Modeling of electric field-induced magnetization switching in multiferroic heterostructures

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Multiferroic heterostructures consist of materials with either pronounced ferroelectric or ferromagnetic effect. The combination of both types of material, be it in layers, columns or inclusions, potentially yields a significant magneto-electric coupling effect even at room temperature. The magnetization in the ferromagnetic material can be controlled by the application of electric fields to the ferroelectric material. In this contribution a linear elastic continuum formulation is coupled with a phase field formulation for the polarization and magnetization in the ferroelectric and the ferromagnetic layer, respectively. The strain transfer at the interface of the layers yields a magneto-electric coupling effect within the heterostructures. The finite element method is used to discretize the arising differential equations. A numerical example provides a proof of concept for the simulation of the magneto-electric coupling effect in multiferroic heterostructures.

1 Introduction

The coupling between ferroelectric and ferromagnetic effects is very weak at room temperature in all known materials. Thus, tailored heterogeneous structures, which consist of at least two different types of materials, have become an important subject of research in the last years. By combining Wairauite, a material with pronounced ferromagnetic effect, with Barium Titanate, a material with pronounced ferroelectric effect, Franke et al. [1] could observe a significant magneto-electric coupling effect at room temperature. Thus, the control of the magnetization direction with electric voltage is possible, which is of high interest in nanoscale electronics. The simulation of such multiferroic heterostructures with the finite element method has been presented in [2]. Thereby, two layers are coupled by the strains along the interface, and the polarization and the magnetization in the layers are described by phase field models.

2 Phase field modeling

The mechanical behavior is governed by the equilibrium $\text{div } \sigma = 0$ and a linear kinematic relation $\epsilon = \frac{1}{2} (\nabla u + (\nabla u)^T)$. For the considered case of decoupled magnetic and electric effects, Maxwell’s equation yields $\text{div } D = 0$ and $\text{div } B = 0$ for the electric displacement $D$ and the magnetic induction $B$ in the ferroelectric and the ferromagnetic layer, respectively. The electric field $E$ and the magnetic field $H$ are computed by $E = -\nabla \varphi$ and $H = -\nabla \psi$ from the electric potential $\varphi$ and the magnetic potential $\psi$. The electric enthalpy is chosen as proposed in [3] and depends on the polarization direction $P$ of the ferroelectric layer. The magnetic enthalpy is chosen as proposed in [4], where the magnetization $M$ is expressed using polar coordinates $\theta$. However, a different finite element discretization scheme is applied for the polar angle $\theta_2$ in order to prevent unphysical interpolated values [5]. The constitutive equations are derived from the enthalpies. For more details, especially on the evolution equation and the finite element discretization, see [2–4].

3 Numerical example

The applicability of the proposed simulation framework is shown with the help of a simple bilayer example. A 3 nm thick ferroelectric BaTiO$_3$ layer is applied onto a 0.3 nm thick ferromagnetic FeGa layer. The length and width of the specimens are 60 nm x 30 nm. A sketch of this layout is given in Fig. 1. For material constants see [2]. Each layer is discretized by $20 \times 10 \times 1$ elements. The nodal deformations $u_{ij}$ are tied pairwise along the interface. Implicit time integration is used.

The boundary conditions are chosen as follows. Minimal Dirichlet boundary conditions are set for the mechanical deformations $u$ in order to prevent rigid body motions. No external mechanical loads are applied. A time-dependent electric potential $\varphi = \pm \varphi(t)$ as defined in Fig. 2 is applied at the front and the back of the ferroelectric layer. All other faces are free of electrical charges. No boundary conditions are set for the magnetic potential $\psi$. The polarization $P$ and the magnetization $\theta$ are initially aligned in $x$-direction with no further boundary conditions for $t > 0$. * Corresponding author: e-mail wolfgang.dornisch@b-tu.de, phone +49 355 69 2822, fax +49 355 69 2473 This is an open access article under the terms of the Creative Commons Attribution License 4.0, which permits use, distribution and reproduction in any medium, provided the original work is properly cited.
Fig. 1: Exemplary layout of the multiferroic heterostructure.

Fig. 2: Applied electric potential difference over the computed time interval of 60 ns.

Fig. 3: Magnetic flux in $y$-direction at the center of the ferromagnetic layer depending on the time step. Additionally, six plots with intermediate polarization and magnetization states are provided.

The results of the simulation are given in Fig. 3 by means of a plot of the $y$-component of the magnetic flux $B$ over the time steps. Furthermore, the initial, four intermediate and the final state of the polarization and the magnetization are given. In the initial state, $B_y = 0$Vs holds since the initial magnetization $M(\theta)$ points in $x$-direction. After application of the electric potential difference, the polarization and after some precessional oscillations also the magnetization changes to be aligned in $y$-direction. This yields a value $B_y = -1.8$Vs as final state. This example shows that the magnetization can be switched by electric voltage and thus magneto-electric coupling is obtained.

4 Conclusion

The provided numerical example shows the applicability of the proposed framework for the simulation of strain-coupled multiferroic heterostructures. More details on the involved methods can be found in [2]. Future work will focus on further possibilities for the fulfillment of the magnetization constraint, on optimization of the layer layout and on the application of mortar methods [6] for non-conforming meshing of the single layers.

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