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Electric-field Control of a Spin “bit” Configuration in MERAM Model: A Monte Carlo Study

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Abstract: Magnetoelectric (ME) effect can be realized in multiferroic composites composed of the alternative ferromagnetic (FM) and ferroelectric (FE) multilayer such as FM layer grown on top of FE layer (FM/FE). In this work, we have shown that the spin orientation in FM layer can be controlled by using the electrical field indirectly via the elastic mechanism between these layers. There is a critical electric field for each FM layer such as Fe, Fe_3O_4, which is the minimum electric field to switch the spin to the different directions in space. The Monte Carlo simulation has been applied for the anisotropy model taken into account the magnetocrystalline anisotropy and shape anisotropy as well as the effective anisotropy field. The particular spin switching, i.e. an angle of 90 degree switching, corresponding to bit “0” and “1” switching in magnetoelectric random access memory (MERAM) will be discussed.

Keywords: magnetoelectric effect, multiferroic composites, electric-field control of magnetism, anisotropy model, Monte Carlo simulation, MERAM

1. Introduction

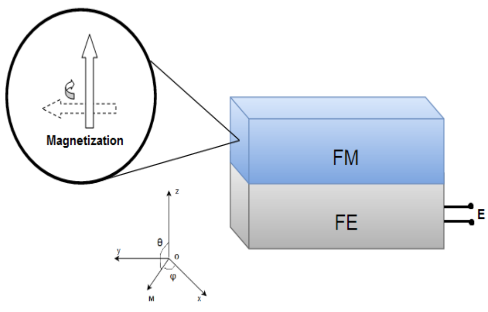

Figure 1. A model of FM/FE composite multiferroic heterostructure.

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Magnetoelectric (ME) effect [1, 2] has been a subject of interest for the physics community due to its variety of applications as well as the physics behind. One also observes a fascinating ME effect in multiferroic composites composed of the multilayer such as the alternative layers of the ferromagnetic (FM) and ferroelectric (FE) layers [3-5]. The ME effects in this composite multiferroic system is a result of the piezoelectric effect in FE layer due to the applied electric field which has been transferred to the FM layer via the magnetostrictive effect. The possibility of controlling magnetism in FM layer by using an applied external electric field has been recently proposed [6-9]. This topic has opened a active research area in the next generation, namely Magnetoelectric Random Access Memory (MERAM).

Table 1. Material parameters, i.e., Young Modulus Y (N/m^2), magnetocystalline coefficients K_1 (MJ/m^2), saturation magnetization M_s (kA/m), the Poisson's ratio v, in-plane effective magnetostriction coefficient λ (ppm) used for simulation

Materials	Fe_3O_4	Fe	CFO
Y	2.3	2.11	1.37
K_1	-0.01	0.048	0.1
M_s	410	1700	350
n	0.26	0.29	0.33
λ	-19	20	-350

For thin ferromagnetic films such as Fe, Fe_3O_4, Ni, Co deposited on ferroelectric substrates, i.e., $Pb[Zr_xTi_{1-x}]O_3$ (PZT), $(1-x)Pb(Zn_{1/3}Nb_{2/3})-xPbTiO_3$ (PZN-PT) [$(0 \le x \le 1)$], $BaTiO_3$, so on which form a class of composite multiferroic heterostructures. In this structure, it is possible to achieve reversible and irreversible spin reorientation transitions by an electric field via strain-driven magnetoelectric coupling. This mechanism has been recently observed experimentally [10, 11]. Similar to this mechanism, the magnetic tunability of ME composite nanostructures has been measured through electric field-induced changes using the ferromagnetic resonance (FMR) field technique [12]

From the theoretical perspective, the control of magnetism, i.e. spin orientation, in FM layer via an external electric field in a FM/FE layer heterostructures with various magnetic films grown on FE substrates has been investigated by several groups [3,4]. There is a little numerical calculation on these subject due to its expensive time computer consumption as well as the challenge in dynamic of spin reorientation performed by the numerical techniques.

In this manuscript, we present a detailed discussion on an electric-field control mechanism of magnetization switching in multiferroic heterostructures by using Monte Carlo (MC) simulation [13]. The FM layers have been chosen for the illustrations such as Fe, CFO and Fe_3O_4 films which can be experimentally deposited on top of the FE layer such as PZN-PT, $BaTiO_3$, PZN substrates. In the next section, we will introduce anisotropy model and the MC technique used for our study. The third section, the results would be presented for two cases: isotropic and non-isotropic biaxial stresses. The conclusion will be the last section.

2. An anisotropy model

Since we are only interested in the spin orientation occurred in FM layer. The anisotropy model is well-known as a simple and standard model to describe the spin in the FM/FE heterostructure [14-16]. The total anisotropy energy of FM film can be described as the sum of different anisotropy terms such as exchange energy, Zeeman energy, magnetocrystalline anisotropy, magnetostatic (shape) anisotropy and magnetoelastic energy.

For a simplicity, we just consider here the re-orientation of magnetization vectors which are strictly rotate from its initial in-plane direction $\overrightarrow{OM_0}$ to another direction $\overrightarrow{OM}$, so an exchange energy can be neglected.

Total free energy F_{tot} could be written as:

$$F_{tot} = F_{mc} + F_{shape} + F_{me} \tag{1}$$

For simplicity, we will ignore the exchange and Zeeman energy. In case of materials with a cubic symmetry, the magnetocrystalline anisotropy energy is expressed as:

$$F_{mc} = K_1\left(m_1^2m_2^2 + m_1^2m_3^2 + m_2^2m_3^2\right) + K_2\, m_1^2m_2^2m_3^2 \tag{2}$$

With K_1 and K_2 are anisotropy constants. Their values depend on the material characteristics and temperature. m_i (i=1,2,3) are the direction cosines of the magnetic easy axis with respect to the principal cubic axis.

If the second term can be neglected, the easy axes are the <100> axes (*i.e.*, the $\pm x$, $\pm y$, and $\pm z$, directions) for $K_1 > 0$. In other hand, the $< 111 >$ directions is favor for a case of $K_1 < 0$.

The shape anisotropy term reads:

$$F_{shape} = \frac{1}{2}\mu_o M_S^2 m_3^2 \tag{3}$$

Here the magnetization is assumed to be uniform with a magnitude characterized by the saturation magnetization M_s, and subtends an angle with the film normal vector. According to this expression, the contribution favors an in-plane preferential orientation for the magnetization.

Through ME coupling, a stress on the magnetic phase is generated by an electric field induced a strain on the piezoelectric phase. This electric field induces the biaxial stresses, consequently, producing the effective anisotropy field $\overrightarrow{H_{eff}}$ which is explained as a negative gradient of magnetoelastic energy on magnetization vector: $\overrightarrow{H_{eff}} = -\overrightarrow{\nabla}_M \cdot F_{me}$

The magnitude of F_{me} and H_{eff} along different direction could be written as:

$$F_{me} = -\overrightarrow{H_{eff}} \cdot \overrightarrow{M_s} \tag{4}$$

$$\begin{cases} H_{eff,x} = \dfrac{3\lambda Y}{M_s(1+v)}\left(|d_{31}-d_{32}|\right)E \\ H_{eff,y} = \dfrac{-3\lambda Y}{M_s(1+v)}\left(|d_{31}-d_{32}|\right)E \\ H_{eff,z} = \dfrac{3\lambda Y}{M_s(1+v)}\left(|d_{31}+d_{32}|\right)E \end{cases} \tag{5}$$

where Y is the Young's Modulus and v is the Poisson's ratio of FE layer, whereas λ is the in-plane effective magnetostriction coefficient, d_{31} and d_{32} are piezoelectric coefficients and E is the applied external electrical field.

In Monte Carlo simulation, the two angles (θ, φ) defining the direction of magnetization vector will be the variables through simulation process. A new orientation $\vec{v}_{att}$ of the magnetization is generated. The attempted direction is chosen in a spherical segment around the present orientation $\vec{v}$. Then the energy difference ΔE between the attempted and the present orientation is proposed. If $\Delta E<0$, the new spin configuration is accepted. If $\Delta E>0$, the magnetization is accepted with a probability which is proportional to exp $(-\Delta E/T)$. Otherwwise, a new orientation of $\vec{v}_{att}$ is rejected. We repeat this process untill reaching a stable configuration. In practice, this process relaxes to the stable configurations after 10000 to 15000 steps and the magnetization is then measured by averaging out the all stable configurations.

We are interested in two cases which correspond to the two type of stresses due to the elastic transferring from FE layer: the isotropic (e.g. $d_{31} = d_{32}$) and non-isotropic (e.g. $d_{31} \neq d_{32}$) biaxial stresses. The materials parameters of these FM films applied for the calculations are shown in Table 1.

3. Results and discussions

3.1. A case of an isotropic biaxial stress

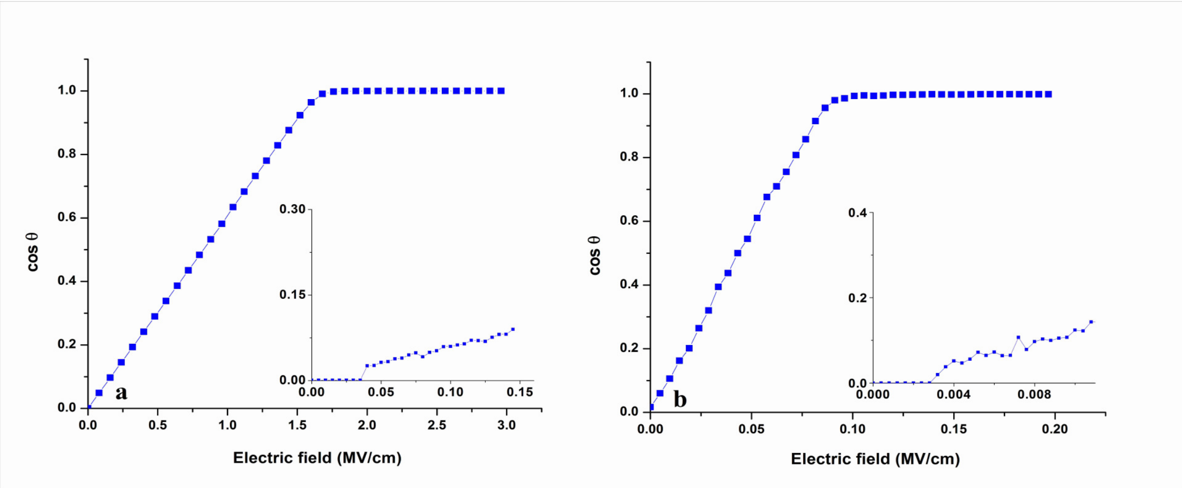

Figure 2. Spin reorientation in Fe/ PZN-PT layer (a) and Fe_3O_4/ PZN-PT(b) induced by an external electric field . In set: the magnification of the small value of the external filed regime.

In case of an insotropic biaxial stress, the boundary condition has been set to $d_{31} = d_{32}$. From Eqn (5), $H_{eff,x}$ and $H_{eff,y}$ can be neglected. The magnitude of magnetoelastic energy can be written as::

$$F_{me} = -\overrightarrow{H_{eff,z}} \cdot \overrightarrow{M_s} \tag{6}$$

The term (6) will be substituted into Eq.4 and included into MC code. In order to perform a magnetization control of an electrical field, we investigate a dependence of $\cos\theta$ on an external electric field for the Fe layer (Fig. 2a) and Fe_30_4 (Fig. 2b). These two materials are well-known as a standard and popular FM layer. The substrate PZN-PT has been selected to be the same for two cases. The different substrates such as $BaTiO_3$, PZT, so on will be investigated easily by changing the material parameters respectively. As shown in Fig. 2, the value of $\cos\theta$ changes smoothly from zero to one as an electric field increases. We should note that, there is another case in which the spin orientation has a step shape similar to the first order transition [4]. In other words, the spin configuration in FM layer are completely controlled by an external electric field. More interestingly, as $\cos\theta=0$ (or θ=π/2) corresponding to the spin vector in-plane film while $\cos\theta=1$(θ=0) the spin vector is perpendicular to the film plane. In principle, this mechanism is similar to the two states system in which we can represent as a spin "bit": a bit "0" corresponds to the spin state at θ=0 and a bit "1" in the other state. Strikingly, we have found that there is a critical electric field E_c which is a minimum value for an electric field to switch from bit "1" to bit "0". Although this critical electric field is small, i.e below 0.1 MV/cm, it is important for a practical application. Since it creates an energy barrier for a forward and backward switching, then prevents the flip and flop randomly between two states. Indeed, in the limit of a small external electric field, the shape anisotropy plays a critical role. If $\cos\theta=0$, shape anisotropy has been set to zero, thus magnetization prefer the in plane orientation. As we increase the external electric field, the contribution of the effective anisotropy field $H_{eff,z}$ is significant.

A general feature shown in Fig. 2 is that the relationship between $\cos\theta$ and an external electric field E is almost linear. There is another electric strength which is necessary to switch the spin completely from bit "1" to bit "0" namely the determined electrical field, E_d. We have found that E_d depends strongly on the materials. For example, Fe film and Fe_3O_4 film on PZN-PT, E_d are 1.68 MV/cm and 0.10 MV/cm respectively.

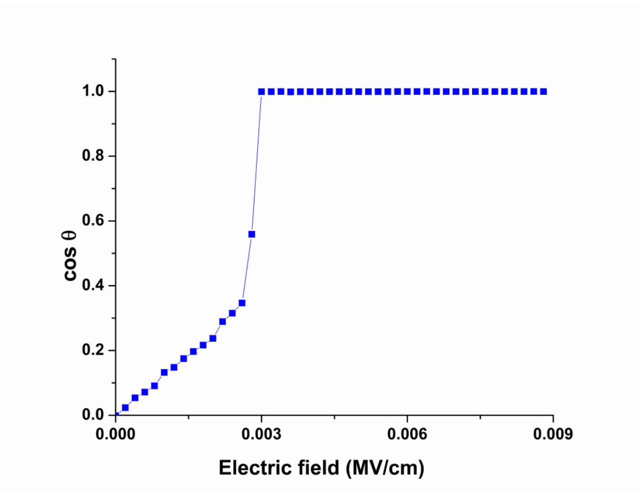

Figure 3. Spin reorientation in CFO/ PZN-PT induced by an external electric field (isotropic biaxial stress case).

Other than Fe and Fe_3O_4, CFO is very popular FM layer. We have done a similar calculation for CFO film. The dependence of the magnetization vector by the external electric field is also represented by a straight line at the start. As an external electric field reaches the value $E = 0.003$ MV/cm, the 90 degree rotation of magnetization suddenly happens (Fig. 3). This value is much smaller than the one found in Fe and Fe_3O_4 films. This is also consistent with the other findings using the analytical approaches [3, 4].

Table 2 summarizes the critical electric field for different FM layers: Fe, Fe_3O_4, CFO. Through the calculation, we realize that the properties of FE layer have great impact on the re-orientation of magnetization. Fig. 4 shows the dependence of the critical electric field E_d of Fe film on piezoelectric coefficient d_{31}. It is obvious that the critical electric field increases with the polarization of FE layer.

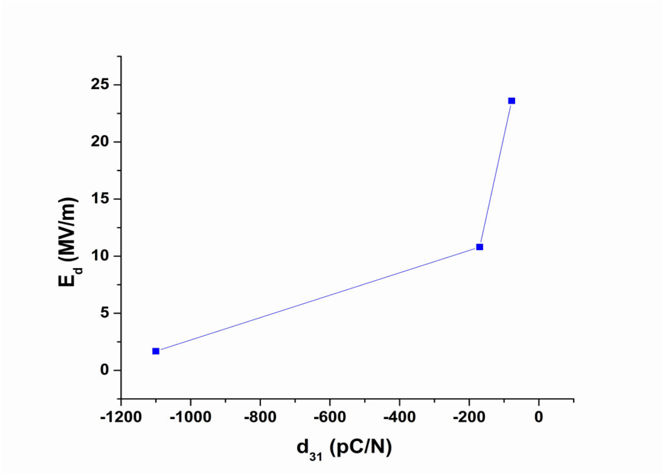

Figure 4. The dependence of determined electric fields E_d of Fe on piezoelectric coefficient d_{31}.

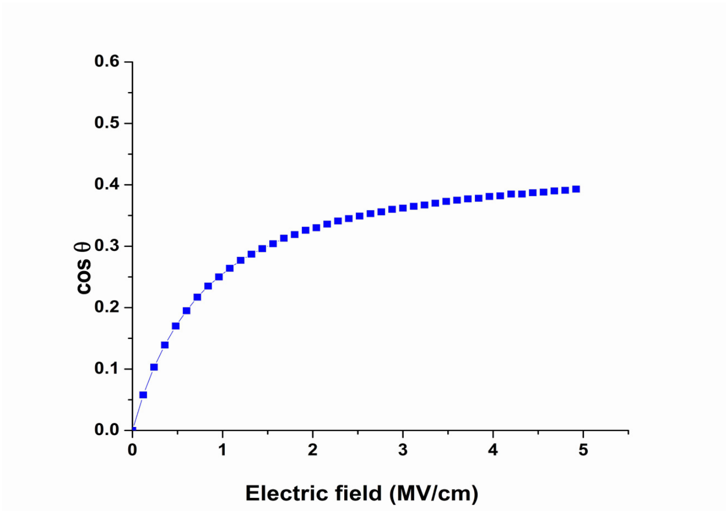

Figure 5. Spin reorientation induced by external electric field of Fe / PZN-PT in non-isotropic biaxial stressess case.

3.2. Non-isotropic biaxial stresses

In several cases, the coupling between FM/FE layers is non-isotropic induced strains. Hence, an electric field applied in the direction of the polarization vector will result in different strains on x and y directions. In other words, the boundary condition has been modified as $d_{31} \neq d_{32}$. As Eqn. 4, we have the contribution of effective magnetic field $\vec{H}_{\mathrm{eff},x}$ and $\vec{H}_{\mathrm{eff},y}$ along x and y direction to total energy:

$$F_{me} = -(\vec{H}_{\mathrm{eff},x} + \vec{H}_{\mathrm{eff},y} + \vec{H}_{\mathrm{eff},z}).\vec{M}_s \tag{7}$$

A single crystal PZN–PT displays large anisotropic in-plane piezoelectric coefficients of d_{31} (-3000 pC/N) and d_{32} (1000 pC/N) and the re-orientation of magnetization vector according to z axis is described in Fig. 5. Interestingly, the change in direction is non-linear and E_d is much larger than the one found in the isotropic cases. The anisotropy effect has a large impact on the switching process. In other words, it is more difficult to rotate spin or reorientate the spin configuration in the presence of the anisotropy couplings.

Table 2. The value of determined electric field E_d for 90 degrees rotation of spin in FM layers

	E_d(MV/cm)		
FM/FE	**PZN-PT**	**BTO**	**PZN**
Fe	1.68	23.6	10.8
Fe_3O_4	0.10	1.08	0.63
CFO	0.003	0.042	0.02

3. Conclusion

The switch of the magnetization vector driven by an electric field applied to the FE layer has been investigated systematically using Monte Carlo simulation. We have found that the applied electric field is able to control the spin configuration in FM layer in the composite multiferroics FM/FE layer. This can be implemented as the MERAM mechanism in some applications. We have studies two type of couplings between the FM/FE layer. In case of isotropic coupling, there is a small critical electric field E_c at which the spin starts to rotate and the determined electric field E_d at wthich the spin completely switch from in-plane direction to the perpendicular direction. We have applied our calculation for different FM layer: Fe, Fe_3O_4 and CFO grown on PZN-PT substrate. We show that E_d depends strongly on the piezoelectric coefficients. In case of anisotropic coupling, the much larger E_d is required to switch the spin completely to the perpendicular direction due to the anisotropy effects. Our study could be implemented in MERAM mechanism.

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