Micromagnetic Study on the Magnetization Reversal of Barium Hexaferrite (BaFe\textsubscript{12}O\textsubscript{19}) Thin Film

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Abstract

This study investigates a magnetization reversal mechanism based on the hysteresis curve of Barium Hexaferrite (BFO) thin film by micromagnetic simulation through parallel and perpendicular magnetization directions along the axes. The hexagonal shape of the BFO film was modeled with thicknesses of 5, 10, and 15 nm and a diameter size ranging from 50 to 100 nm. It was found that the coercivity field \( H_C \) and the saturation field \( H_S \) of the BFO film decreased as the diameter size increased and thickness decreased. It was observed that the nucleation field \( H_N \) increased as the diameter size increased. An analysis of energies showed that the demagnetization energy was dominantly influenced by the diameter and thickness in comparison to the anisotropic energy. From the hysteresis curve, the switching time was also investigated. Interestingly, the switching time was faster for the thinner BFOs with a diameter under 70 nm. For particles larger than 70 nm in diameter, the switching time showed fluctuation irrespective of the BFO thickness. Based on these results, a diameter size of 70 nm is proposed as the critical size for producing the equal time for switching domain polarity.

Keywords: micromagnetics, magnetization reversal, hysteresis, barium hexaferite

Introduction

Magnetoplumbite-type Barium ferrite (BaFe\textsubscript{12}O\textsubscript{19}, BFO) is one of the well-known permanent magnet materials that has been widely applied to sensors, toys, motors, microwave absorbers, and magnetic storage media [1-3]. A BFO with a hexagonal close packed (HCP) crystal structure consists of 64 ions per primitive unit cells with a P6\textsubscript{3}/mmc space group that has high uniaxial magnetic anisotropy energy [2, 4, 5]. On the other hand, good chemical stability, high temperature and corrosion resistances, and high mechanical hardness make BFO an attractive material to exploit further potential applications [6, 7]. Based on author’s knowledge, most of the previous
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studies involving BFO materials have focused on the material preparation methods, influence of dopants, and macroscale magnetic properties stimulated by practical applications [8–10]. There are many popular methods to produce BFO particles such as using solid state reaction, mechanical alloying, coprecipitation, sol-gel, and hydrothermal methods [11–13]. In recent years, some efforts have been made toward the growth of nanostructure BFO thin film of BFO due to its potential application in ultrahigh density magnetic recording [14]. While methods have been effective in producing bulk quantities of single-phase BFO particles, discussions about the growth of nanostructure grains and the properties of single-domain particles of Barium ferrites are lacking. The magnetic configuration of individual nanostructures has also been rarely discussed, although several facilities, such as Lorentz microscopy, magnetic force microscopy, scanning tunneling microscopy, and Kerr microscopy, have been employed to study local magnetic behaviors [15, 16]. The limited resolution of those experimental facilities made the observations of the magnetic configuration in nanoscale insufficient. Alternatively, a simulation approach using the micromagnetic method can be performed to analyze a specific behavior of local magnetization based on the Landau-Lifshitz-Gilbert equation [17]. According to most studies, the micromagnetic method is powerful for the study of next generation ultrahigh density magnetic recording materials, including spintronics developments, due to the continuum approach that bridges the molecular and macroscopic analysis of the ferromagnetic system [18, 19].

This study investigated the magnetization behavior of a single BFO thin film in the presence of an external magnetic field in order to obtain its hysteresis curves for both in-plane and out-plane directions at a size interval ranging from 50 to 100 nm. Our previous study has shown that the critical size of a single hexagonal BFO nanostructure was around 430 nm, which agrees with the analytical Kittel formula [20, 21]. This means that the simulations in the present study are in the regime of single-domain particles. The influence of hexagonal size on the coercivity, anisotropic field, nucleation field, and switching time, along with domain configuration are discussed in detail.

**Materials and Methods**

To produce the hysteresis curve of the BFO film, micromagnetic simulation was performed using public software, the Object Oriented Micro-Magnetic Framework (OOMMF) based on the Landau-Lifshitz-Gilbert (LLG) equation [18-22]. A hexagonal shape BFO film was used as illustrated in Figure 1(a), with respect to the diameter size and thickness variation. The diameter size varied from 50 to 100 nm and the thicknesses t were 5, 10, and 15 nm. Material parameters, such as saturation magnetization, $M_s = 275$ kA/m, magnetocrystalline anisotropy constant, $K_1 = 96$ kJ/m$^3$, and exchange constant, $A = 2 \times 10^{-11}$ J/m, were used in this simulation [23]. The damping constant $\alpha$ was fixed at 0.1 and the cell size was $2.5 \times 2.5 \times 5$ nm$^3$ taking into consideration that the exchange length of BFO $l_{ex} = \sqrt{2A/\mu_0M_s^2}$ was around 6.5 nm [4,19]. The initial spin configuration of BFO was set to random, as shown in Fig. 1(b), and the temperature was 0 K. Then, the magnetic field was applied from -1000 mT to +1000 mT in x direction ($H_x$) and z direction ($H_z$) in order to observe magnetization behavior on the hard and easy axes direction, respectively.

**Results and Discussion**

The hysteresis curve of the BFO film diameter and thickness variation is displayed in Figure 2(a–c). The hysteresis curve closely showed a rectangular pattern corresponding to its easy axis direction. Interestingly, the domain structures only exhibited single-domain structure magnetization and followed the Stoner-Wohlfarth prediction [24]. This was understandable because the dimensions of the simulated BFO were below the critical size, which was around 525 nm [20, 21, 25], and the single-domain structure was easily formed. Then, the coercivity field was observed from the z direction magnetization for the diameter and thickness variation, as depicted in Figure 2(d). The coercivity field ($H_c$) decreased as the diameter size of BFO increased, while it increased as the thickness increased. The decreasing of $H_c$ was found to be linear with the increasing diameter. The coherent rotation of magnetization along the easy axis contributed to the smoothly decreasing coercivity field as the diameter increased. The value of $H_c$ was around 400–520 mT, which was approximately close to the results of Zhang’s work at low temperature [26]. The reduction of $H_c$ in hexaferrite nanostructures has also been observed experimentally by some researchers.
The study by Mosleh et al. [27] showed that an annealing temperature could have an increasing effect on $H_c$ due to the particle size increase. Our results similarly showed that the thicker BaFe$_{12}$O$_{19}$ film has a larger coercivity value, which particularly occurred in the single-domain particle size regime.

Concerning easy axis magnetization, we observed the saturation field ($H_s$) in relation to easy axis magnetization, as given in Figure 3(a), for the diameter and thickness variation. The saturation field decreased as the diameter increased, whereas it increased as the thickness increased. The decreasing trend of the saturation field followed the coercivity field. In this sense, the particle dimension and ratio influenced intrinsic magnetic properties, such as the saturation field. It is known that at larger volume of the film uses a larger amount of energy.
equally with the given magnetic field. However, our simulation found that the thickness of the film more strongly affected the $H_s$ values than the film diameter, thus the ratio of the film became important as shown in Figure 3(a). The energy densities of BFO, such as the demagnetization and anisotropy energies, were also analyzed. The energies are represented in Figure 3(b) through the diameter and thickness variation. Interestingly, it was also observed that the demagnetization energy decreased as the diameter of the BFO thin film increased, while the anisotropy energy was relatively constant as the diameter and thickness increased. Therefore, the demagnetization energy was highly affected by the thin film geometry over the anisotropic energy, as shown in the Figure 3(b). This result, according to which the demagnetization energy is affected by changing the BFO dimension agrees with the report by Goolaup [25]. As indicated in Figure 3, the saturation field and the demagnetization energy were related to the changes in diameter. The demagnetization energy originated from the demagnetization or magnetostatics field in the magnetic system [4].

Furthermore, the BFO hysteresis curve in x direction was also produced, as shown in Figure 4 for the diameter and thickness variation. The hysteresis curve showed a typical S-curve for all the diameter and thickness variations, as usually found in the hard axis magnetization direction. An interesting aspect of the hysteresis curve in the x direction was in respect to the nucleation field ($H_N$), where the magnetic field abruptly decreased just as it was reported in Permalloy (Py) [28, 29]. It was shown that $H_N$ changed as the diameter and thickness increased. For the cases in which the thicknesses were $t = 5$ nm and $t = 10$ nm, the nucleation field tend to increase as the diameter increased. However, for thickness $t = 15$ nm, the nucleation field showed small fluctuation from 50 nm to 70 nm, and above 70 nm it became constant. This result was obtained irrespective to changes in the diameter. Based on the energy analysis shown in Figure 3(b), the anisotropy energy of the 10 nm and 15 nm thicknesses were lower for $d = 60$ in comparison to the thickness of 5 nm. These characteristics contributed to the total energy that affected the slightly reduced nucleation field. In comparison to the thickness 5 nm, the anisotropy energy was insensitive to diameter. Therefore, the total energy was only contributed to by the demagnetization energy that monotonously increased the nucleation field.

Figure 5 shows the domain structure evolution of the BFO thin film, which was applied using a quasi-static field in the x direction for the case $d = 100$ nm with respect to the thicknesses $t = 5$, 10, and 15 nm. The saturation magnetization was obtained by giving an external magnetic field around 1000 mT and denoted by position 1 (x positive) and position 4 (x negative) with the single-domain structure. Then, the domain structure started to

Figure 4. The BFO Hysteresis Curve in the x Direction Magnetic Field with Respect to the Thickness Variation (a) $t = 5$ nm, (b) $t = 10$ nm, (c) $t = 15$ nm, and (d) the Nucleation field ($H_N$) in Relation to the Diameter and Thickness Variation
change after the magnetic field was applied in the opposite direction. It was found that the domain structure still maintained a single-domain structure and the vector magnetization direction also changed, as presented at positions 2 and 5 around the field magnitude of 340 mT ($t = 5$ nm), 380 mT ($t = 10$ nm), and 420 mT ($t = 15$ nm). Interestingly, the domain showed a single-domain structure again at zero magnetic field (positions 3 and 6) with the vector magnetization preferred to the easy axis magnetization for all thicknesses. These results showed that the magnetization rotation during the domain switching process was coherent and in agreement with the theoretical and experimental prediction [30, 31].

Besides the coercivity, nucleation, and saturation field, the switching time of BFO thin film was also determined based on the hysteresis curve in x direction magnetic field. The switching time was defined by the time needed to switch the domain magnetization from a different polarization, such as positive to negative polarization. It was observed that the switching time increased as the diameter size increased. Interestingly as can be seen in Figure 6, the switching time increased as the thickness increased, until the diameter was around 70 nm. Above the 70 nm diameter, the switching time showed a fluctuation that was irrespective to the BFO thickness. It was also found the relatively equal switching time occurred at the diameter 70 nm for all thicknesses. This means that the 70 nm diameter size of the BFO thin film was the critical size for switching domain polarity. Above the 70 nm diameter, the switching process could be affected by incoherent rotation and domain wall motion [32]. These results suggest that the switching time in the hard-magnetic orientation was also influenced by the nucleation field $H_N$. In comparison to Figure 4(d), the switching time tended to produce the same characteristics. For the thickness of 5 nm, an increase of the film diameter also increased the switching time significantly.
However, for the thicknesses of 10 nm and 15 nm, the switching time increased only slightly and corresponded with the insensitive trend of the nucleation field for the same film size.

Conclusion

In this paper, we investigated the magnetic hysteresis curve characteristics of Barium Hexaferrite (BFO) nano thin film by micromagnetic simulation methods. The hexagonal shape of the BFO film was simulated using varied the thicknesses of 5, 10, and 15 nm and a diameter size ranging from 50 to 100 nm. This diameter size interval was below the single-domain critical size. It was observed that the coercivity of the hexaferrite thin film slightly decreased as the diameter size increased. However, the coercivity increased as the thickness increased. For the hard axis orientation magnetic field, it was found that the nucleation field $H_N$ values are changed as the BFO diameter and thickness increased. For thicknesses of 5 and 10 nm, the $H_N$ values were increased as the diameter increased. This shows that the demagnetization energy values were predominantly influenced by diameter and thickness size in comparison to anisotropic energy values. Therefore, the increase in the saturation field was contributed to by increasing the demagnetization energy as the BFO thickness increases. Interestingly, it was also shown that the switching time is faster for a thinner BFO of a diameter that is under 70 nm. For a particle larger than 70 nm in diameter, the switching time showed fluctuation that seemed to be irrespective of the BFO thickness. Therefore, the diameter size of 70 nm is proposed as the critical size for producing the equal time for switching domain polarity.

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