FAST TRACK COMMUNICATION

Polarization and magnetization dynamics of a field-driven multiferroic structure

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Abstract

We consider a multiferroic chain with a linear magnetoelectric coupling induced by electrostatic screening at the ferroelectric/ferromagnet interface. We study theoretically the dynamic ferroelectric and magnetic response to external magnetic and electric fields by utilizing an approach based on coupled Landau–Khalatnikov and finite-temperature Landau–Lifshitz–Gilbert equations. Additionally, we make comparisons with Monte Carlo calculations. It is demonstrated that for material parameters corresponding to BaTiO3/Fe the polarization and the magnetization are controllable by external magnetic and electric fields, respectively.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

Magnetic nanostructures have been intensively researched [1] due to their versatile use in technology. Multiferroics, i.e., systems that exhibit a coupled ferroelectric and ferromagnetic order, have received much attention recently [2–4]. A variety of potential applications of multiferroics rely on a possible control of magnetism (electric polarization) with electric (magnetic) fields due to the magnetoelectric coupling. Indeed, recent experiments have demonstrated the existence of both effects [5–7]. Furthermore, a number of interesting phenomena associated with the coupled polarization/magnetization dynamics at interfaces and in bulk have been reported, such as the electrically controlled exchange bias [8], the electrically controlled magnetocrystalline anisotropy [9] and the influence of electric field on the spin-dependent transport [10]. Theoretically, recent Monte Carlo calculations for a three-dimensional spinel lattice were performed to study the magnetic-field induced polarization rotation [11, 12].

In this work we investigate theoretically and numerically the field-driven dynamics of the electric polarization and the magnetization of a ferroelectric/ferromagnetic system that shows a magnetoelectric coupling at the interface. For this purpose we consider a two-phase multiferroic chain consisting of 50 polarization sites and 50 localized magnetic moments, as sketched in figure 1. The ferromagnetic (FM) part of the chain is a normal metal (e.g., Fe), whereas the ferroelectric (FE) part is BaTiO3 (figure 1). Recently this system has been shown to exhibit a magnetoelectric coupling [13, 14] and has been realized experimentally [15]. The multiferroic coupling arises as a result of an accumulation of spin-polarized electrons or holes at the FE-insulator/FM-metal interface when the FE is polarized [16]. At the metal/insulator interface, the screening of the polarization charge alters the FE-polarization orientation, resulting in a linear change of the surface magnetization. The resulting magnetization in the FM structure decays exponentially away from the interface. Taking the FM material as an ideal metal with a screening length of around [17] 1 Å, the exchange interaction between the additional surface magnetization and the FM part is thus limited to only the first site. Switching to dimensionless units, we introduce the reduced polarization \( p_j(t) = P_j(t)/P_S \) and magnetic moment \( S_i(t) = \mu_i(t)/\mu_S \) vectors, where \( P_S \) is the spontaneous polarization of (bulk) BaTiO3 and \( \mu_S \) is the magnetic moment at saturation of (bulk) Fe.

2. Theoretical formalism

The total energy of the FE/FM system in a very general one-dimensional case consists of three parts

\[
E_S = F_{FE} + F_{FM} + E_C.
\]
The coupling constant as $\lambda$ and the multiferroic interface. In what follows, we vary $\kappa$ and the FM parts due to imperfections and are expressed by the screening charge at the interface and the local magnetic fields.

Various pinning effects that may emerge in both the FE and FM parts due to imperfections and are expressed by $\kappa_{\text{FE}}$ and $J_i$, $D_i$, respectively, are not considered here, i.e., $\kappa_{\text{FE}} \equiv \kappa_{\text{FM}}, J_i \equiv J, D_i \equiv D$.

We consider that the linear FE/FM coupling appears as a result of the exchange interaction of the magnetization induced by the screening charge at the interface and the local magnetization in the ferromagnet (for details we refer to [18]) and can be written as

$$E_c = \lambda p_S \mu_S \mathbf{p}_0 \cdot \mathbf{S}_0.$$  (4)

The meaning of the quantities appearing in these equations is explained in table 1.

Based on the parameters obtained from ab initio calculations for the BaTiO$_3$/Fe-interface [13, 19], we estimate the coupling constant as $\lambda = J a_{\text{Fe}}\alpha_{\text{Fe}}/(\epsilon_{\text{Fe}}\delta_{\text{Fe}} a_{\text{Fe}}^2) \approx 2 \times 10^{-6}$ s F$^{-1}$, where the surface ME-coupling constant is $\alpha_S = 2 \times 10^{-10}$ G cm$^{-2}$. We find this value is too low to obtain a sizable ME-response for the one-dimensional multiferroic interface. In what follows, we vary $\lambda$ and explore the dependence of the multiferroic dynamics on it.

The polarization dynamics is governed by the Landau-Khalatnikov (LKh) equation [20, 21], i.e.,

$$\gamma_i p_S \frac{dp_i}{dt} = H_{\text{FE}}^{\text{ij}} = -\frac{1}{a^3 p_S} \frac{\delta F_{\text{FE}}}{\delta p_j},$$  (5)

where $\gamma_i$ is the viscosity constant (table 1) and $H_{\text{FE}}^{\text{ij}}$ stands for the total external and internal fields acting on the local polarization. The magnetization dynamics obeys the Landau-Lifshitz–Gilbert [22] (LLG) equation of motion

$$\frac{d\mathbf{S}}{dt} = \frac{\gamma}{1 + \alpha_{\text{FM}}^2} \left[ \mathbf{S} \times H_{\text{FM}}^{\text{ij}}(t) \right] - \frac{\gamma \alpha_{\text{FM}}^2}{1 + \alpha_{\text{FM}}^2} \left[ \mathbf{S} \times \mathbf{S} \times H_{\text{FM}}^{\text{ij}}(t) \right].$$  (6)

where $H_{\text{FM}}^{\text{ij}}$ is the Gilbert damping parameter. The total effective field acting on $\mathbf{S}$ is defined as the sum of deterministic and stochastic parts $H_{\text{FM}}^{\text{ij}}(t) = -\frac{\delta F_{\text{FM}}}{\delta \mathbf{S}_i} + \zeta_{\text{FM}}(t)$. The characteristics of the additive white noise associated with the thermal energy $k_B T$ are [23] $\langle \zeta_{\text{FM}}(t) \rangle = 0$ and $\langle \zeta_{\text{FM}}(t) \zeta_{\text{FM}}(t + \Delta t) \rangle = 2k_B T \gamma \alpha_{\text{FM}}^2 \delta_{ij} \delta(\Delta t)$. Here $i$ and $j$ index the corresponding sites in the FM material. $k$ and $l$ are the Cartesian components of $\zeta$ and $\Delta t$ is the time interval. The coupled equations of motion (5) and (6) are solved numerically in reduced units, re-normalizing the energy (1) over doubled anisotropy strength $D$. Thus, the dimensionless time in both equations is $t = \omega_D t = y B_A t = \gamma D t / \mu_S$ and the reduced effective fields are $H_{\text{FM}}^{\text{ij}}(t) / B_A$, $H_{\text{FE}}^{\text{ij}} = H_{\text{FE}}^{\text{ij}} / (\gamma \gamma_i p_S B_A)$.

To endorse our results we conducted kinetic Monte Carlo (MC) simulations for the description of the dynamics of an FE/FM chain subjected to external magnetic and electric fields. The electric dipoles and the magnetic moments are understood as three-dimensional classical unit vectors, which are randomly updated with the standard Metropolis algorithm [24]. The period of the external field is chosen to be 600 MC steps per site.

In the following, the system is described via the reduced total polarization $p_S(t)$

$$p_S(t) = \frac{1}{N_{\text{FE}}} \sum_{j=0}^{N_{\text{FE}}-1} p_j(t),$$  (7)

and the reduced net magnetization $S_S(t)$

$$S_S(t) = \frac{1}{N_{\text{FM}}} \sum_{i=0}^{N_{\text{FM}}-1} S_i(t).$$  (8)

3. Results of numerical simulations

To demonstrate the response of the FE/FM chain to external fields using the LKh and the LLG equations we used a damping parameter $\alpha_{\text{FM}} = 0.5$, which is significantly higher than the

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**Table 1. Parameters used in the numerical calculations.**

| FE material (BaTiO$_3$) |
|-------------------------|
| Number of sites $N_{\text{FE}}$ | 50 |
| Polarization [26] $p_S$ (C m$^{-2}$) | 0.265 |
| Initial state $p_j(t = 0)$ ($p_S$) | [0.0, 0.0, 1.0] |
| Constant [20] $\gamma$ (V m s$^{-1}$) | 2.5 $\times$ 10$^{-3}$ |
| Constant $\alpha_{\text{FE}}$ (V m C$^{-1}$) | $-2.77 \times 10^7$ |
| Constant $\alpha_{\text{FE}}$ (V m C$^{-1}$) | $1.70 \times 10^6$ |
| FE interaction $\kappa_{\text{FE}}$ (V m C$^{-1}$) | $1.0 \times 10^8$ |
| Lattice constant [27] $a$ (m) | 0.4 $\times$ 10$^{-9}$ |
| FE/FM coupling $\lambda$ (s F$^{-1}$) Parameter |

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**FM material (Fe)**

| Number of sites $N_{\text{FM}}$ | 50 |
| Gyromagnetic ratio $\gamma$ ((T s)$^{-1}$) | $1.76 \times 10^{11}$ |
| Moment per site [28] $\mu_S$ ($\mu_B$) | 2.2 |
| Initial state $S_i(t = 0)$ ($\mu_S$) | [0.14, 0.14, 0.98] |
| Anisotropy strength [29] $D$ (J) | $1.0 \times 10^{-22}$ |
| Exchange strength [29] $J$ (1) | $1.33 \times 10^{-21}$ |
| Damping $\alpha_{FM}$ Parameter |
The hysteresis loops for the external electric field of the form \( B_x(t) = B_{0c} \cos \omega t \). The loops (a) and (b) are obtained by using the LLG equations; (c) and (d) are calculated using the MC method. In both methods, parameters are chosen such that (b) are obtained by using the LKh and the LLG equations; (c) and (d) are calculated using the MC method. In both methods, parameters are omitted; the hysteresis curves are averaged over 100 ((a), (b)) and 200 ((c), (d)) subsequent periods.

Irrespective of the temperature and the calculational method, only several first spin sites follow the electric field due to the voltage produces an oscillating magnetic field. The situation generally, the depolarizing field may well be sizable and thus affects the dynamics [30–32]. Here we estimate the strength of \( \varepsilon_{DF} \) by introducing a one-dimensional SC at the interface \( Q_{SC} = P_{3a} \alpha^2 \) (table 1). As a result, the electric field induced by the SC is opposite to the local polarization (figure 1) and can be written as \( \varepsilon_{DF} = -Q_{SC}/(4\pi \varepsilon_0 \varepsilon_{FE} a^2 n_j^2) e \), where \( \varepsilon_0 = 8.85 \times 10^{-12} \text{ A s V}^{-1} \text{m}^{-1} \) is the permittivity of free space, \( \varepsilon_{FE} \approx 2000 \) is the dielectric constant in barium titanate and \( n_j \) is the index numbering the polarization sites starting from the interface, e.g. \( n_{j=0} = 1 \). Thus, the strength of the depolarizing field calculated for \( n_{j=0} = 1 \) and upon the other parameters is \( \varepsilon_{DF} \approx 2 \times 10^6 \text{ V m}^{-1} \), which is at least one order of magnitude smaller than the amplitudes of the applied electric field (≈4 \( \times 10^7 \text{ V m}^{-1} \)). Keeping in mind that \( \varepsilon_{DF} \) decays in the FE away from the interface we can neglect the depolarizing field.

4.2. Effect of induced electric and magnetic fields

According to Maxwell’s equations an oscillating magnetic field induces an oscillating electric field, and an alternating voltage produces an oscillating magnetic field. The situation...
Figure 3. Hysteresis loops of the total reduced polarization/magnetization as a function of external electric field of the form $E_z(t) = E_0 z \cos \omega t$. The curves (a) and (b) are obtained by using the LKh and the LLG equations; (c) and (d) are calculated using the MC method. Parameters are chosen such that $E_c \approx a^3 P_S E_z \approx J, i.e. \lambda = 240 \text{s F}^{-1}, B_0 z = 0 \text{T}, E_0 z = 4.07 \times 10^7 \text{V m}^{-1}, \omega = 3.61 \times 10^{11} \text{s}^{-1}, \alpha = 0.5$. 20 first periods (1/ω) are omitted; the hysteresis loops are averaged over 100 ((a), (b)) and 200 ((c), (d)) subsequent periods.

Figure 4. Response of the one-dimensional multiferroic structure to the time-dependent magnetic field $B_z(t) = B_0 z \cos \omega t$ plotted for various frequencies $\omega$. The field-free precessional time in the FM part is $T_{\text{pre}} = T_{\text{pre}} \approx 4 \text{ps}$. The curves (a) and (b) are obtained by using the LKh and the LLG equations; (c) and (d) are calculated using the MC method. Parameters are $T_0 = 0 \text{K}, \alpha = 0.5, B_0 = 6.65 B_A$ and $\lambda = 240 \text{s F}^{-1}$. Several first periods are omitted.

becomes especially important for the second case, since even small induced magnetic fields aligned perpendicularly to the inducing field, and hence to the initial state of the magnetization, can sufficiently assist the switching at appropriate frequencies [33, 34].

From Faraday’s law of Maxwell’s equations $\nabla \times E = \mu_S \mu_0 \partial H / \partial t$ and for the given applied magnetic field $B_z(t) = B_0 z \cos \omega t$, the induced electric field acting on the FE polarization is oriented perpendicularly to the inducing field ($XY$-plane, figure 1). Its amplitude for relative magnetic permittivity in BaTiO$_3$ [35] $\varepsilon_{\text{Fe}} \approx 1$ and $\varepsilon_{\text{FM}} \approx 5000$ scales as $E_0^{\text{ind}} = \alpha_{\text{Fe}} \mu_{\text{Fe}} / (\mu_{\text{FM}}) B_0 z \omega \approx 2 \text{V m}^{-1}$.

Likewise, when an external electric field $E_z(t) = E_0 z \cos \omega t$ is applied, according to Ampere’s law of Maxwell’s equations $\nabla \times B = \mu_S \mu_0 \varepsilon_{\text{Fe}} \partial E / \partial t$, the direction of the induced field is perpendicular to the inducing field. The amplitude of the induced magnetic field in iron for $a_{\text{FM}} = 0.28 \times 10^{-9} \text{m}$ and $\varepsilon_{\text{FM}} \approx 1$ (since iron is assumed to be an ideal metal) is $B_0^{\text{ind}} = a_{\text{FM}} \mu_{\text{FM}} \mu_0 \varepsilon_{\text{FM}} B_0 z \omega \approx 2 \times 10^{-3} \text{T}$.

Our calculations with the estimated (and even larger) amplitudes of the induced electric field show no influence on the $Z$-projection of the FE polarization. This is a consequence of the uncoupled nature for the projections of the FE polarization (cf equation (5)). Both numerical methods give
Figure 5. Response of the one-dimensional multiferroic structure to the time-dependent electric field $E_z(t) = E_0 \cos \omega t$ plotted for various frequencies $\omega$. The field-free precessional time in the FM part is $T_{FM}^{\text{prec}} \approx 4 \text{ ps}$. The curves (a) and (b) are obtained by using the LKh and the LLG equations; (c) and (d) are calculated using the MC method. Parameters are $T_0 = 0 \text{ K}$, $\alpha = 0.5$, $E_0 = 4.07 \times 10^7 \text{ V m}^{-1}$ and $\lambda = 240 \text{ s}^{-1}$. Several first periods are omitted.

a slightly enhanced (less than 1%) ME response in the presence of the induced magnetic field. Therefore, the effect of the induced electric and magnetic fields can be deemed irrelevant for the considered multiferroic chain and for the chosen range of frequencies.

4.3. Frequency dependence of the magnetoelectric response

A variation of the frequency $\omega$ of the external electric and magnetic fields can also affect the ME response of the multiferroic chain. Figure 4 demonstrates the response of the multiferroic interface to an external magnetic field. The periods of the external magnetic field should be compared with a characteristic field-free precessional time $T_{FM}^{\text{prec}} \approx 4 \text{ ps}$ which is valid for bulk iron. As one expects, magnetic fields with longer periods favor better saturation of the magnetization (figure 4(b)). The response of the total electric polarization to the external magnetic field becomes enhanced with increasing period of B-field. This is confirmed by both numerical methods (figures 4(a) and (c)).

The multiferroic response to an external electric field is shown in figure 5 for which the situation of very short electric fields (less than or around $T_{FM}^{\text{prec}}$) is addressed. The magnetization does not relax quickly enough, resulting in a hysteresis which is similar to the ferroelectric one. Additionally, we obtain an increase of the net magnetization response (figure 5(b)). This feature can also be observed using the MC method (figure 5(d)).

5. Summary

The main result obtained using two independent methods—the direct solution of the LKh and the LLG equations (5) and (6) and the kinetic MC method—is that, due to the coupling at the interface of FE/FM, the ferromagnetic subsystem responds to an external electric field and the ferroelectric subsystem responds to an external magnetic field. The use of both methods allowed a comparison of dynamical and statistical approaches for studying coupling phenomena at the FE/FM interface. Additionally, the LKh/LLG equations provide an insight into the real time temporal behavior, while the MC approach is very useful to inspect the temperature influence on both sides of the interface.

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