Micromagnetic studies of the domain structure of BaFe$_{12}$O$_{19}$ cubes in zero magnetic field

D Djuhana$^*$, C Kurniawan, and J W Utomo

Department of Physics, Faculty of Mathematics and Natural Sciences (FMIPA)
Universitas Indonesia, Depok 16424, Indonesia

Center for Physics Research, The Indonesian Institute of Sciences (LIPI), Kawasan Puspitek No. 441-442 Serpong, Banten 15314, Indonesia

Corresponding author: dede.djuhana@sci.ui.ac.id

Abstract. This article reports an investigation of the domain structure of cube-shaped BaFe$_{12}$O$_{19}$ models in zero magnetic field using the public-domain OOMMF micromagnetic simulator to model cubes with sides varying from 100 to 900 nm. A Bloch wall appears in BaFe$_{12}$O$_{19}$ cubes larger than about 510 nm and a single-domain structure appeared below 510 nm. The transition from single- to multiple-domain structure in the cube-shaped models occurred near the size predicted by analytical solutions of Kittel’s equation. Analysis of the magnetization energy showed that the exchange energy increased with increasing size once the Bloch wall was formed. We also calculated the width of the Bloch walls from the full width at half maximum of the transverse component of the magnetization vector. The domain wall width increased, as the modeled cubes grew larger.

1. Introduction
Barium hexaferrite (BaFe$_{12}$O$_{19}$) is a very popular magnetic material owing to its high magnetocrystalline anisotropy, excellent chemical stability, and high Curie temperature ($T_c$) [1-3]. BaFe$_{12}$O$_{19}$ is used widely in permanent magnets, microwave absorbers, and memory storage materials [4-7]. In addition to experimental methods, numerical simulations of micromagnetic phenomena are an effective tool to understand magnetic domain structure in ferromagnetic materials [8,9]. We have previously studied the transition from single-domain (SD) structures to multi-domain (MD) structures in BaFe$_{12}$O$_{19}$ for hexagonal and cylindrical models. The transition occurred around diameters of 430 and 410 nm for the hexagonal and cylindrical models, respectively [10]. However, the two models differed greatly from theoretical predictions, by around 18%. This disagreement indicates that a better theoretical model is needed to predict the domain structure in BaFe$_{12}$O$_{19}$, especially the size at which the transition from SD to MD structures occurs.

In this article, we report an investigation of the domain structure of microscale cubes of BaFe$_{12}$O$_{19}$ using public-domain micromagnetic simulation software. A transition from SD to MD structure appeared when the size of the cube passed through a critical value. We also calculated the width of the domain wall and the magnetization energy in terms of the side length of the cube. Finally, we analytically solved for the critical transition side length and domain wall width using Kittel's equation for comparison with the numerical results.

2. Simulation method
Investigations of the domain structure of BaFe$_{12}$O$_{19}$ were performed in the OOMMF public-domain micromagnetic software [11] using the Landau–Lifshitz–Gilbert (LLG) [12] equation:

$$\frac{d\mathbf{m}}{dt} = \gamma \mathbf{m} \times \mathbf{H}_{\text{eff}} + \alpha \mathbf{m} \times \frac{d\mathbf{m}}{dt}$$
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Figure 1. Geometry and dimensions of BaFe$_{12}$O$_{19}$ cube-shaped model with random initial magnetization. The cube side was varied from 100 to 900 nm in this simulations.

Figure 2. BaFe$_{12}$O$_{19}$ cubes show (a) SD structure with sides of 500–nm and (b) MD structure with a Bloch wall between domains with sides larger than 510 nm. The colour in this plot represents magnetization in the $z$ direction.

where $\gamma$ is the gyromagnetic ratio 2.21 $\times$ 10$^{-5}$ m/A·s, $\alpha$ is the damping factor, $\vec{m}$ is the magnetization vector, and $\vec{H}_{\text{eff}}$ is the effective field vector. The sides of the model BaFe$_{12}$O$_{19}$ cubes were varied from 100 to 1 $\mu$m, and the simulation cell size was 10 $\times$ 10 $\times$ 10 nm. This cell volume was chosen because the exchange length of BaFe$_{12}$O$_{19}$ is 20.8 nm [13]; hence, the calculations will be adequate at this resolution. The following material parameters of BaFe$_{12}$O$_{19}$ were used: the magnetization saturation $M_s = 2.75 \times 10^5$ A/m, exchange constant $A = 2 \times 10^{-11}$ J/m, anisotropy constant $K = 96 \times 10^3$ J/m$^3$, and damping factor $\alpha = 0.01$ [14]. The simulation was performed in a zero magnetic field with the spin configuration initially random, as depicted in figure 1. The domain structure was observed once the magnetization system reached the equilibrium state after about 10 ns.

3. Results and discussion

After the system reached equilibrium, we observed SD structure in cubes with sides smaller than 510 nm, and MD structure in cubes with sides larger than 510 nm. A Bloch wall formed in cubes with sides larger than 510 nm. Figure 2 shows the domain structure in cubes with 500-nm and 510-nm sides, respectively. The transition from SD to MD structure indicates a critical size for this
Figure 3. The magnetization energies of BaFe$_{12}$O$_{19}$ cubes with side lengths (a) $L = 500$ nm and (b) $L = 510$ nm. The demagnetization energy is dominant over the exchange energy with SD structure, while the exchange energy shows increasing once MD structure appears.

Figure 4. (a) Determination of the width of Bloch wall in BaFe$_{12}$O$_{19}$ domain structure from the FWHM of the transverse magnetization ($M_y$) and (b) width BaFe$_{12}$O$_{19}$ Bloch wall related to the side length of a BaFe$_{12}$O$_{19}$ cube. The dashed line plots the domain wall width obtained by theoretical calculations.

ferromagnetic material. For comparison, we also calculated the critical size of cube-shaped BaFe$_{12}$O$_{19}$ structures using Kittel's formula $D_c = (2 \times 9\sigma_w) / \mu_0 M_s^2$ with the domain wall energy $\sigma_w = 2\sqrt{AK_1}$. The predicted critical size is around 525 nm with 3% error, as reported previously [15-17]. The difference between this prediction and our numerical results is caused by the discretization involved in the micromagnetic simulation calculations.

We also analyzed magnetization energies of demagnetization energy and exchange energy. For the SD case, the demagnetization energy was higher than the exchange energy at equilibrium. The exchange energy therefore approaches the demagnetization energy when multiple domains appear. On the other hand, the exchange energy tends to increase for cubes larger than the critical size. Magnetization energy profiles for the cubes with 500-nm and 510-nm sides are shown in figure 3.

In further calculations, we determined the width of the BaFe$_{12}$O. Bloch wall using the full width at half maximum (FWHM) of the transverse magnetization component ($M_y$). The FWHM was calculated using Gaussian fitting of the transverse magnetization, as shown in figure 4a. The width of the BaFe$_{12}$O. Bloch wall in cubes with size lengths 510 to 900 nm is presented in figure 4b. The width of the Bloch wall increased as the cube side length increased. To understand this relation, we calculated the width of the domain wall based on an approximation of Kittel's equation $W_{DW} = \pi \sqrt{A / K_1}$ and found
a value of 45.35 nm [17,18]. Comparing these values, the width of the BaFeO. Bloch wall obtained from the FWHM value is close to the theoretical prediction.

4. Conclusions
We have systematically investigated the domain structure of cubic BaFeO, using micromagnetic simulations with no external magnetic field. A Bloch wall structure appears in BaFeO, cubes with side lengths larger than 510 nm, and the cubes exhibit SD structure when the side length is less than 510 nm. The exchange energy tends to increase with side length when the micromagnetic structure has multiple domains. We have also calculated the width of the Bloch wall from the FWHM of the transverse magnetization component. The domain wall is wider in larger cubes of BaFeO. Theoretical calculations were also used to predict the transition regime and the domain wall width using Kittel’s equation. Interestingly, the micromagnetic simulation results are close to the theoretical predictions. The results of the above numerical simulations suggest that micromagnetic domain structures are influenced by energy contributions in a ferromagnetic system, which are determined in part by the scale of the material.

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