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DISSIPATIVE RESPONSE IN FERROIC MATERIALS: CONTINUUM MODELING AND SIMULATION OF ELECTRO-MAGNETO-MECHANICAL COUPLING

ALEXANDER HUMER, ASTRID PECHSTEIN AND MICHAEL KROMMER

Institute of Technical Mechanics
Johannes Kepler University
Altenberger Str. 69, 4040 Linz, Austria
e-mail: alexander.humer@jku.at, web page: http://www.jku.at/tmech

Abstract. Ferroic materials are characterized by the presence of electric/magnetic dipoles that can be irreversibly re-oriented under sufficiently strong loading. Upon poling, an initially random distribution of dipoles on the microscopic domain scale results in a non-vanishing state of remanent polarization/magnetization on the macroscopic level. The remanent switching of dipoles constitutes the "smartness" in materials and their usage both as sensors and as actuators. Once being poled, material properties are typically assumed to be constant and uni-directional in engineering problems. To extend the operational range of ferroic transducers and open perspectives for novel applications, we seek for an accurate understanding of the evolution of the polarization/magnetization, which requires both physical and geometric non-linearities to be included in the modeling. To describe irreversible changes of the remanent state, we transfer phenomenological concepts and algorithms of associative elasto-plasticity to the field of electro-magneto-mechanics. To describe the dissipative response in a thermodynamically consistent manner, the principle of maximum dissipation is adopted. As in elasto-plasticity, constitutive equations for dissipative internal forces that drive the evolution of the remanent polarization/magnetization then follow as associated flow rules. To simplify the algorithmic treatment, we introduce the notion of dissipation functions, by which the constrained optimization problem is converted into an unconstrained problem, which can be efficiently solved by standard means. The vectors of remanent polarization/magnetization enter the model as additional internal variables. The constitutive response is governed by thermodynamic potentials, i.e., the free energy and dissipation functions. We derive a (mixed) variational formulation, identify appropriate function spaces for the dependent fields involved, and introduce a finite-element discretization. Representative numerical examples demonstrate the efficacy of the framework in electro-magneto-mechanically coupled problems.

Key words: Ferroic materials, Hysteretic response, Electro-magneto-mechanical coupling, Ferroelectric materials, Magnetostriction, Mixed finite elements

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1 ELECTRO-MAGNETO-MECHANICAL COUPLING IN FORROICS

A main aim of the present paper is to develop a phenomenological model that captures both the reversible and dissipative response of ferroic materials to electro-magneto-mechanical stimuli. In particular, we describe reversible *piezoelectric coupling* and the effects of *electrostriction and magnetostriction*. Beyond the reversible domain, the state of electric/magnetic domains, i.e., regions of polycrystals characterized by a uniform spontaneous polarization or magnetization, are no longer constant but evolve irreversibly under sufficiently strong electro-magnetic-mechanical loads, which is typically referred to as *domain-switching*.

Macroscopically, such irreversible response, which is the defining property of ferroic materials, is reflected in *hysteretic phenomena*. For the sake of brevity, we refer to the seminal book of Eringen and Maugin [1] for a description of diverse phenomena and their underlying (microscopic) processes. Modeling and simulation of electro-magneto-mechanical coupling is by no means a new topic. In the context of ferroelectric materials, we mention contributions by Kamlah [2], Landis [3], Klinkel [4] and Miehe et al. [5]. More recently, mixed-finite elements for ferroelectric continua have been presented in [6, 7, 8, 9]. A geometrically non-linear setting for ferroelectrics has been considered in [10, 11].

In what follows, we develop the constitutive relations of electro-magneto-mechanics within a unified thermodynamically consistent framework. A novel approach to describe ferroelastic switching is presented and we develop a mixed finite-element formulation.

Speaking of deformation, kinematics is the starting point of our reasoning. Let $\boldsymbol{u}$ denote the displacement field of material points that constitute material bodies, we introduce the symmetric part of the displacement gradient as (linearized) strain tensor $\boldsymbol{\varepsilon} = \left(\operatorname{grad} \boldsymbol{u} + (\operatorname{grad} \boldsymbol{u})^T\right)/2$. We split the strain tensor into a reversible mechanical (elastic) part $\boldsymbol{\varepsilon}_{me}$ and *eigenstrains* $\boldsymbol{\varepsilon}^*$:

$$\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}_{me} + \boldsymbol{\varepsilon}^*, \qquad \boldsymbol{\varepsilon}^* = \boldsymbol{\varepsilon}^*_{re} + \boldsymbol{\varepsilon}^*_{ir}. \tag{1}$$

The eigenstrain, in turn, is composed from reversible and irreversible (remanent) parts, i.e., $\boldsymbol{\varepsilon}^*_{re}$ and $\boldsymbol{\varepsilon}^*_{ir}$, respectively. The former accounts for reversible deformation induced by electro-magneto-mechanical coupling, whereas the latter is related to the domain state, i.e., the states of remanent polarization and magnetization, respectively.

In the present paper, we translate the notion of eigenstrains from mechanics to electromagnetic fields. Hence, we split the electric polarization vector $\boldsymbol{p}$ into a *dielectric part* $\boldsymbol{p}_d$, which accounts for the material's susceptibility to electric fields, and an *eigenpolarization* $\boldsymbol{p}^*$:

$$\boldsymbol{p} = \boldsymbol{p}_d + \boldsymbol{p}^*, \qquad \boldsymbol{p}^* = \boldsymbol{p}^*_{re} + \boldsymbol{p}^*_{ir}. \tag{2}$$

In analogy the kinematic quantitites, the (electric) eigenpolarization is composed from a reversible part $\boldsymbol{p}^*_{re}$, which is induced mechanically, and an irreversible part $\boldsymbol{p}^*_{ir}$, i.e., the macroscopic avarage of the spontaneous polarization of the domains a polycrystal is composed of. The magnetic analog to the (electric) polarization is the *magnetic polarization* vector $\boldsymbol{i}$, which is related to the common notion of *magnetization* through the vacuum permeability μ_0, i.e.,

$\boldsymbol{i} = \mu_0 \boldsymbol{m}$. Accordingly, we decompose $\boldsymbol{i}$ in analogy to (2) into

$$\boldsymbol{i} = \boldsymbol{i}_m + \boldsymbol{i}^*, \qquad \boldsymbol{i}^* = \boldsymbol{i}^*_{re} + \boldsymbol{i}^*_{ir}, \tag{3}$$

i.e., we introduce a magnetic part $\boldsymbol{i}_m$ and a magnetic eigenpolarization $\boldsymbol{i}^*$, which, in turn, is composed from a reversible contribution $\boldsymbol{i}^*_{re}$ and an irreversible part $\boldsymbol{i}^*_{ir}$.

To keep the presentation compact, we introduce a set of electro-magnetic polarization fields $\mathfrak{p}$, and a dual set $\mathfrak{q}$, which comprises the electric field and the magnetic field strength:

$$\mathfrak{p} = \{\boldsymbol{p}, \boldsymbol{i}\}\,, \qquad \mathfrak{d} = \{\boldsymbol{d}, \boldsymbol{b}\}\,, \qquad \mathfrak{q} = \{\boldsymbol{e}, \boldsymbol{h}\}\,. \tag{4}$$

For subsequent use, we have also combined electro-magnetic *flux-densities*, i.e., the dielectric displacement $\boldsymbol{d}$ and the magnetic flux density $\boldsymbol{b}$, which are defined by

$$\boldsymbol{d} = \varepsilon_0 \boldsymbol{e} + \boldsymbol{p}, \qquad \boldsymbol{b} = \mu_0 \boldsymbol{h} + \boldsymbol{i}, \tag{5}$$

in a set of vectors denoted by $\mathfrak{d} = \mathfrak{c}\mathfrak{q} + \mathfrak{p}$ with $\mathfrak{c} = \{\varepsilon_0, \mu_0\}$. Wherever $\mathfrak{d}$, $\mathfrak{p}$ and $\mathfrak{q}$ occur in what follows, we imply that both electric and magnetic fields are to be substituted if needed.

2 BALANCE LAWS OF ELECTRO-MAGNETO-STATICS

2.1 Quasi-static Maxwell's equations in matter

Using the above notation, we briefly recall the fundamental balance laws of electro-magneto-statics, i.e., we assume (quasi-)static conditions for all fields involved. We consider non-conducting continua, for which the volume density of free charges is zero ($q_e = 0$) and free surface currents vanish ($\boldsymbol{j}_f = \boldsymbol{0}$). Under these assumptions, the local forms of Gauss' laws of conservation of charge and magnetism, Faraday's law of induction and Ampère's law can be compactly formulated as:

$$\operatorname{div} \mathfrak{d} = 0, \qquad \operatorname{curl} \mathfrak{q} = \boldsymbol{0} \;\leftrightarrow\; \mathfrak{q} = -\operatorname{grad} \phi, \qquad \phi = \{\phi_e, \phi_m\}, \tag{6}$$

where the set ϕ comprises scalar-valued electric and magnetic potentials ϕ_e and ϕ_m, respectively. At a body's surfaces, the jump of the normal component of the dielectric displacement $\boldsymbol{d}$ equals the free surface charge density σ_f. As no magnetic charges are known to exist ($\sigma_m = 0$), we introduce the set σ within our notation to formulate the jump conditions as

$$\boldsymbol{n} \cdot [\![\mathfrak{d}]\!] = \sigma, \qquad \sigma = \{\sigma_f, 0\}\,, \qquad \boldsymbol{n} \times [\![\mathfrak{q}]\!] = \boldsymbol{0}, \tag{7}$$

i.e., the tangential component of electro-magnetic fields $\mathfrak{q}$ must vanish identitically.

2.2 Equilibrium relations

From a mechanics point of view, non-homogeneous electro-magnetic fields are reflected by sources in the balance equations of thermodynamics. In the (local) balance of linear momentum, couplings with electro-magnetic fields enter as a force density $\mathfrak{f}_{em}$, i.e.,

$$\operatorname{div} \boldsymbol{\sigma}_{me} + \boldsymbol{f} + \mathfrak{f}_{em} = \boldsymbol{0}, \qquad \mathfrak{f}_{em} = (\operatorname{grad} \mathfrak{q})^T \cdot \mathfrak{p}, \tag{8}$$

where $\boldsymbol{\sigma}_{me}$ denotes Cauchy's stress tensor and $\boldsymbol{f}$ is a volume density of mechanical forces. The electro-magnetic forces are (non-uniquely) represented as the divergence of *Maxwell stresses* $\mathfrak{s}$, which are defined by

$$\mathfrak{f}_{em} = \operatorname{div} \mathfrak{s}, \qquad \mathfrak{s} = \mathfrak{q}\mathfrak{d} - \frac{1}{2}\left(\mathfrak{c}_0 \mathfrak{q} \cdot \mathfrak{q}\right) \mathbf{I}. \tag{9}$$

Introducing the notion of *total* stresses $\boldsymbol{\sigma} = \boldsymbol{\sigma}_{me} + \mathfrak{s}$, the balance of linear momentum reduces to the classical form as in the uncoupled case,

$$\operatorname{div} \boldsymbol{\sigma} + \boldsymbol{f} = \mathbf{0}, \qquad \boldsymbol{\sigma} = (\boldsymbol{\sigma})^T, \tag{10}$$

where the symmetry of the total stresses is established by electro-magnetic couples which enter the balance of angular momentum. Again, we refer to Eringen and Maugin [1] for a detailed derivation and boundary conditions on the mechanical fields.

3 THERMODYNAMIC FRAMEWORK

Prior to specifying the nature of eigenstrains and eigenpolarization, we outline the thermodynamic foundation which the constitutive model—and subsequently also the numerical framework—is built upon. Still, we first need to decompose the remanent eigenstrains $\boldsymbol{\varepsilon}^*_{ir}$ into two parts to account for the phenomenon of *ferroelasticity*. Ferroelasticity describes the fact that ferroic domains re-orient under sufficiently strong mechanical loads. As opposed to domain switching under electro-magnetic loads, no macroscopic polarization can be induced by mechanical loads, see, e.g., [2]. Therefore, we split the remanent eigenstrains into a component $\boldsymbol{\varepsilon}^*_{ir,\mathfrak{p}}$ related to the state of polarization and a ferroelastic part $\boldsymbol{\varepsilon}^*_{ir,f}$:

$$\boldsymbol{\varepsilon}^*_{ir} = \boldsymbol{\varepsilon}^*_{ir,\mathfrak{p}} + \boldsymbol{\varepsilon}^*_{ir,f} \tag{11}$$

We introduce the *free energy*-type of thermodynamic potential ψ, which we postulate as a function of strains $\boldsymbol{\varepsilon}$, electro-magnetic fields $\mathfrak{q}$, (eigen-)polarization fields $\mathfrak{p}$, $\mathfrak{p}^*$ as well as remanent strains $\boldsymbol{\varepsilon}^*_{ir,f}$ and the remanent polarization $\mathfrak{p}^*_{ir}$, respectively:

$$\psi = \psi(\boldsymbol{\varepsilon}, \mathfrak{q}, \mathfrak{p}, \mathfrak{p}^*, \boldsymbol{\varepsilon}^*_{ir,f}, \mathfrak{p}^*_{ir}) \tag{12}$$

The second law of thermodynamics in the form of the *Clausius-Duhem inequality* demands the dissipation D, i.e., the rate of dissipated energy, to be equal or greater than zero:

$$D = P - \dot{\psi} \geq 0, \qquad P = \boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}} - \mathfrak{d} \cdot \dot{\mathfrak{q}}. \tag{13}$$

In the above relation, P denotes the power of stresses $\boldsymbol{\sigma}$ and flux densities $\mathfrak{d}$ and the rates of their dual variables, i.e., strains and electro-magnetic fields. Substituting the rate of ψ, i.e.,

$$\dot{\psi} = \frac{\partial \psi}{\partial \boldsymbol{\varepsilon}} : \dot{\boldsymbol{\varepsilon}} + \frac{\partial \psi}{\partial \mathfrak{q}} \cdot \dot{\mathfrak{q}} + \frac{\partial \psi}{\partial \mathfrak{p}} \cdot \dot{\mathfrak{p}} + \frac{\partial \psi}{\partial \mathfrak{p}^*} \cdot \dot{\mathfrak{p}}^* + \frac{\partial \psi}{\partial \boldsymbol{\varepsilon}^*_{ir,f}} : \dot{\boldsymbol{\varepsilon}}^*_{ir,f} + \frac{\partial \psi}{\partial \mathfrak{p}^*_{ir}} \cdot \dot{\mathfrak{p}}^*_{ir}, \tag{14}$$

we can identify the constitutive relations for the total stress tensor $\boldsymbol{\sigma}$ and flux densities $\mathfrak{d}$, along with the dissipative forces $\boldsymbol{\sigma}^*$ and $\mathfrak{q}^*$ that drive the evolution of the ferroelastic deformation $\boldsymbol{\varepsilon}^*_{ir,f}$ and the remanent polarization $\mathfrak{p}^*_{ir}$:

$$\boldsymbol{\sigma} = \frac{\partial \psi}{\partial \boldsymbol{\varepsilon}}, \qquad \mathfrak{d} = \frac{\partial \psi}{\partial \mathfrak{q}}, \qquad \boldsymbol{\sigma}^* = \frac{\partial \psi}{\partial \boldsymbol{\varepsilon}^*_{ir,f}}, \qquad \mathfrak{q}^* = \frac{\partial \psi}{\partial \mathfrak{p}^*_{ir}}. \tag{15}$$

Note that the polarization $\mathfrak{p}$ and the eigenpolarization $\mathfrak{p}^*$ are *internal* variables that we have included for modeling purposes. Their work-conjugates must vanish identically, i.e.,

$$\mathbf{0} = \frac{\partial \psi}{\partial \mathfrak{p}}, \qquad \mathbf{0} = \frac{\partial \psi}{\partial \mathfrak{p}^*}, \tag{16}$$

which allows us to reduce the Clausius-Duhem inequality to

$$D = \boldsymbol{\sigma}^* : \dot{\boldsymbol{\varepsilon}}^*_{ir,f} + \mathfrak{q}^* \cdot \dot{\mathfrak{p}}^*_{ir} \geq 0. \tag{17}$$

The dissipative driving forces $\boldsymbol{\sigma}^*$ and $\mathfrak{q}^*$ are bound by the *coercive stress* σ_y and the *coercive (electro-magnetic) field strength* $\mathfrak{q}_c = \{e_c, h_c\}$, i.e., they must remain within the respective admissible ranges, which are defined in terms of *switching functions* $f_{\boldsymbol{\sigma}^*}$ and $f_{\mathfrak{q}^*}$:

$$\mathbb{E}_{\boldsymbol{\sigma}^*} = \left\{ \boldsymbol{\sigma}^* \mid f_{\boldsymbol{\sigma}}(\boldsymbol{\sigma}^*) \leq 0 \right\}, \qquad f_{\boldsymbol{\sigma}^*}(\boldsymbol{\sigma}^*) = \|\operatorname{dev} \boldsymbol{\sigma}^*\| - \sqrt{\frac{2}{3}}\sigma_y, \tag{18}$$

$$\mathbb{E}_{\mathfrak{q}^*} = \left\{ \mathfrak{q}^* \mid f_{\mathfrak{q}}(\mathfrak{q}^*) \leq 0 \right\}, \qquad f_{\mathfrak{q}^*}(\mathfrak{q}^*) = \|\mathfrak{q}^*\| - \mathfrak{q}_c. \tag{19}$$

In the above relations, $\operatorname{dev} \boldsymbol{\sigma}^* = \boldsymbol{\sigma}^* - (\operatorname{tr} \boldsymbol{\sigma}^*/3)\mathbf{I}$ denotes the deviatoric part of the driving stresses, which accounts for the fact that domain switching is assumed as *volume-preserving*, i.e., $\operatorname{tr} \boldsymbol{\varepsilon}^*_{ir} = 0$ must hold, see, e.g., [2] for ferroelectric materials.

Although the microscopic mechanisms underlying domain switching and plasticity differ fundamentally, both phenomena share similarities from a macroscopic point view, even more so as ferroelastic switching, i.e., irreversible changes of the domain state under mechanical forces, is concerned. Not least for this reason, we postulate the *principle of maximum dissipation*, which constitutes the thermodynamic foundation of associative plasticity, see, e.g., Simo and Hughes [12], in the present context of ferroic materials. In other words, for given rates of ferroelastic eigenstrains $\dot{\boldsymbol{\varepsilon}}^*_{ir,f}$ and the irreversible eigenpolarization $\dot{\mathfrak{p}}^*_{ir}$, we assume the conjugate driving forces such that the dissipation is maximal:

$$D = \sup_{\boldsymbol{\sigma}^* \in \mathbb{E}_{\boldsymbol{\sigma}^*}} \boldsymbol{\sigma}^* : \dot{\boldsymbol{\varepsilon}}^*_{ir,f} + \sup_{\mathfrak{p}^* \in \mathbb{E}_{\mathfrak{q}^*}} \mathfrak{q}^* \cdot \dot{\mathfrak{p}}^*_{ir}. \tag{20}$$

Hence, the evolution of the eigenfields is governed by a *constrained optimization problem*, which can be solved by means of Lagrange multipliers, which are subject to the classical KKT-conditions for loading/unloading. Within the proposed framework, we adopt the concept of a *dissipation function*, which allows us to forgo much computational burden. The dissipation

function Φ is defined such that its derivatives with respect to rates of remanent fields give the respective driving forces. To model a rate-independent response, we choose the following positively homogeneous function of degree one,

$$\Phi = \sqrt{\frac{2}{3}}\sigma_y \|\dot{\boldsymbol{\varepsilon}}^*_{ir,f}\| + \mathfrak{q}_c \|\dot{\mathfrak{p}}^*_{ir}\|. \tag{21}$$

As the dissipation function Φ is not differentiable at zero, derivatives do not exist for vanishing rates $\|\dot{\boldsymbol{\varepsilon}}^*_{ir,f}\| = 0$ and $\|\dot{\mathfrak{p}}^*_{ir}\| = 0$. For convex functions, the notion of a *sub-differential*, see, e.g., [13], can be used instead, which gives the following relationships for the driving forces:

$$\boldsymbol{\sigma}^* \in \partial_{\dot{\boldsymbol{\varepsilon}}^*_{ir,f}} \Phi, \qquad \mathfrak{q}^* \in \partial_{\dot{\mathfrak{p}}^*_{ir}} \Phi. \tag{22}$$

By direct computation, we can convince ourselves that the principle of maximum dissipation is *a priori* satisfied by the above dissipation function, i.e., $D = \Phi$.

4 CONSTITUTIVE MODELS FOR THE COUPLED RESPONSE OF FERROICS

To further specify the constitutive model, we split the potential ψ into a reversible mechanical and electro-magnetic parts ψ_{me}, ψ_{em} and a component ψ^* related to the eigenpolarization:

$$\psi = \psi_{me} + \psi_{em} + \psi^* \tag{23}$$

The reversible mechanical (elastic) part is quadratic in the elastic strains, i.e.,

$$\psi_{me} = \frac{1}{2}\boldsymbol{\varepsilon}_{me} : \mathbb{c} : \boldsymbol{\varepsilon}_{me} = \frac{1}{2}\left(\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^*\right) : \mathbb{c} : \left(\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^*\right), \tag{24}$$

where $\mathbb{c}$ denotes the fourth-rank tensor of elastic moduli. For the electro-magnetic part, we first introduce the co-energy $\hat{\psi}_{em}$, which is meant to describe the linear response of ferroic materials to electro-magnetic fields. For this purpose, we take it as quadratic in $\mathfrak{p} - \mathfrak{p}^*$,

$$\hat{\psi}_{em} = \frac{1}{2}\left(\mathfrak{p} - \mathfrak{p}^*\right) \cdot \left(\mathfrak{c}_0 \boldsymbol{\chi}\right)^{-1} \cdot \left(\mathfrak{p} - \mathfrak{p}^*\right) + \frac{1}{2}\mathfrak{c}_0 \mathfrak{q} \cdot \mathfrak{q}, \tag{25}$$

where the last term accounts for the free-space contribution and $\boldsymbol{\chi}$ is a second-rank tensor of electric/magnetic susceptibility $\boldsymbol{\chi} = \{\boldsymbol{\chi}_e, \boldsymbol{\chi}_m\}$. Upon a (partial) Legendre transform, we obtain the corresponding free energy-type potential as

$$\psi_{em} = \hat{\psi}_{em} - \left(\mathfrak{p} - \mathfrak{p}^*\right) \cdot \mathfrak{q} - \mathfrak{c}_0 \mathfrak{q} \cdot \mathfrak{q} = \frac{1}{2}\left(\mathfrak{p} - \mathfrak{p}^*\right) \cdot \left(\mathfrak{c}_0 \boldsymbol{\chi}\right)^{-1} \cdot \left(\mathfrak{p} - \mathfrak{p}^*\right) - \left(\mathfrak{d} - \mathfrak{p}^*\right) \cdot \mathfrak{q}, \tag{26}$$

where the definition (5) of flux densities $\mathfrak{d}$ has been used. Since eigenstrains are of non-mechanical origin and the inelastic components of ψ are assumed to be independent of strains, we already find the constitutive equation for the stress tensor as

$$\boldsymbol{\sigma} = \frac{\partial \psi}{\partial \boldsymbol{\varepsilon}} = \frac{\partial \psi_{me}}{\partial \boldsymbol{\varepsilon}} = \mathbb{c} : \left(\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^*\right). \tag{27}$$

In what follows, we particularize the constitutive response for two types of coupled behavior, i.e., ferroelectric ceramics and magnetostrictive materials.

4.1 Dissipative response of ferroelectric materials

In poled ferroelectrics, electric fields induce a reversible eigenstrain due to the *converse piezoelectric effect*, i.e.,

$$\boldsymbol{\varepsilon}^*_{re} = \boldsymbol{e} \cdot \mathbb{d}(\boldsymbol{p}^*_{ir}), \tag{28}$$

where $\mathbb{d}$ denotes the third-rank tensor of piezoelectric constants. In the present context, we do not assume the domain state as constant. The piezoelectric effect is inherently linked to the domain state, which is reflected by the dependency of $\mathbb{d}$ on the remanent polarization $\boldsymbol{p}^*_{ir}$.

The remanent polarization is a measure for the orientation of ferroelectric domains in the material. Upon poling, an irreversible (isochoric) eigenstrain $\boldsymbol{\varepsilon}^*_{ir,p}$ is induced:

$$\boldsymbol{\varepsilon}^*_{ir,p} = \frac{3}{2}\frac{\varepsilon_{sat}\beta}{\|\boldsymbol{p}^*_{ir}\|^2}\left\{\boldsymbol{p}^*_{ir}\boldsymbol{p}^*_{ir} - \frac{1}{3}\left(\boldsymbol{p}^*_{ir}\cdot\boldsymbol{p}^*_{ir}\right)\mathbf{I}\right\}, \qquad \beta = \frac{\|\boldsymbol{p}^*_{ir}\|}{p_{sat}}, \tag{29}$$

where β denotes the ratio of the current remanent polarization to the saturation polarization p_{sat}; ε_{sat} is the corresponding maximum remanent eigenstrain. To model a linear reversible response of ferroelectrics, we set $\hat{\psi}^*_{re} = 0 \leftrightarrow \psi^*_{re} = -(\boldsymbol{p}^* - \boldsymbol{p}^*_{ir})\cdot\boldsymbol{e}$. The irreversible co-potential $\hat{\psi}^*_{ir}$ governing the rate-independent behavior during switching is chosen as

$$\begin{aligned}\hat{\psi}^*_{ir} = &-\frac{H^*\varepsilon^2_{sat}}{2}\sum_{k=1}^{3}\left\{\frac{1}{3}\log\left((1-\gamma)\varepsilon_{sat}+2\lambda_k\right)+\frac{2}{3}\log\left((1-\gamma)\varepsilon_{sat}-\lambda_k\right)+\gamma\right\}\\ &-\frac{p^2_{sat}}{\varepsilon_0\chi^*}\left\{\log(1-\beta)+\beta\right\}, \qquad \gamma = \sqrt{\frac{2}{3}}\frac{\|\boldsymbol{\varepsilon}^*_{ir,f}\|}{\varepsilon_{sat}}.\end{aligned} \tag{30}$$

where χ^* and H^* represent "hardening" parameters and λ_k, $k = 1, 2, 3$ are the principal values of the ferroelastic eigenstrains. The corresponding free energy then follows upon the Legendre transform

$$\psi^*_{ir} = \hat{\psi}^*_{ir} - \boldsymbol{p}^*_{ir}\cdot\boldsymbol{e}. \tag{31}$$

With ψ fully specified, the relations (16) for the internal variables both give

$$\mathbf{0} = \frac{\partial\psi}{\partial\boldsymbol{p}} = \frac{\partial\psi}{\partial\boldsymbol{p}^*} = (\varepsilon_0\boldsymbol{\chi})^{-1}\cdot(\boldsymbol{p}-\boldsymbol{p}^*) - \boldsymbol{e} \;\leftrightarrow\; \boldsymbol{p}-\boldsymbol{p}^* = (\varepsilon_0\boldsymbol{\chi})\cdot\boldsymbol{e}. \tag{32}$$

The constitutive relation (15) for the dielectric displacement allows us to identify $\boldsymbol{p}^*_{re}$ as

$$\boldsymbol{d} = \boldsymbol{\sigma} : \frac{\partial\boldsymbol{\varepsilon}^*}{\partial\boldsymbol{e}} + \varepsilon_0\left(\mathbf{I}+\boldsymbol{\chi}\right)\cdot\boldsymbol{e} + \boldsymbol{p}^*_{ir} \quad\rightarrow\quad \boldsymbol{p}^*_{re} = \boldsymbol{\sigma} : \frac{\partial\boldsymbol{\varepsilon}^*}{\partial\boldsymbol{e}} = \mathbb{d}^T : \boldsymbol{\sigma}. \tag{33}$$

4.2 Reversible response of magnetostrictive materials

As a second example, we consider the magneto-mechanical coupling in *magnetostrictive* materials. Here, we focus on the non-linear reversible response and assume remanent eigenstrains and the magnetization to vanish; so do the corresponding parts of the free energy:

$$\boldsymbol{\varepsilon}^*_{ir} = \mathbf{0}, \qquad \boldsymbol{i}^*_{ir} = \mathbf{0}, \qquad \psi^* = \psi^*_{re}, \qquad \psi^*_{ir} = 0. \tag{34}$$

We introduce reversible eigenstrains that have a quadratic dependency on the magnetization:

$$\boldsymbol{\varepsilon}^*_{re} = \boldsymbol{\varepsilon}^*_{re}(\boldsymbol{i}) = \frac{3}{2}\frac{Q_m}{\mu_0^2}\left(\boldsymbol{i}\boldsymbol{i} - \frac{1}{3}\left(\boldsymbol{i}\cdot\boldsymbol{i}\right)\mathbf{I}\right), \tag{35}$$

where Q_m is a material constant describing isochoric magnetostriction. The reversible part ψ^*_{re}, which is related to the corresponding co-energy by

$$\psi^*_{re} = \hat{\psi}^*_{re} - \boldsymbol{i}^*\cdot\boldsymbol{h}, \tag{36}$$

may be specified, e.g., in analogy to electrostrictive materials [14] such that its derivative given by

$$\frac{\partial\hat{\psi}^*_{re}}{\partial\boldsymbol{i}^*} = \frac{1}{\varepsilon_0\chi^*}\left(1-\beta^m\right)^{-1/m}\boldsymbol{i}^*, \qquad \beta = \frac{\boldsymbol{i}^*}{\|\boldsymbol{i}^*\|}, \tag{37}$$

where χ^* is a magnetic susceptibility and m a non-dimensional "shape" parameter. From this free energy, we recover the definition (5) of the magnetic flux density:

$$\boldsymbol{b} = -\frac{\partial\psi}{\partial\boldsymbol{h}} = \mu_0\boldsymbol{h} + \boldsymbol{i}. \tag{38}$$

The constitutive equations (16) for the internal variables, i.e., the polarization fields $\boldsymbol{i}$ and $\boldsymbol{i}^*$, respectively, give the relations

$$\mathbf{0} = -\boldsymbol{\sigma} : \frac{\partial\boldsymbol{\varepsilon}^*}{\partial\boldsymbol{i}} + \left(\mu_0\boldsymbol{\chi}\right)^{-1}\cdot\left(\boldsymbol{i}-\boldsymbol{i}^*\right) - \boldsymbol{h}, \qquad \mathbf{0} = -\left(\mu_0\boldsymbol{\chi}\right)^{-1}\cdot\left(\boldsymbol{i}-\boldsymbol{i}^*\right) + \frac{\partial\hat{\psi}^*_{re}}{\partial\boldsymbol{i}^*}, \tag{39}$$

from which we obtain the magnetic field intensity as

$$\boldsymbol{h} = -\boldsymbol{\sigma} : \frac{\partial\boldsymbol{\varepsilon}^*}{\partial\boldsymbol{i}} + \frac{\partial\hat{\psi}^*_{re}}{\partial\boldsymbol{i}^*}. \tag{40}$$

4.3 Stress-based formulation

The finite-element formulation presented below is established upon the *Hellinger-Reissner* mixed variational principle of continuum mechanics, in which stresses serve as independent variable alongside the displacement field. In the electro-magnetic domain, the flux densities $\mathfrak{d}$ are used as independent fields, i.e., we return to the co-energies introduced in previous sections. For this reason, we introduce the potential Ω by another (partial) Legendre transform of the free energy, i.e.,

$$\Omega = \psi - \boldsymbol{\sigma} : \boldsymbol{\varepsilon} + \mathfrak{d}\cdot\mathfrak{q} = \psi_{me} - \boldsymbol{\sigma} : \boldsymbol{\varepsilon} + \hat{\psi}_{em} + \hat{\psi}^*. \tag{41}$$

For the case of a linear elastic mechanical response, we can directly invert the constitutive relation (27) for the strains that become dependent variables in what follows:

$$\boldsymbol{\varepsilon} = \mathbb{c}^{-1} : \boldsymbol{\sigma} + \boldsymbol{\varepsilon}^*. \tag{42}$$

For the ferroelectric response, the electric field as dependent variable follows as

$$\boldsymbol{e} = \left(\mathbf{I}+\boldsymbol{\chi}\right)^{-1}\cdot\left(\boldsymbol{d} - \boldsymbol{p}^*_{ir} - \boldsymbol{\sigma} : \frac{\partial\boldsymbol{\varepsilon}^*}{\partial\boldsymbol{e}}\right); \tag{43}$$

the magnetic field of the magnetostrictive model has already been given in (40).

5 FINITE-ELEMENT FORMULATION

Let V denote the body of interest with boundary ∂V. In the quasi-static case, we use a (pseudo-)time t to define load histories. For a finite interval $[t, t+\Delta t]$, the respective increments $\Delta\boldsymbol{\sigma}$, $\Delta\boldsymbol{\varepsilon}^*_{ir,f}$, $\Delta\mathfrak{d}$, and $\Delta\mathfrak{p}^*_{ir}$ are found as critical point of the incremental algorithmic potential

$$\int_V \left(\Omega(t+\Delta t) - \Omega(t)\right) dv + \int_t^{t+\Delta t}\int_V \Phi dv dt - \Delta W_{ext} \to \max_{\Delta\boldsymbol{\sigma}} \min_{\Delta\boldsymbol{\varepsilon}^*_{ir,f}} \min_{\Delta\mathfrak{d}} \min_{\Delta\mathfrak{p}^*_{ir}}. \tag{44}$$

The stress tensor needs to be explicitely balanced with the external forces and the flux densities are required to satisfy Gauss' laws explicitly. Dividing the algorithmic potential by Δt and letting $\Delta t \to 0$, we obtain

$$\int_V \left(\dot\Omega + \partial_t\left\{(\mathfrak{f} - \operatorname{div}\boldsymbol{\sigma})\cdot\boldsymbol{u} - (\operatorname{div}\mathfrak{d})\,\phi + \Phi\right\}\right) dv - P_{ext} \to \max_{\dot{\boldsymbol{\sigma}}} \max_{\dot\phi} \min_{\dot{\boldsymbol{\varepsilon}}^*_{ir,f}} \min_{\dot{\mathfrak{d}}} \min_{\dot{\mathfrak{p}}^*_{ir}} \min_{\dot{\boldsymbol{u}}}, \tag{45}$$

where the local balance laws have been introduced by means of Lagrange multipliers, which turn out as the displacment field $\boldsymbol{u}$ and electro-magnetic potentials ϕ.

We use non-standard mixed finite elements to discretize the problem in space. Flux densities $\mathfrak{d}$ are discretized using divergence-conforming elements of Brezzi-Douglas-Marini (BDM) type [15]. To satify Gauss' laws in weak sense, a single Lagrange multiplier per element suffices. The remanent polarization is interpolated with discontinous polynomial functions. Displacements and stresses are discretized by elements of mixed continuity that were originally developed for thin elastic structures [16] and later extended to ferroelectric materials [7, 8] and elasto-plastic continua [17]. In particular, only the tangential component of displacements and the normal component of the stress vector (TDNNS) are continous accross element faces. The ferroelastic strains $\boldsymbol{\varepsilon}^*_{ir,f}$ are discretized by discontinuous polynomial functions.

6 NUMERICAL EXAMPLES

6.1 Ferroelectric and ferroelastic response

As first example, we consider a homogeneous ferroelectric specimen under uni-axial electro-mechanical loads (in $\boldsymbol{e}_3$-direction), for which the material parameters are listed in Tab. (1). Figure 1 shows the polarization hysteresis (left) and the butterfly hysteresis of the strain (right) when applying an electric field up to $\pm 2e_c$. The proposed model can capture the typical

Table 1: Material parameters of soft PZT similar to [2].

Young's modulus E	$80\,\mathrm{GPa}$	Poisson ratio ν	0.3
linear susceptibility χ_e	1355.32	coercive field e_c	$1\,\mathrm{kV\,mm^{-1}}$
susceptibility at switching χ^*	338829.91	saturation polarization p_{sat}	$0.3\,\mathrm{C\,m^{-2}}$
piezo coefficient d_{31}	$-2.1\times10^{-10}\,\mathrm{m\,V^{-1}}$	yield stress σ_y	$50\,\mathrm{MPa}$
piezo coefficient d_{33}	$4.2\times10^{-10}\,\mathrm{m\,V^{-1}}$	saturation strain ε_{sat}	0.002
piezo coefficient d_{15}	$5.2\times10^{-10}\,\mathrm{m\,V^{-1}}$	hardening stiffness H^*	$5\,\mathrm{GPa}$

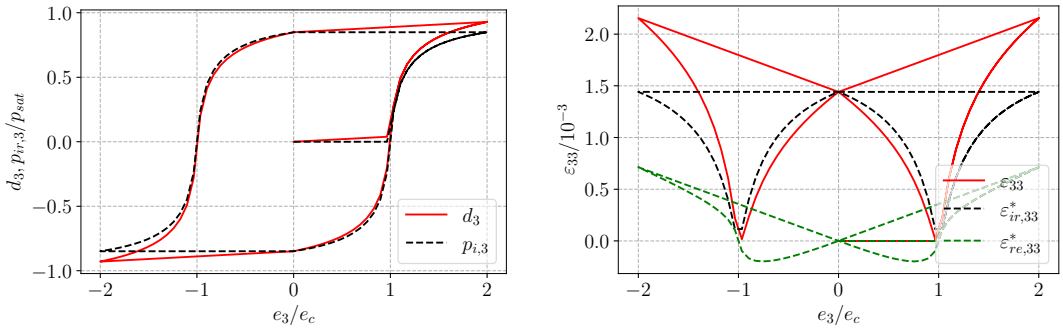

Figure 1: Electric (left) and butterfly (right) hysteresis under uni-axial electric loading.

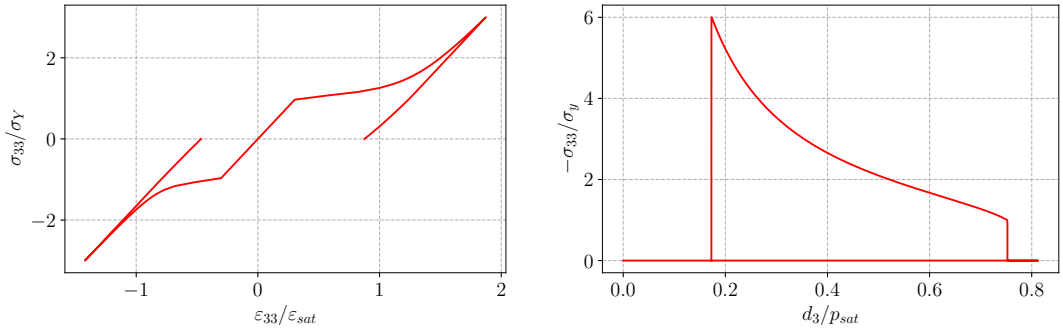

Figure 2: Ferroelastic hysteresis of an unpolarized specimen (left) and depoling under compressive stresses (right).

ferroelectric hysteresis under varying electric fields. Subjecting an unpoled specimen to tensile/compressive mechanical loads $\boldsymbol{\sigma} = \sigma_{33}\boldsymbol{e}_3\boldsymbol{e}_3$ results in the (idealized) non-symmetric ferroelastic lock-up behavior, see Figure 2 (left). For this purpose, twice the coercive stress is applied as tensile and compressive load, respectively. Figure 2 (right) illustrates the mechanical depoling of poled ferroelectrics. Subsequent to poling by means of electric field of $e_3 = 3e_c/2$, a compressive load of $\sigma_{33} = -6\sigma_y$ is applied, by which the specimen is depoled.

6.2 Magnetostrictive response

The reversible response of a magnetostrictive composite made from Terfenol-D is studied as a second example. To (qualitatively) replicate the measurements of isotropic specimen under a compressive load of $16.3\,\mathrm{MPa}$ reported in [18], the parameters listed in Tab. 2 have been used. We impose a magnetic field strength up to $h_0 = \pm 150\,\mathrm{kA\,m^{-1}}$ to the pre-stressed specimen.

Table 2: Material parameters of a Terfenol-D composite.

Young's modulus E	$22.4\,\mathrm{GPa}$	Poisson ratio ν	0.4
linear susceptibility χ_m	0	shape parameter m	2
susceptibility χ^*	9	magnetostriction Q_m	$1.78 \times 10^{-3}\,\mathrm{mm^2\,kA^{-2}}$
saturation polarization i_{sat}	$0.5\,\mathrm{T}$		

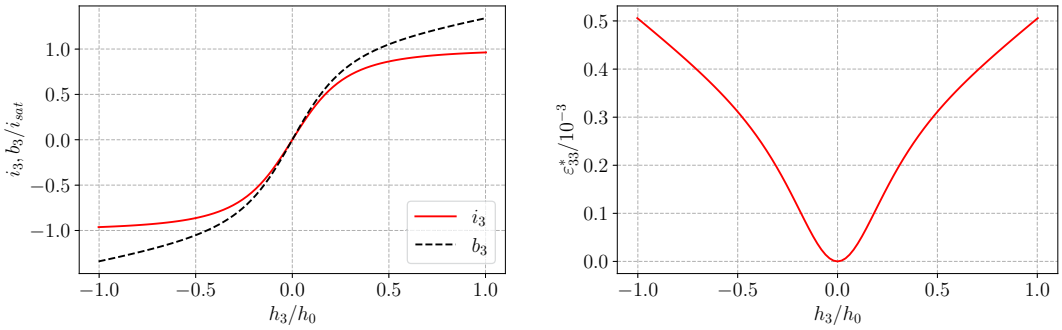

Figure 3: Magnetostrictive response of a Terfenol-D composite: magnetic fields (left) and eigenstrain (right).

Figure 3 illustrates the non-linear response of the material to the applied field: The (normalized) magnetic polarization $\boldsymbol{i}$, which equals the eigenpolarization $\boldsymbol{i}^*$, initially shows a linear response, but quickly saturates as the magnetic field strength increases (left). Figure 3 (right) shows the magnetically induced eigenstrain (in load direction). Initially quadratic, the non-linearity of the magnetic polarization reduces the sensitivity of strains as the magnetization saturates for higher field strength.

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