

Modelling and simulation of multi-physics applications in case of sudden transformations of material properties

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Abstract. Within this paper, we present a practical approach to generate and simulate coupled models for switching domains in material sciences, for example in crystal structures of ferroelectric materials or magnetic shape memory alloys (MSMA). Instead of developing combined averaged FE-models, we propose an approach by augmenting existing mechanical and electromagnetic FE-code. The necessary domain variables and inequalities are described and the implementation in COMSOL Multiphysics by smoothing the discontinuities is shown for MSMA. The simulation results are compared with experimental data and remaining deviations are discussed. The individual strengths and weaknesses of our approach compared to averaged models result in different use cases.

Introduction

With growing computational power, micromechanical models gain increasing attention in material sciences. Particularly interesting problems are numerical models for switching domains, for example in crystal structures [1]. One typical application are ferroelectric materials, which include piezoelectric and electrostrictive effects. The latter are mainly caused by domain reorientation [2]. Another application of switching domain simulations are magnetic shape memory alloys (MSMA) [3].

Ferroelectric materials and MSMA are made both of a tetragonal crystal lattice (in the relevant low-temperature phase) that moves into specific orientations depending on the external load. Beside the reaction of both materials to mechanical stresses, ferroelectric materials are susceptible to electrical fields and MSMA to magnetic fields additionally [4]. The behaviour is mostly analogue and will be first described using MSMA as an example.

Magnetic shape memory alloys The lattice of MSMA's martensitic phase has a shorter c-axis having a higher magnetic permeability in that direction – the so-called easy axis, marked with an arrow in Fig. 1 – compared to the a- and b-axes – denoted as hard axes. It is advantageous from an energetic point to align the easy axis with an external magnetic field or compressive mechanical load. The energy difference creates a driving force towards a reorientation [5]. If the energy difference exceeds a certain threshold – the so-called twinning stress σ_{tw} – the concerning domain orientation switches along diagonal twin boundaries as shown in Fig. 1. Section 1.1 briefly describes a common mathematical model by Likhachev and Ullakko [6] with discrete domain variables denoting the lattice orientation and the governing switching conditions.

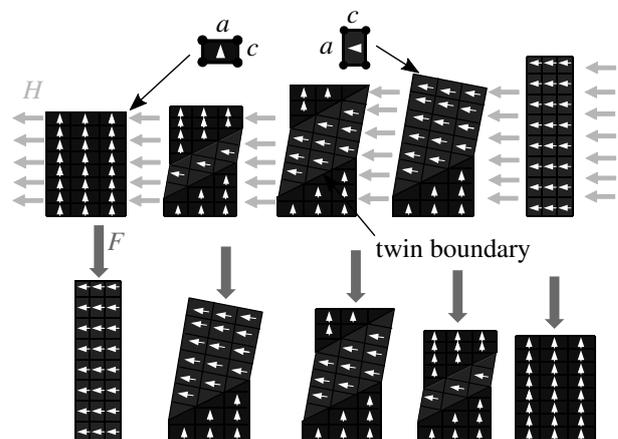


Figure 1: Domain wall movement of a MSM-element under magnetic influence and mechanical load.

Ferroelectric materials The lattice of ferroelectric materials has a longer c-axis with an ionic dipole

moment, which translates to a polarization on a continuum scale [7]. For MSMA, the direction of the c -axis is typically neglected, because the magnetic 180° -domain motion is almost unconstrained [8]. In contrast, for ferroelectric materials the polarization direction is important. It is advantageous from an energetic point to align the polarization with an external electric field and to move the c -axis out of a compressive mechanical load. An example of each case is shown in Fig. 2. Section 1.1 presents a corresponding mathematical model by Hwang and McMeeking [7] with discrete domain variables denoting the lattice orientation and the governing switching conditions.

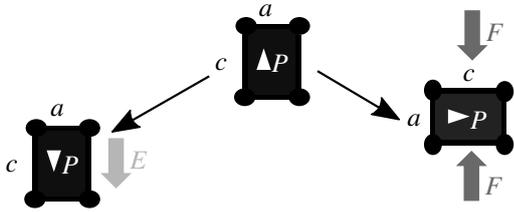


Figure 2: 180° -domain motion of ferroelectric material under electrical influence (left) and 90° -domain motion under compressive mechanical load (right).

Modelling An efficient way to model the macroscopic behaviour of switching domain materials are averaged energy-based models, using continuous phase variables denoting multiple lattice orientations coexistent in a continuum. Their simulation procedure is typically a magneto-static analysis with a special constitutive material model including the continuous phase variables.

For MSMA, one of the most popular models is given by Kiefer and Lagoudas [8]. It formulates the Gibbs free energy as the sum of the Gibbs energy of all possible martensitic variants weighted by their domain variables and a mixing term. The magnetic part contains the magnetic anisotropy energy for a crystal alignment different from the external field and the Zeeman energy for a magnetization direction outside the magnetic easy axis. The mixing term is approximated by analytical hardening functions. Section 1.2 presents some of the necessary equations.

A different modelling approach is presented in [9]. There, the mechanical energy is expressed as a piecewise quadratic function in terms of the strain instead of the stress. A Stoner-Wohlfarth hysteresis model covers

the magnetic anisotropy energy and the Zeeman energy. Additionally, all three possible crystal orientations are taken into account instead of the two-dimensional simplification. [10] gives a more comprehensive overview of the different models available.

In contrast to the averaged concepts, section 2 presents the proposed approach of using fundamental mechanical and electromagnetic models that are coupled with discrete phase variables and the inequalities from section 1.1. To improve convergence, adequate smoothing techniques are applied. In section 3, for validation our approach is compared with experimental data. Finally, the presented modelling techniques are categorised for different use cases in section 4.

1 Mathematical models

This section extends the literature work and presents the used mathematical description of MSMA and ferroelectric materials as well as different averaged models of MSMA.

1.1 Material behaviour

MSMA One way to model the magnetic (F_M) and mechanical (F_{mec}) driving forces for a typical configuration with a unidirectional magnetic field using the energy differences is given in [6] by

$$F_M(H) = G_h(H) - G_e(H) = - \int_0^H M_h(\tilde{H}) d\tilde{H} + \int_0^H M_e(\tilde{H}) d\tilde{H}, \quad (1)$$

$$F_{mec}(\boldsymbol{\sigma}) = \epsilon_0 (\sigma_{xx} - \sigma_{yy}), \quad (2)$$

with the free magnetization energy G , the magnetization curves $M(H)$ in the easy (e) and hard (h) direction, as well as the absolute value H of the magnetic field. The transformation strain $\epsilon_0 = 1 - \frac{c}{a}$ can be calculated from the lattice lengths, σ_{ij} are components of the stress tensor $\boldsymbol{\sigma}$.

The magnetic driving force can be generalized to a magnetic stress for different field directions H_i (again, only the absolute value is used) [3]:

$$\begin{aligned} \sigma_{M,i}(H_i) &= \frac{1}{\epsilon_0} (G_h(H_i) - G_e(H_i)) \\ &= \frac{1}{\epsilon_0} \left(- \int_0^{H_i} M_h(\tilde{H}) d\tilde{H} + \int_0^{H_i} M_e(\tilde{H}) d\tilde{H} \right). \end{aligned} \quad (3)$$

In typical applications, the loads act in one plane as shown in Fig. 3. Therefore, only two domain states are relevant, modelled with a variable $p \in \{0, 1\}$ with $p = 0$ for the easy axis in x -direction and $p = 1$ for y -direction. The switching conditions are then described by

$$\begin{aligned} \sigma_{M,x}(H_x) + \sigma_{xx} > \sigma_{tw} + \sigma_{yy} + \sigma_{M,y}(H_y) &\rightarrow p = 0, \\ \sigma_{M,y}(H_y) + \sigma_{yy} > \sigma_{tw} + \sigma_{xx} + \sigma_{M,x}(H_x) &\rightarrow p = 1. \end{aligned} \quad (4)$$

If none of these inequalities is true, the phase variable p remains constant.

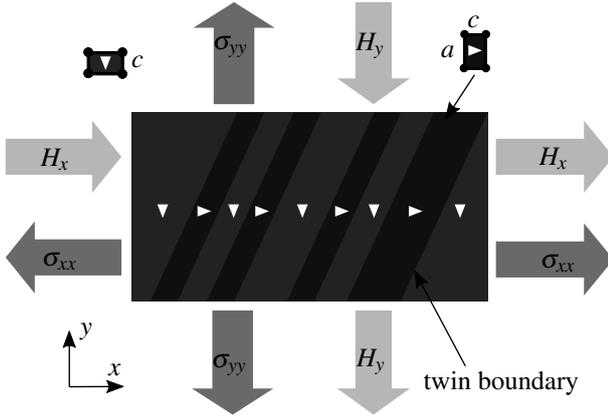


Figure 3: Directional magnetic and mechanical loads of an MSM-element.

Ferroelectric materials For ferroelectric materials, the electric field E and the polarization P have to be considered instead of magnetic field and magnetization. With three lattice axes and two polarization directions each, six states are possible in general. The critical field energy $W_E = 2P_0E_0$ for the switching can be calculated from the so-called spontaneous polarization P_0 and field E_0 , at which the polarization switches [7]. To switch to one of the six states, the electrical or mechanical work has to exceed the corresponding threshold

$$E_i \partial P_i + \sigma_{jk} \partial \epsilon_{jk} \geq 2P_0E_0. \quad (5)$$

If multiple switches are possible, the energetically most favourable is chosen.

1.2 Averaged energy-based models

As the full model of Kiefer and Lagoudas [8] is rather complex, we only show a simplified version not taking into account 180° -domain walls (which have already

been neglected in section 1.1). The Gibbs energy is in this case

$$\begin{aligned} G = & -\frac{1}{2\rho} \boldsymbol{\sigma} : \mathbf{S} \boldsymbol{\sigma} - \frac{\mu_0}{\rho} \underbrace{M_{\text{sat}} [(1-p)\mathbf{e}_x + p\mathbf{e}_y]}_{\mathbf{M}} \cdot \mathbf{H} \\ & + G_{\text{an}}(p, \boldsymbol{\theta}) + \frac{1}{\rho} f(p, \boldsymbol{\epsilon}_r) + G_0(T), \end{aligned} \quad (6)$$

with the mass density ρ , the stress $\boldsymbol{\sigma}$, the isotropic elastic compliance S , the vacuum permeability μ_0 , the magnetization \mathbf{M} the magnetic field \mathbf{H} , the saturation magnetization M_{sat} , the phase p , the magnetic anisotropy energy G_{an} dependent on the angle $\boldsymbol{\theta}$ between the magnetization and the easy axes of both phases, the hardening function f dependent on the phase p as well as the reorientation strain $\boldsymbol{\epsilon}_r$ and a reference state G_0 which is constant for isothermal problems. The term $\mathbf{M} \cdot \mathbf{H}$ describes the Zeeman energy.

From this energy, the driving force $\pi_p = -\rho \frac{\partial G}{\partial p}$ can be derived, which can be solved for the closed-form solution of the phase $p(\boldsymbol{\sigma}, \mathbf{H})$. The hardening function describes the hysteretic nature with two different analytical expressions dependent on the direction of the phase change $\left| \frac{\partial p}{\partial t} \right|$. The required fitting parameters can be obtained from a single constant-stress hysteresis loop.

2 Extended fundamental models

Different techniques to directly simulate the switching as described in section 1.1 are used. For ferroelectric materials, in [7] and [2] a basic linear piezoelectric model is applied and extended with specific code for the respective switching criterion. Only one domain can change per analysing step. The switched domains are used to update some of the effected parameters in the linear stiffness matrix, other changes are only updated every loading step to speed up the convergence. The highly nonlinear model demands that only a few domains – each represented by a single element – can be simulated effectively.

For MSMA, a finer mesh inside the diagonal domains (also called slices, shown in Fig. 3) is required to accurately capture the local flux inside. Our approach is based on the work of [3]. There, (4) is evaluated by averaging for each domain. While in [3] representative points in the middle of each slice are used, we average over all elements within the domain.

The BH-curves describing the magnetization behaviour for both axes are according to [11]. For an anisotropic implementation in COMSOL Multiphysics, those have to be transferred into $\mu_r(B)$ using

$$B = \mu_0 (H + M) = \mu_0 \mu_r H. \quad (7)$$

Input and output curves for both axes depicted in Fig. 4. The resulting magnetic stress according to (3) is shown in Fig. 5. The energy difference resulting in σ_M represents the area between the two blue curves in Fig. 4. Above $5 \cdot 10^5$ A/m, the curves are identical and therefore a saturation is reached.

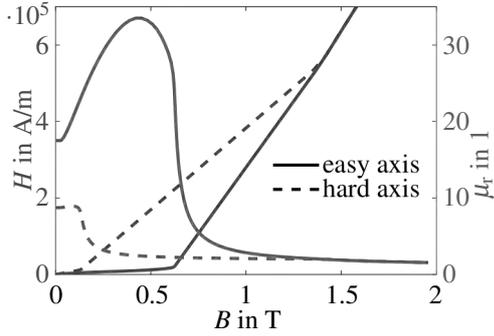


Figure 4: HB- and $\mu_r(B)$ -curves for easy and hard axis used in the simulation model.

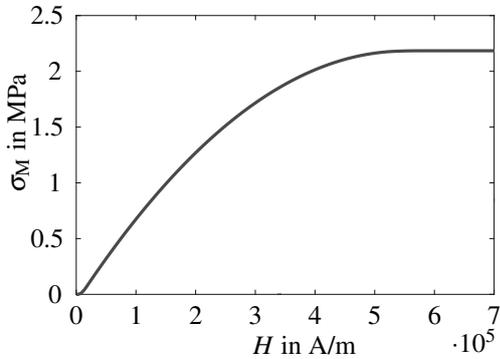


Figure 5: Magnetic stress curve $\sigma_M(H)$ used for simulation.

For each slice, the inequalities (4) to identify the phase p_i for the next iterative step based on the last p_{i-1} are implemented in the following smoothed way

$$p_i = s_1 (p_{i-1} + e_1 - e_2),$$

$$e_1 = s_2 (\sigma_{M,x}(H_x) + \sigma_{xx} - \sigma_{tw} - \sigma_{yy} - \sigma_{M,y}(H_y)), \quad (8)$$

$$e_2 = s_2 (\sigma_{M,y}(H_y) + \sigma_{yy} - \sigma_{tw} - \sigma_{xx} - \sigma_{M,x}(H_x)),$$

where the inequalities are replaced by differences e_1 and e_2 which are smoothed by s_2 . The output is limited to $[0, 1]$ by the saturation function s_1 . The functions s_1 and s_2 are shown in Fig. 6. As stresses are typically above 1 hPa, the phase usually switches directly between 0 and 1. A lower gradient in s_2 improves the convergence but generates more intermediate phases, not given in reality.

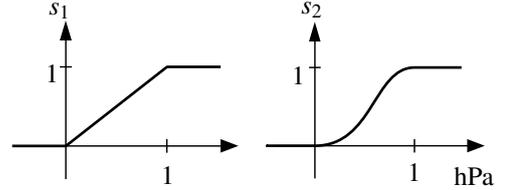


Figure 6: Smoothing functions used in (8).

Currently, it is not possible to measure the material parameters width and twinning stress for each slice individually. However, averaged measurements published in [12] allow to estimate typical distributions. While we keep the width constant at 0.1 mm to get a better mesh, the twinning stresses σ_{tw} of the slices are randomly distributed around 0.4 MPa as shown in Fig. 7.

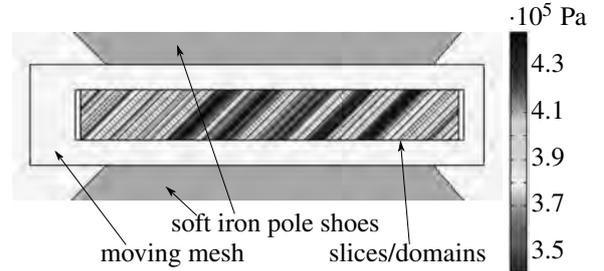


Figure 7: Random twinning stress distribution $\sigma_{tw}(x)$.

Based on a coupled magnetic and mechanical simulation, we are able to calculate the phase of each domain. The phase induces a strain in each slice of the mechanical model and determines the assignment of the corresponding magnetic permeability to the global coordinates.

As discontinuous jumps lead to severe convergence problems, we added smoothing to the load stepping by using a low-pass filter. This can be done in a time-dependent solver by introducing additional ODEs

$$-p_{s,i} + p_i - d_p \frac{\partial p_{s,i}}{\partial t} = 0, \quad (9)$$

with the index s indicating the smoothed variable and the damping d_p . The Index i cycles through all slices. The smoothing is not only beneficial from a numerical point of view but describes the behaviour also under real conditions, as the domain reorientation does not occur instantaneously in reality. It is even more efficient to use a static parametric solver and to replace the derivate with the difference quotient

$$-p_{s,i} + p_i - d_p \frac{p_{s,i} - p_{s,i-1}}{I_i - I_{i-1}} = 0, \quad (10)$$

where instead of the time t , the coil current I is used as a measure for the excitation. The proposed approach to add one variable per slice has little impact on the computational cost compared to the fine mesh needed for the magnetic simulation. An efficient way to implement the different variables and constants given in (8) for each slice is to use COMSOL's Java interface to loop over the domains.

The result of an intermediate load step can be seen in Fig. 8. Red domains have a vertical easy axis, blue domains indicate vertical hard axis. Thus, an external vertical flux is diagonally orientated in the blue domains and almost vertically in the red slices to minimize the magnetic resistance. The crooked outline of the MSM element is caused by the mechanical strain in the switched red regions, as the elongation also causes a transverse contraction. To include the geometric non-linearity in the magnetic simulation, a moving mesh domain has been set up on the surrounding air as shown in Fig. 7.

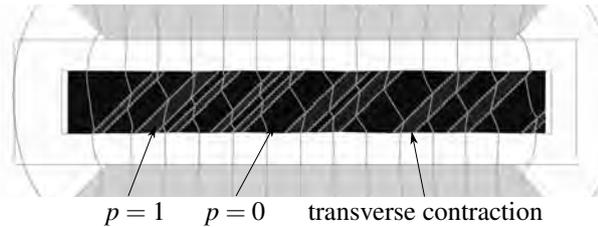


Figure 8: Distribution of the phase variable p (marked blue and red) for an intermediate magnetic field, magnetic flux lines in light grey.

3 Results

Simulated results in Fig. 9 show the expected hysteretic strain-excitation behaviour for an MSMA-element under axial compressive load. In accordance with (4),

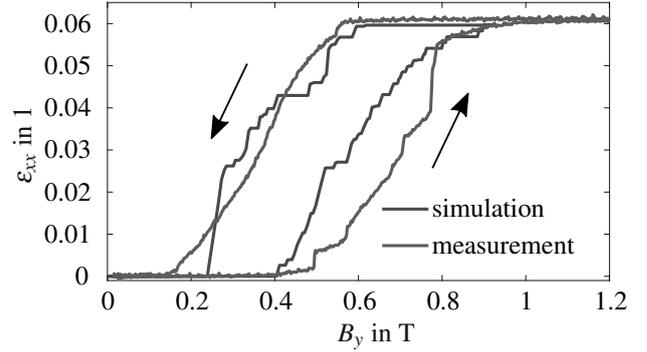


Figure 9: Simulated and measured strain of a loaded MSM-element over the driving flux density (averaged over the element).

the magnetic stress σ_M has first to overcome the compressive mechanical stress $\sigma_{xx} = -0.5$ MPa induced by the load and the twinning stress σ_{tw} until each segment switches. Because from this point a bigger part of the flux passes through that slice, the field in neighbouring domains decreases and the excitation has to be even bigger until the next segment switches. The hysteresis is mainly caused by the dissipative nature of σ_{tw} , which inhibits switching in both directions.

In non-switched domains (marked in blue), the flux is oriented diagonally almost perpendicular to the twin boundaries to minimize the magnetic reluctance. This local behaviour can only be replicated by modelling those slices instead of a continuum. For the same reason, our model offers better results than averaged models when simulating the inhomogeneous flux in the air next to the MSMA which helps to understand the spread of measurements of the magnetic flux at different positions on the MSMA surface. This becomes even more important for MSMA with a single highly mobile twin boundary instead of the discussed multiple fine twins. The local effects in this so-called Type II MSMA are discussed in [13].

For comparison, the curve of a measurement provided by ETO MAGNETIC for the equal load σ_{xx} is depicted in the same diagram. It can be seen, that the startpoints and endpoints of the elongation with increasing flux densities are quite similar. The shown measured result starts to move slower while other analysed samples have a more linear shape. The difference is mainly caused by the unique distribution of the twinning stresses σ_{tw} inside the slices and can indeed lead to different results. As the material parameters differ

between probes and can change over time, the efficient measurement of material parameters for a particular probe remains a complex challenge.

Comparing simulation and measurement, the starting point again fits quite well, but the final state is reached earlier in case of the simulation. This might be caused by the design of the pole shoes as shown in Fig. 7, which is chosen to begin the switching in the middle. In contrast, the experimental test setup has bigger pole shoes extending the outer sections.

4 Conclusion

Our proposed method directly uses the governing inequalities (4) which are comparably easy to understand. While we showed the implementation only for MSMA, the analogies with ferroelectric materials allow the application for this material class as well. More in general, our method could be applied for the implementation of new physical phenomena with switching domains – maybe even other discontinuous processes – without the need to derive a specific combined model. Due to the highly non-linear behaviour of inequalities, several smoothing techniques have to be applied. While they help to achieve convergence, the simulation is still rather inefficient, because the step size has to be lower at (smoothed) switches with high gradients in many variables. Hence, in many applications energy models with averaged phase variables are superior, once they have been developed. Other applications benefit from the proposed model accurately describing local effects, as averaged models cannot fully reflect inhomogeneous fields inside and around the sample.

Further investigations with varying mesh settings, damping and tolerances might lead to improved performance. The presented version is used for a quasi-static load case, transient analyses should be possible with the static parametric implementation of the damping as the phase is not directly dependent on the time.

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