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Citation: Appl. Phys. Lett. **98**, 112505 (2011); doi: 10.1063/1.3567542

View online: http://dx.doi.org/10.1063/1.3567542

View Table of Contents: http://apl.aip.org/resource/1/APPLAB/v98/i11

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APPLIED PHYSICS LETTERS **98**, 112505 (2011)

Phase-field simulation of strain-induced domain switching in magnetic thin films

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(Received 19 December 2010; accepted 23 February 2011; published online 16 March 2011)

The strain-induced magnetic domain switching in epitaxial $CoFe_2O_4$ (CFO) thin films was studied using phase-field method. In particular, we investigated the domain switching from an initial in-plane direction to out-of-plane under the action of in-plane elastic strains. An abrupt switching feature is observed for a single-domain film while the switching of a multidomain CFO thin film is gradual. Typical magnetic domain structures as a result of the biaxial isotropic in-plane strains are presented. © *2011 American Institute of Physics*. [doi:10.1063/1.3567542]

Mechanical strain controlled magnetic domain or magnetization switching in thin films via magnetoelastic coupling is a critically important mechanism for realizing the applications of multiferroics and spintronics.[1] It will allow us to switch magnetization directly using electric voltages rather than usual current or magnetic field through a combination of magnetoelastic and electromechanical couplings in magnetic/ferroelectric (FE) artificial multiferroic heterostructures.[2] This indirect electric voltage-control of magnetization is also known as a converse magnetoelectric (ME) effect,[2,3] which can potentially be utilized to develop totally new spintronic or ME devices with much lower power consumption and higher speed. Examples include voltage-driven magnetic random access memories,[4,5] microwave devices,[6] and the logic circuits.[7] Such voltage-induced magnetization switching has been widely studied in various magnetic/FE composite structures,[8–13] and realized by direct experimental observation of magnetic domain switching based on, for example, the magnetic force microscopy[11,12] or the Lorentz microscopy.[13]

Theoretically, our previous thermodynamic calculations have shown that the magnetic easy axis (i.e., the spontaneous magnetization) of a magnetic thin film can be switched from an initial in-plane direction to out-of-plane under the action of a piezostrain.[3] However, a single-domain for the magnetic film was assumed for simplicity. To incorporate the possibility of multidomains and give a more intuitional demonstration on such strain-induced domain switching in magnetic thin films, in this letter, we employ the phase-field approach which has been used to predict the domain structure evolution in ferroelectric thin films,[14–16] bulk ferromagnets,[17] ferromagnetic shape memory alloys,[18,19] as well as the vertical ME composite heterostructures.[20] Cobalt ferrite ($CoFe_2O_4$, CFO) with strong magnetoelastic coupling and high Curie temperature[9] is chosen as the representative magnetic material. By taking into account the specific geometric size of a CFO film, the effect of a biaxial isotropic in-plane strain on the corresponding domain structure change is investigated.

In a phase-field model, the magnetic domain structure is described by the spatial distribution of a magnetization field $\mathbf{M}=M_s\mathbf{m}=M_s(m_1,m_2,m_3)$, where M_s and m_i represent the saturation magnetization and the direction cosine, respectively. The corresponding domain structures can thus be obtained from the temporal evolution of local magnetization configuration described by the well-known Landau-Lifshitz-Gilbert (LLG) equation, i.e.,

$$(1+\alpha^2)\frac{\partial \mathbf{M}}{\partial t} = -\gamma_0 \mathbf{M}\times\mathbf{H}_{\mathrm{eff}} - \frac{\gamma_0\alpha}{M_s}\mathbf{M}\times(\mathbf{M}\times\mathbf{H}_{\mathrm{eff}}), \quad (1)$$

where γ_0 and α are the gyromagnetic ratio and the damping constant, respectively. $\mathbf{H}_{\mathrm{eff}}$ is the effective magnetic field, given as $\mathbf{H}_{\mathrm{eff}}=-(\mu_0 M_s)(\partial F_{tot}/\partial \mathbf{m})$. Here μ_0 denotes the vacuum permeability, and F_{tot} is the total free energy of a multidomain magnetic film,

$$F_{tot} = F_{mc} + F_{ms} + F_{ex} + F_{elas}, \quad (2)$$

where F_{mc}, F_{ms}, F_{ex}, and F_{elas} are the magnetocrystalline anisotropy, magnetostatic, magnetic exchange, and elastic energy, respectively. F_{elas} is given by

$$F_{elas} = \frac{1}{2}\int c_{ijkl}e_{ij}e_{kl}dV = \frac{1}{2}\int c_{ijkl}(\varepsilon_{ij}-\varepsilon_{ij}^0)(\varepsilon_{kl}-\varepsilon_{kl}^0)dV, \quad (3)$$

where e_{ij} is elastic strain, ε_{ij} total strain, and c_{ijkl} the elastic stiffness tensor. ε_{ij}^0 is the stress-free strain describing the stress-free deformation of a cubic ferromagnet associated with the local magnetization change,

$$\varepsilon_{ij}^0 = \begin{cases} \frac{3}{2}\lambda_{100}\left(m_i m_j - \frac{1}{3}\right) & (i=j), \\ \frac{3}{2}\lambda_{111} m_i m_j & (i\neq j), \end{cases} \quad (4)$$

where λ_{100} and λ_{111} are the magnetostrictive constants. By considering a mixed boundary condition for the film-substrate system,[14] the calculation of elastic energy F_{elas} can be obtained through a combination of Khachaturyan's mesoscopic elastic theory[21] and the Stroh's formalism of anisotropic elasticity.[22]

The details for obtaining F_{mc}, F_{ms}, and F_{ex} are given in Refs. 3 and 17. To incorporate the effect of sample shape on

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0003-6951/2011/98(11)/112505/3/$30.00

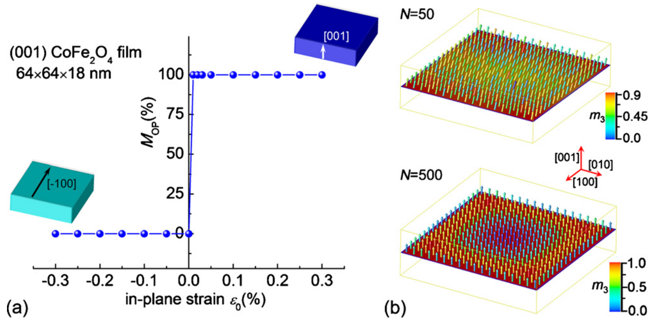

FIG. 1. (Color online) (a) Out-of-plane magnetization, i.e., M_{OP}, as a function of the biaxial in-plane strain ε_0 in a (001)-oriented CoFe$_2$O$_4$ film of $64\times64\times18$ nm. The insets illustrate the corresponding magnetic domain structures at $\varepsilon_0=\pm0.3\%$. (b) Temporal evolution of the local magnetization vectors at $\varepsilon_0=0.01\%$, $t=N\Delta\tau$.

domain structures, a finite-size boundary condition is used herein for F_{ms}, with the demagnetization factor N in the magnetostatic energy[17] obtained numerically.

The temporal evolution of the local magnetization and thus the domain structures are obtained by numerically solving the LLG equation using the semi-implicit Fourier spectral method.[23] The film-substrate system is discretized int o a three-dimensional array of cubic cells of $64\Delta x\times64\Delta x\times128\Delta z$ with finite-size boundary conditions along the three principle cubic axes as mentioned above. The thicknesses of the substrate and the film are set as $h_s=36\Delta z$ and $h_f=18\Delta z$, respectively. To investigate the effect of sample size on the domain structures, we consider two different sets of grid sizes in real space, i.e., $\Delta x=\Delta z=1$ nm and $\Delta x=3$ nm, $\Delta z=1$ nm, corresponding to the CFO films with a size of $64\times64\times18$ nm and $192\times192\times18$ nm, respectively. Note that different grid size along different directions in the later case would lead to anisotropic domain wall energies along the x and z directions, which should be considered in determining the exchange stiffness constant in reduced unit, i.e., $A^*=2A/\mu_0M_s^2l_d^2$ with A denoting the exchange constant and l_d the cell size along different crystal axes.[17] Each simulation starts with an initial random configuration with arbitrary magnetization orientations and proceeds for long enough time to ensure a stabilized magnetization distribution with a normalized time step $\Delta\tau=0.01$. The material parameters of CFO films are listed in Ref. 24.

Let us first consider the (001)-oriented CFO films with a geometric size of $64\times64\times18$ nm. Figure 1(a) shows the change in out-of-plane magnetizations, i.e., M_{OP}, under the action of a biaxial in-plane strain $\varepsilon_{11}=\varepsilon_{22}=\varepsilon_0$ which may arise from the lattice and/or thermal mismatch between the film and a substrate.[14] A single-domain appears due to the relatively small size of the film.[25] The magnetization of the film switches abruptly from its initial in-plane direction $[\bar{1}00]$ to a perpendicular direction [001], as the in-plane strain ε_0 exceeds a critical value of about 0.01% [Fig. 1(a)]. This abrupt feature qualitatively agrees with our previous analytical calculations with a single-domain assumption.[3] Switching to other energetically degenerate orientations, i.e., the [100], [010], and $[0\bar{1}0]$ in-plane directions and the $[00\bar{1}]$ out-of-plane directions is also possible, depending on the initial random magnetization distribution. The temporal evolution of the local magnetization vectors at the critical strain of 0.01% is shown in Fig. 1(b), illustrating a typical coherent magnetization rotation process in single-domain magnetic thin films.[26]

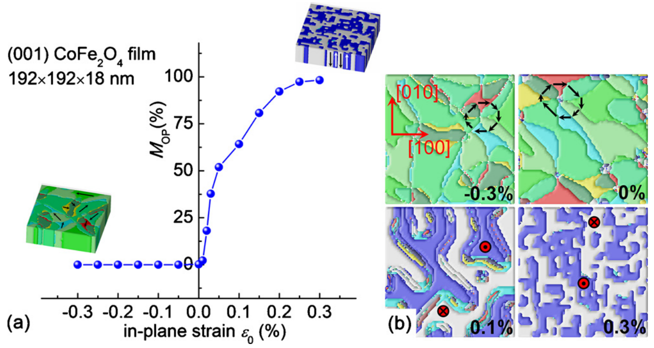

FIG. 2. (Color online) Out-of-plane magnetization, i.e., M_{OP}, as a function of the biaxial in-plane strain ε_0 in a (001)-oriented CoFe$_2$O$_4$ film of $192\times192\times18$ nm. The insets show the typical magnetic domain structures at their corresponding in-plane strains of $\varepsilon_0=\pm0.3\%$ with each color indicating a specific magnetization orientation (see the arrows). (b) Top view of the magnetic domain structures at $\varepsilon_0=-0.3\%$, 0%, 0.1%, and 0.3%, respectively. The arrows, as well as the symbols $\otimes$ and $\odot$, denote the directions of local magnetization vectors.

A somewhat different strain-induced domain switching feature is exhibited for the (001) CFO film with a relatively larger size of $192\times192\times18$ nm, which presents a mosaic-like multidomain structure [Fig. 2(a)]. In this case, the out-of-plane domains grow gradually as the positive (tensile) in-plane strain ε_0 increases. It becomes saturated (i.e., almost only out-of-plane domains being present) at a strain of about 0.3%. This magnetization switching process takes place through domain wall motion, common in a multidomain magnetic film, in contrast to the coherent rotation in a single-domain film [see Fig. 1(b)].[26] On the other hand, the magnetic directions for the domains under a negative (compressive) ε_0 are along the in-plane directions. Figure 2(b) shows the top view of the corresponding magnetic domain structures. As seen, the in-plane magnetic domains under zero or negative strains (−0.3%) form a magnetic flux closure structure (see the arrow circles) driven by the demagnetization field. A Néel-type 180° magnetic domain wall[27] is revealed using a vector plot of local magnetization vectors (not shown here).

Moreover, it can be seen from Fig. 2(b) that the domain wall thickness δ becomes thinner with increasing negative or positive strains with increasing number of domains and interfaces, resulting from the competition between the exchange anisotropy energy and elastic anisotropy.[28] Among them, the reduction in the domain wall thickness induced by negative strains can be estimated analytically as[5]

$$\delta = 2\sqrt{2}\sqrt{\frac{A}{K_A}}, \quad K_A = K_1 + \frac{1}{2}\mu_0 M_s^2 + \frac{3}{2}\lambda_{100}(c_{11}-c_{12})\left(1+\frac{2c_{12}}{c_{11}}\right)\varepsilon_0, \tag{5}$$

which agrees with the phase-field simulation results (see Fig. 3). However, the decrease in wall thickness upon positive strains cannot be understood directly using Eq. (5), mainly due to the presence of a relatively complex magnetic domain wall structure associated with out-of-plane domain switching. Corresponding magnetic vector plots indicate that the Néel-type 180° in-plane domain wall, the Bloch-type 90° and

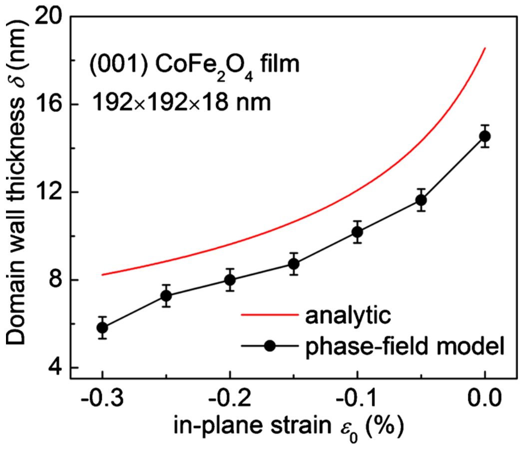

FIG. 3. (Color online) Variation trends of magnetic domain wall thickness δ with the negative in-plane strains, obtained from both the analytic calculation based on Eq. (5) and the phase-field simulations.

180° out-of-plane domain wall[27] coexist during the domain switching process, and eventually become 180° Bloch-type-like [e.g., the magnetic domain structure at $\varepsilon_0=0.3\%$ in Fig. 2(b)] through domain wall motion.

In conclusion, the effect of a biaxial in-plane strain on magnetization switching as well as the magnetic domain structures in epitaxial CFO films were studied using phase-field simulations. It is shown that the magnetic domains can be switched from an initial in-plane to an out-of-plane direction under isotropic in-plane elastic strains. By carefully considering the magnetostatic and magnetic exchange energy contribution, abrupt and gradual magnetization switching features are observed for a single-domain (corresponding to a relatively small geometric size) and multidomain (corresponding to a larger size) CFO films, respectively. Such strain-induced domain switching in magnetic thin films provides routes for an electric voltage-control of magnetization in artificial magnetic/ferroelectric multiferroic heterostructures through piezoelectrically controlled strains.

This work was supported by the NSF under Grant No. DMR-1006541. The computer simulations were carried out on the LION and Cyberstar clusters at the Pennsylvania State University supported in part by the NSF grants (Grant Nos. DMR-0820404, DMR-0908718, DMR-9983532, and DMR-0122638) and in part by the Materials Simulation Center and the Graduated Education and Research Services at the Pennsylvania State University. This work was also financially supported by the NSF of China (Grant Nos. 50832003 and 50921061), the National Basic Research Program of China (Grant No. 2009CB623303), and in part by the China Scholarship Council.

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[25] Here, in the film size ($64\times64\times18$ nm) is comparable to or even smaller than the typical domain wall length δ of CFO films, which can be roughly estimated to be about 24 nm from $\delta=2\sqrt{2A/K_1}$ (Ref. 5). A more practical estimation of the domain wall length can also be done numerically as discussed in the text.
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