure 1(a). Such a situation happens when magnetic domains are stochastically changed by the external...
trigger such as optical irradiation. We modeled the internal domain as the 8 × 8-site square lattice with the site separation of 2 nm, as illustrated in Figure 1(b). The magnetic recovery process at individual sites can be simulated by considering precession and damping factors, as indicated in Figure 1(c).

To obtain the temporal evolution of the system, we performed numerical calculation based on the LLG eq. [11]. The LLG eq.,

$$\frac{dM}{dt} = -\gamma M \times H_{\text{eff}} + \frac{\alpha}{M_S} M \times \frac{dM}{dt},$$  \hspace{1cm} (1)

describes the motion of magnetization in a magnetic material, where $M$ is the magnetization, $H_{\text{eff}}$ is the effective magnetic field, $\gamma$ is the gyromagnetic ratio, $\alpha$ is the Gilbert’s damping factor, and $M_S$ is the saturation magnetization. The first and second term in the right-hand side of the equation corresponds to the precession and damping kinetics of the magnetization respectively, which can be seen in Figure 1(c).

By substituting Eq. (1) to the second term of the right-hand side of itself, we obtain

$$\frac{dM}{dt} = \frac{\gamma}{1 + \alpha^2} \left[ M \times H_{\text{eff}} + \frac{\alpha}{M_S} M \times (M \times H_{\text{eff}}) \right].$$  \hspace{1cm} (2)

In our calculation, we set $||M|| = M_S$ for simplicity, deriving a normalized form of Eq. (2):

$$\frac{d\mathbf{m}}{dt} = -\frac{\gamma}{1 + \alpha^2} \left[ \mathbf{m} \times H_{\text{eff}} + \alpha \mathbf{m} \times (\mathbf{m} \times H_{\text{eff}}) \right],$$  \hspace{1cm} (3)

where $\mathbf{m} = M/||M||$ is the normalized vector of magnetization.

We numerically solved Eq. (3) by the four-dimensional Runge-Kutta method with a time step of $\Delta t = 2$ ps. For the effective magnetic field $H_{\text{eff}}$, we considered five terms:

$$H_{\text{eff}} = H_{\text{ext}} + H_K + H_A + H_D + H_{\text{DMI}},$$

where $H_{\text{ext}}$ is the applied external magnetic field, $H_K$ is the anisotropic magnetic field, $H_A$ is the exchange magnetic field, $H_D$ is the demagnetization field, and $H_{\text{DMI}}$ is the DMI magnetic field. In our calculation, we set

$$H_{\text{ext}} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ H_0 \end{pmatrix},$$

$$H_K = \begin{pmatrix} 0 \\ 0 \\ 2K_u m_z \\ M \end{pmatrix},$$

$$H_A = 2A \frac{\partial}{\partial m} \left[ \left( \frac{\partial m}{\partial x} \right)^2 + \left( \frac{\partial m}{\partial y} \right)^2 \right],$$

$$H_{\text{DMI}} = \frac{2D}{M} \begin{pmatrix} \frac{\partial m_z}{\partial x} \\ \frac{\partial m_z}{\partial y} \\ \frac{\partial m_z}{\partial x} + \frac{\partial m_x}{\partial y} + \frac{\partial m_y}{\partial x} \end{pmatrix},$$

where $H_0$ is the strength of the applied magnetic field, $K_u$ is the anisotropic energy, $D$ is the DMI, and $A$ is the exchange stiffness constant. The parameters were set as given in Table 1. We used the gyromagnetic ratio of an electron for $\gamma$. The parameters $\alpha$, $M_S$, $A$ were set referring to the results of previous studies on the femtomagnetism [2, 12, 13]. Parameters $K_u$ and $D$ are flexible parameters that can be determined by the experimental cases. We adopted the reasonable values of the real materials [4]. We calculated the spatial derivatives by differentiating them with spatial step, $\Delta x = \Delta y = 2$ nm, which is the size of the lattice. We first set the original magnetization state to be the one with the magnetization of all sites pointing to the $+z$ direction. We, then, made the initial magnetization-reversed states by randomly selecting

![Figure 1: (a) A concept of a transient magnetic domain, surrounded by the original state. (b) An 8 × 8 square lattice surrounded by a boundary (green region). In the initial state, a number of the sites (colored in red) were selected randomly and reversed the magnetization, while the others were unchanged (colored in blue). (c) An illustration of motion of magnetization. The blue, red, and green arrows show the direction of magnetization, damping, and precession respectively. The black thin arrow shows the direction of the external magnetic field.](image)

<table>
<thead>
<tr>
<th>Parameter name</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gilbert’s damping factor</td>
<td>$\alpha = 0.3$</td>
</tr>
<tr>
<td>Saturation magnetization</td>
<td>$M_s = 2.00 \text{MA m}^{-1}$</td>
</tr>
<tr>
<td>Gyromagnetic ratio</td>
<td>$\gamma = 1.76 \times 10^{11} \text{rad s}^{-1} \text{T}^{-1}$</td>
</tr>
<tr>
<td>Applied external field</td>
<td>$\mu_0 H_0 = 3.6 \text{T}$</td>
</tr>
<tr>
<td>Anisotropy energy</td>
<td>$K_u = 0.314 \text{MJ m}^{-3}$</td>
</tr>
<tr>
<td>DMI coefficient</td>
<td>$D = 62.8 \mu \text{m}^2$</td>
</tr>
<tr>
<td>Exchange stiffness constant</td>
<td>$A = 0–37.70 \text{pJ m}^{-1}$</td>
</tr>
</tbody>
</table>
various number of sites and reversing their magnetization to the \( -z \) direction. For the boundary condition, we assumed magnetization of the boundary sites to be constant during the process, since we considered a transient magnetic domain surrounded by the original state. In the following section, we show a picture on micromagnetic dynamics in magnetic materials, provided by the present simulation.

III. RESULTS AND DISCUSSION

Figure 2(a) shows a recovery of the magnetization along the \( z \) direction, \( M_z \), after various case of the initial reversed states. In the simulation, all the 64 sites originally have the up orientation, and the net magnetization is \( M_z = 64 \). The reversed magnetization, induced by optical pumping, was treated in the initial condition. Amount of \( M_z \) is described by the number of the reversal sites. In all cases, the net magnetization was kept constant at first, followed by the recovery. Intriguingly, the dynamics appears essentially different when a sign of the initial \( M_z \) value is negative. The reversal magnetization is enhanced before the recovery process, as indicated by symbols in Figure 2(a). Moreover, in the case of the 60 reversal sites, all of them transiently have the down orientation and the net magnetization is \( M_z = -64 \). Figure 2(b) schematically draws a cycle of the dynamic behavior. After the optical pumping of the original state (i), occupations of the opposite magnetization sites become dominant (ii). Subsequently, the transient net magnetization is completely reversed (iii), followed by the recovery to the original state (i). The enhancement of the reversal magnetization is due to the exchange interaction term, \( H_A \), while the recovery proceeds by the external field term, \( H_{ext} \), as in all the cases.

Since it is intriguing to observe the transient state of the totally reversed magnetization, (i) in Figure 3, we further examined the exchange-interaction dependence by simulating with different values of the exchange stiffness constant, \( A \). When there is no interaction (\( A = 0 \)), the initial state of the 60 reversed state returned to the original state, (II). At the finite \( A \) values (6.28–17.59 \( \text{pJ m}^{-1} \)), the reversed magnetization is enhanced and becomes fully opposite. Above that region, the transient state disappears, and the recovery curves become complicated. Eventually, the magnetization transits to the state (III) at \( A = 32.67 \) and 37.70 \( \text{pJ m}^{-1} \) in the present simulation. As schematically illustrated in Figure 3, the state (III) is composed of the in-plane antiparallel ordering. The simulation predicts existence of varieties of the transient magnetization states, depending on the exchange interaction in a matter.

In addition, we investigated effects of DMI in the magnetization recovery. Figure 4 shows simulation results with different DMI constants. The recovery time was found to become, in general, short by large DMI values. This finding may help understanding or exploring spin dynamics of multiferroic materials, for examples, that show intriguing magnetoelectric effects by DMI.

The present simulations demonstrate intriguing magnetic evolutions in the transient magnetic domain. Today, varieties of experiments have been made to study magnetization dynamics, controlled by magnetic fields, optical rays or spin-
currents, for example. We hereby propose one possible experiment, time-resolved magneto-optical measurement, to examine our results. The magneto-optical effects, such as Faraday effect [14] or magneto-optical Kerr effect (MOKE) [15], have been standard techniques to probe magnetization of a sample [9, 10]. The time-resolved measurements, typically by the pump-probe method, have unveiled magnetization or spin dynamics in a material. With femtosecond laser pulse as a pump, recent investigations have discovered the ultrafast events of demagnetization or magnetization-reversal [5–8]. The phenomena match with the initial conditions, adopted in the simulation (Figure 2 and Figure 3). It is inferred that the initial amount of the reversal state depends on strength of the photo-induced magnetization, and it can be controlled by the photon flux of the incident optical beam.

The induced magnetic reversal state is not permanent and returns to the initial state when one applies a constant magnetic field on the sample. With parameters adopted in the present simulation, we expect to observe the phenomena at picosecond timescale. This behavior should be observed by time-resolved magneto-optical measurements with femtosecond time-resolution. It is suitable to conduct a time-resolved MOKE measurement with different pump intensity on materials, such as GdFeCo [2, 5–7], that has been reported to show the ferromagnetism [6, 16]. In addition, the element-selective non-linear spectroscopy, developed recently, may probe magnetization dynamics of specific 2D sublattice at the interface that matches with the present model [17–20].

IV. CONCLUSION

Focusing on the recovery process of the magnetization dynamics, triggered extrinsically, we performed a numerical simulation on a magnetic nanodomain in the femtosecond time scale. We solved the Landau-Lifshitz-Gilbert equation with a square lattice. We found that the temporal evolutions depend on the initial condition. Furthermore, we discovered the magnetization reversal state that is enhanced or completed transiently. The dynamical behavior may be observed on the appropriate sample by a time-resolved magneto-optical measurement with the pump-probe method.

Acknowledgements

The research was made under the SACLAC Basic Development Program 2018-2020. The XFEL experiments were performed at the BL1 of SACLAC with the approval of the Japan Synchrotron Radiation Research Institute (JASRI) (Proposal No. 2020A8019). We appreciate Souliman EL MOUSSAOUI for discussion. T. S. acknowledges support by Forefront Physics and Mathematics (FoPM) WINGS Program, the University of Tokyo.

Note

This paper was presented at the 9th International Symposium on Surface Science (Online) from November 28 to December 1, 2021.

References

