Weierstraß–Institut für Angewandte Analysis und Stochastik

im Forschungsverbund Berlin e.V.

Preprint ISSN 0946 – 8633

An energetic material model for time-dependent ferroelectric behavior: Existence and uniqueness

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submitted: 7th March 2005

Research supported by the European Union via HPRN-CT-2002-00284 "Smart Systems: New Materials, Adaptive Systems and their Nonlinearities. Modelling, Control and Numerical Simulation."

Preprint No. 1014

Berlin 2005

2000 Mathematics Subject Classification. 82D45, 74G25, 74C05.

Key words and phrases. Ferroelectric material model, existence of solutions, energetic formulation.

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Abstract

We discuss rate-independent engineering models for multi-dimensional behavior of ferroelectric materials. These models capture the non-linear and hysteretic behavior of such materials. We show that these models can be formulated in an energetic framework which is based on the elastic and the electric displacements as reversible variables and interior, irreversible variables like the remanent polarization. We provide quite general conditions on the constitutive laws which guarantee the existence of a solution. Under more restrictive assumptions we are also able to establish uniqueness results.

1 Introduction

Ceramic materials and single crystals showing ferroelectric behavior are being used in many applications in electronics and optics. A crystal is ferroelectric if it has a spontaneous polarization which can be reversed in sense or reoriented by the application of an electric field, larger than the coercive field. Reversal is also known as switching. A large number of applications of ferroelectric ceramics also exploit properties that are an indirect consequence of ferroelectricity, such as dielectric, piezoelectric, pyroelectric, and electro-optic properties. Piezoelectricity is the ability of certain crystalline materials to develop an electrical charge proportional to a mechanical stress. It was discovered by the Curie brothers in 1880. Piezoelectric materials also show a converse effect, where a geometric strain (deformation) is produced on the application of a voltage. The permanent electric dipole moment possessed by all pyroelectric (polar) materials may, in certain cases, be reoriented by the application of an electric field. The above comments are meant to point out that ferroelectric crystals are necessarily both pyroelectric and piezoelectric.

Ferroelectricity is a phenomenon which was discovered in 1921. The name refers to certain magnetic analogies, though it is somewhat misleading, as it has no connection with iron (ferrum) at all. Ferroelectricity has also been called Seignette electricity, as Seignette or Rochelle Salt (RS) was the first material found to show ferroelectric properties, such as a spontaneous polarization on cooling below the Curie point, ferroelectric domains, and a ferroelectric hysteresis loop. A huge leap in the research on ferroelectric materials came in the 1950's, leading to the widespread use of barium titanate ($BaTiO_3$) based ceramics in capacitor applications and piezoelectric transducer devices. Since then, many other ferroelectric ceramics including lead titanate ($PbTiO_3$), lead zirconate titanate (PZT), lead lanthanum zirconate titanate (PLZT), and relaxor ferroelectrics like lead magnesium niobate (PMN), have been developed and utilized for a variety of applications. With the development of ceramic processing and thin film technology, many new applications have emerged. The biggest uses of ferroelectric ceramics have been in areas such as dielectric ceramics for capacitor applications, ferroelectric thin films for non volatile memories, piezoelectric materials for medical ultrasound imaging and actuators, and electro-optic materials for data storage and displays.

The model proposed in Section 2 captures these specific features of the non-linear behavior of ferroelectrics, by keeping in the mean time the general perspective for treating multi-axial behavior and complex geometries. It is based on the rate-independent, three-dimensional models used in the engineering literature, see [MB89, KJ98, HFLM99, Kam01, HF01, SB01, ML02, KW03, RS04]. These models work in the framework of small deformations and the quasistatic approximation for the elastic and electrostatic equilibria.

However, certain internal variables Q, like the remanent polarization, are history dependent by an activation threshold and thus, lead to a rate-independent evolution process.

We show that, using as primary reversible variables the elastic displacement $u : \Omega \to \mathbb{R}^d$ and the electric displacement $D : \mathbb{R}^d \to \mathbb{R}^d$, the process can be written in an energetic formulation which is based on the stored-energy functional

$$\mathcal{E}(t, u, D, Q) = \int_\Omega W(x, \varepsilon(u), D, Q) + \alpha(x, \nabla Q)\,\mathrm{d}x + \int_{\mathbb{R}^d\setminus\Omega} \frac{1}{2\epsilon_0}|D|^2\,\mathrm{d}x - \langle \ell(t), (u, D)\rangle$$

and an dissipation potential of the form

$$\mathcal{R}(\dot{Q}(t)) = \int_\Omega R(x, \dot{Q}(t, x))\,\mathrm{d}x.$$

This energetic formulation was originally developed for shape-memory alloys in [MT99, MTL02], but is now shown to apply for many different rate-independent material models such as finite-strain elastoplasticity, damage, brittle fracture, delamination and vortex pinning in superconductors, see [Mie04b] for a survey.

The theory is based on a purely static stability condition (S) and the energy balance (E) which have to hold for all $t \in [0, T]$:

$$\begin{aligned}
&\text{(S)}\quad \mathcal{E}(t, u(t), D(t), Q(t)) \le \mathcal{E}(t, \widehat{u}, \widehat{D}, \widehat{Q}) + \mathcal{R}(\widehat{Q}-Q(t)) \text{ for all } \widehat{u}, \widehat{D}, \widehat{Q};\\
&\text{(E)}\quad \mathcal{E}(t, u(t), D(t), Q(t)) + \textstyle\int_0^t \mathcal{R}(\dot{Q}(s)))\,\mathrm{d}s\\
&\qquad\qquad = \mathcal{E}(0, u(0), D(0), Q(0)) - \textstyle\int_0^t \langle \dot{\ell}(s), (u(s), D(s))\rangle\,\mathrm{d}s.
\end{aligned}$$

The major advantage of the formulation is that it does involve neither derivatives of the constitutive functions W, α and R nor derivatives of the solution (u, D, Q), since the dissipation integral $\int_0^t \mathcal{R}(\dot{Q}(s)))\,\mathrm{d}s$ can be reformulated as a total variation.

We employ the abstract existence result for (S) & (E) from [MM05, FM04, Mie04b], which is reported in in Section 3, and apply it to our ferroelectric model at hand in Section 4. We provide conditions on the constitutive functions W, α and R which allow us to prove existence of solutions for (S) & (E) in suitable function spaces. In the last Section 5 we discuss the question of uniqueness, which leads to severe restrictions on the constitutive functions W and α.

2 Modeling for ferroelectric materials

Here we give a general description of a class of time-dependent models for ferroelectric materials. These models are rate-independent and thus do not display any time relaxation effects, however they are able to capture history dependence or hysteresis via internal variables which need a nonzero activation energy to invoke changes. The models are in fact a subclass of the theory of standard generalized materials like plasticity, and what is called a yields function there is called the switching function here.

Our class of models is stimulated by the engineering models from [KJ98, Kam01, ML02, KW03, RS04]. However, we will rephrase the theory there in a such a way that it can be formulated in terms of two energetic functionals, namely the stored energy $\mathcal{E}$ and the pseudo-potential $\mathcal{R}$ for the dissipation. Thus, we will be able to take advantage of the recently developed energetic approach to rate-independent models, see [MT04, MM05, FM04] and the survey [Mie04b].

The basic quantities in the theory are the elastic displacement field $u : \Omega \to \mathbb{R}^d$ and the electric displacement field $D : \mathbb{R}^d \to \mathbb{R}^d$. Here the electric displacement is also defined outside the body, as interior polarization of a ferroelectric material generates an electric field E and displacement D in all of $\mathbb{R}^d$ via the static Maxwell equation in $\mathbb{R}^d$. Commonly, the polarization P is used for modeling, it is defined via

$$D = \epsilon_0 E + P,$$

where ϵ_0 the dielectric constant (or permetivity) in the medium surrounding the body Ω. In contrast to D and E, the polarization P is defined only inside the body Ω and set equal to 0 outside. Our formulation stays with D, since it leads to a simple and consistent thermomechanical model.

In addition we use internal variables $Q : \Omega \to \mathbb{R}^{d_Q}$ which, for instance, may be taken as a remanent strain $\varepsilon_{\mathrm{rem}}$ or a remanent polarization P_{rem}.

The stored-energy functional has the following form:

$$\mathcal{E}(t,u,D,Q) = \int_\Omega \Big(W(x,\varepsilon(u),D,Q) + \alpha(x,\nabla Q) \Big)\,\mathrm{d}x + \int_{\mathbb{R}^d\setminus\Omega} \frac{1}{2\epsilon_0}|D|^2\,\mathrm{d}x - \langle \ell(t),(u,D)\rangle, \tag{2.1}$$

where W is the Helmholtz free energy and $\varepsilon(u)$ is the infinitesimal strain tensor given by

$$\varepsilon(u) = \frac{1}{2}(\nabla u + \nabla u^{\mathsf{T}}) \in \mathbb{R}^{d\times d}_{\mathrm{sym}} := \{\, \varepsilon \in \mathbb{R}^{d\times d} \,:\, \varepsilon = \varepsilon^{\mathsf{T}} \,\}. \tag{2.2}$$

The nonlocal term $\alpha(x,\nabla Q)$ in $\mathcal{E}$ usually takes the form $\frac{\kappa}{2}|\nabla Q|^2$ with $\kappa > 0$. This term penalizes rapid changes of the internal variable by introducing a length scale which determines the minimal width of interfaces between domains of different polarization.

The external loading $\ell(t)$ depends on the process time t and is usually given by

$$\langle \ell(t),(u,D)\rangle = \int_{\mathbb{R}^d} E_{\mathrm{ext}}(t,x)\cdot D(x)\,\mathrm{d}x + \int_\Omega f_{\mathrm{vol}}(t,x)\cdot u(x)\,\mathrm{d}x + \int_{\Gamma_{\mathrm{Neu}}} f_{\mathrm{surf}}(t,x)\cdot u(x)\,\mathrm{d}a(x),$$

where E_{ext}, f_{vol} and f_{surf} are applied, external fields.

For the dissipation potential $\mathcal{R}$ we take the very simple ansatz

$$\mathcal{R}(\dot Q) = \int_\Omega R(x,\dot Q(x))\,\mathrm{d}x, \tag{2.3}$$

where $R(x,\cdot) : \mathbb{R}^{d_Q} \to [0,\infty)$ is a convex function which is positively homogeneous of degree 1. Note that the dissipation potential acts on the rate $\dot Q = \frac{\partial}{\partial t}Q$ of the internal variable only. The classical way to describe dissipation in ferroelectrics is a switching function in the form

$$\Phi(x,X_Q) \le 0 \quad \text{with } X_Q = \frac{\partial}{\partial Q}W - \mathrm{div}(\mathrm{D}\alpha(x,\nabla Q)).$$

This is equivalent to our dissipation potential R by the relation

$$R(x,\dot Q) = \max\{\, \dot Q\cdot X_Q \,:\, \Phi(x,X_Q) \le 0 \,\}.$$

To formulate the rate-independent evolution law we use the thermomechanically conjugated forces

$$\sigma = \frac{\partial}{\partial \boldsymbol{\varepsilon}} W \in \mathbb{R}^{d\times d}_{\mathrm{sym}}, \quad E = \begin{cases} \frac{\partial}{\partial D} W & \text{on } \Omega, \\ \frac{1}{\epsilon_0} D & \text{on } \mathbb{R}^d \backslash \Omega \end{cases}, \quad X_Q \in \mathbb{R}^{d_Q},$$

where σ is the stress tensor and E the electric field. The elastic equilibrium equation and the Maxwell equations read

$$\begin{aligned} &-\operatorname{div} \sigma + f_{\mathrm{vol}}(t,\cdot) = 0 && \text{in } \Omega, \\ &\operatorname{div} D = 0 \text{ and } \operatorname{curl}(E - E_{\mathrm{ext}}(t,\cdot)) = 0 && \text{in } \mathbb{R}^d, \end{aligned} \tag{2.4}$$

where $\operatorname{curl} E$ is defined as $\nabla E - (\nabla E)^{\mathsf{T}}$ for general dimensions. Thus, these equations are static and respond instantaneously to changes of the loadings $f_{\mathrm{vol}}(t,\cdot)$ and $E_{\mathrm{ext}}(t,\cdot)$.

The evolution of Q follows a force balance which uses the multi-valued dissipational force

$$\partial R(x,\dot{Q}) = \{\, X \in \mathbb{R}^{d_Q} \ : \ R(x,V) \geq R(x,\dot{Q}) + X\cdot(V - \dot{Q}) \text{ for all } V \in \mathbb{R}^{d_Q} \,\},$$

which is the subdifferential of the convex function $R(x,\cdot)$. The force balance takes the simple form

$$0 \in \partial R(x,\dot{Q}) + X_Q\,. \tag{2.5}$$

We now want to rewrite these equations, at least formally, as equations in function spaces. For this purpose we introduce a suitable state space $\mathcal{Y} = \mathcal{F} \times \mathcal{Q}$ as follows. The space $\mathcal{F}$ contains the functions u and D and takes the form

$$\mathcal{F} = \mathcal{H} \times \mathrm{L}^2_{\mathrm{div}}(\mathbb{R}^d), \text{ where } \mathrm{L}^2_{\mathrm{div}}(\mathbb{R}^d) := \{\, \psi \in \mathrm{L}^2(\mathbb{R}^d;\mathbb{R}^d) \ : \ \operatorname{div} \psi = 0 \,\}$$

and $\mathcal{H}$ is a closed affine subspace of $\mathrm{H}^1(\Omega;\mathbb{R}^d)$. The space $\mathcal{Q}$ contains the internal state functions Q and is taken to be $\mathrm{W}^{1,q_Q}(\Omega;\mathbb{R}^{d_Q})$ for a suitable $q_Q > 1$.

The definition of the space $\mathrm{L}^2_{\mathrm{div}}(\mathbb{R}^d)$ already includes Gauß' law, which is part of our Maxwell's equations. Using the well-known fact (cf. [Tem84, Thm. 1.4]) that the total space $\mathrm{L}^2(\mathbb{R}^d;\mathbb{R}^d)$ decomposes in an orthogonal way into the two closed subspaces $\mathrm{L}^2_{\mathrm{div}}(\mathbb{R}^d)$ and

$$\mathrm{L}^2_{\mathrm{curl}}(\mathbb{R}^d) = \{\, \psi \in \mathrm{L}^2(\mathbb{R}^d;\mathbb{R}^d) \ : \ \operatorname{curl} \psi = 0 \,\}$$

we obtain the following result.

Proposition 2.1 *Denote by $\mathrm{D}_D\mathcal{E}(t,u,D,Q)[\widehat{D}]$ the Gâteaux derivative of $\mathcal{E}$ in the direction $\widehat{D}$. Then, we have*

$$\Big(\forall\, \widehat{D} \in \mathrm{L}^2_{\mathrm{div}}(\mathbb{R}^d): \ \mathrm{D}_D\mathcal{E}(t,u,D,Q)[\widehat{D}] = 0\Big) \iff \operatorname{curl}\big(\frac{\partial}{\partial D}\widetilde{W} - E_{\mathrm{ext}}(t,\cdot)\big) = 0 \text{ in } \mathbb{R}^d,$$

where $\widetilde{W} = W$ for $x \in \Omega$ and $\widetilde{W} = \frac{1}{2\epsilon_0}|D|^2$ else.

Proof: The directional derivative takes the form

$$\mathrm{D}_D\mathcal{E}(t,u,D,Q)[\widehat{D}] = \int_\Omega \big(\frac{\partial}{\partial D} W - E_{\mathrm{ext}}(t)\big)\cdot\widehat{D}\,\mathrm{d}x + \int_{\mathbb{R}^d\backslash\Omega} \big(\frac{1}{\epsilon_0} D - E_{\mathrm{ext}}\big)\cdot\widehat{D}\,\mathrm{d}x,$$

where $\widehat{D}$ is allowed to vary in all of $\mathrm{L}^2_{\mathrm{div}}(\mathbb{R}^d)$. Hence, the integrand is orthogonal to this space, which means that it lies in $\mathrm{L}^2_{\mathrm{curl}}(\mathbb{R}^d)$ as desired. ■

Thus, we implement the Maxwell equations simply by choosing a suitable function space and the condition $\mathrm{D}_D\mathcal{E}(t,u,D,Q)=0$.

Similarly, the elastic equilibrium is obtained by $\mathrm{D}_u\mathcal{E}(t,u,D,Q)=0$, as by the symmetry of σ the operator "div" is adjoint to $u\mapsto\boldsymbol{\varepsilon}(u)$. The dissipative force balance can also be rewritten in functional form and thus the full problem may be written as

$$\begin{gathered}\mathrm{D}_u\mathcal{E}(t,u(t),D(t),Q(t))=0,\quad \mathrm{D}_D\mathcal{E}(t,u(t),D(t),Q(t))=0,\\ 0\in\partial\mathcal{R}(\dot{Q}(t))+\mathrm{D}_Q\mathcal{E}(t,u(t),D(t),Q(t)).\end{gathered}\tag{2.6}$$

Here the total derivative $\mathrm{D}_Q\mathcal{E}$ takes the form

$$\mathrm{D}_Q\mathcal{E}(t,u(t),D(t),Q(t))=\frac{\partial}{\partial Q}W(x,u,D,Q)-\mathrm{div}\,\big[\mathrm{D}\alpha(x,\nabla Q)\big].$$

In fact, our theory is not based on the force balance (2.6). Instead, following [MT99, MTL02, MT04], we use a weaker formulation which is based on energies only. This energetic formulation avoids derivatives of $\mathcal{E}$ and of the solution (u,D,Q). Under suitable smoothness and convexity assumptions (see Section 5) the energetic formulation is equivalent to (2.6). We call (u,D,Q) an ***energetic solution*** of the problem associated with $\mathcal{E}$ and $\mathcal{R}$, if for all $t\in[0,T]$ the *stability condition* (S) and the *energy balance* (E) hold:

$$\begin{aligned}&\text{(S)}\quad \mathcal{E}(t,u(t),D(t),Q(t))\le\mathcal{E}(t,\widehat{u},\widehat{D},\widehat{Q})+\mathcal{R}(\widehat{Q}-Q(t))\ \text{for all}\ \widehat{u},\widehat{D},\widehat{Q};\\ &\text{(E)}\quad \mathcal{E}(t,u(t),D(t),Q(t))+\textstyle\int_0^t\mathcal{R}(\dot{Q}(s)))\,\mathrm{d}s\\ &\qquad\quad =\mathcal{E}(0,u(0),D(0),Q(0))-\textstyle\int_0^t\langle\dot{\ell}(s),(u(s),D(s))\rangle\,\mathrm{d}s.\end{aligned}\tag{2.7}$$

Using the abstract result from Section 3, we will show in Section 4 that the energetic formulation (S) & (E) has solutions for suitable initial data, if the constitutive functions W, α and R satisfy reasonable continuity and convexity assumptions. In Section 5 we will discuss stronger conditions which imply uniqueness.

Before this, we want to display the constitutive choices given in the above-mentioned engineering works. Note that most of these papers are not based on the Helmholtz free energy W (denoted by ψ in the engineering literature, cf. [ML02]), they use either the Gibbs energy $g=\widetilde{G}(\sigma,E,Q)$ defined via $g=\sigma{:}\boldsymbol{\varepsilon}+E{\cdot}D-W$ (cf. [KJ98, Kam01, KW03]) or the enthalpy function $h=H(\boldsymbol{\varepsilon},E,Q)$ with $h=W-E{\cdot}D$ (cf. [SG04, RS04]). The latter choice has the advantage that the physically more relevant quantities $(\boldsymbol{\varepsilon}(u),D,Q)$ can be treated as the basic unknowns but there is the disadvantage that H has a saddle-point structure rather than convexity. Our choice of treating $(\boldsymbol{\varepsilon}(u),D,Q)$ has the advantage that it is reasonable to assume that the Helmholtz free energy is convex; and thus minimization techniques are available.

To put the models in the above-mentioned papers into our framework we transform everything into the variables $(\boldsymbol{\varepsilon}(u),D,Q)$ and use W. The basic assumption is that the strain $\boldsymbol{\varepsilon}$ and the electric displacement D can be split additively into an "elastic" and a "remanent" part

$$\boldsymbol{\varepsilon}=\boldsymbol{\varepsilon}_{\mathrm{el}}+\boldsymbol{\varepsilon}_{\mathrm{rem}}(Q)\quad\text{and}\quad D=D_{\mathrm{el}}+P_{\mathrm{rem}}(Q)$$

and that ε and D occur in W only via the elastic part. Moreover, $\varepsilon_{\rm rem} = \varepsilon_{\rm rem}(Q)$ and $P_{\rm rem} = P_{\rm rem}(Q)$ are assumed to be given constitutive functions of the internal variables.

Thus, in all the works the special choice

$$W(\varepsilon, D, Q) = \widetilde{W}(\varepsilon - \varepsilon_{\rm rem}(Q), D - P_{\rm rem}(Q), Q)$$

is made.

The papers [ML02, RS04] use the special choices

$$P_{\rm rem} = Q \quad \text{and} \quad \varepsilon_{\rm rem}(Q) = c_1\, \mathrm{dev}(Q \otimes Q)$$

and the constitutive functions take the form

$$\widetilde{W}(\varepsilon_{\rm el}, D_{\rm el}, Q) = \frac{1}{2}\left\langle \begin{pmatrix} C(Q) & -B(Q) \\ -B(Q)^{\mathsf T} & A(Q) \end{pmatrix} \begin{pmatrix} \varepsilon_{\rm el} \\ D_{\rm el} \end{pmatrix}, \begin{pmatrix} \varepsilon_{\rm el} \\ D_{\rm el} \end{pmatrix} \right\rangle + W_{\rm hard}(Q). \tag{2.8}$$

Here C is the elastic tensor of order 4, B is the piezoelectric tensor of order 3 and A the inverse of the dielectric tensor of order 2. Whereas C and A may be chosen independently of Q, the dependence of B on Q crucial for the ferroelectric effect. For treating polarization induced piezoelectricity a typical choice is

$$\begin{aligned} B_{ijk}(P_{\rm rem}) = \tfrac{1}{P_{\rm sat}|P_{\rm rem}|^2}\Big(& d_{||} P_{{\rm rem}\,i} P_{{\rm rem}\,j} P_{{\rm rem}\,k} + d_{\perp}(|P_{\rm rem}|^2\delta_{ij} - P_{{\rm rem}\,i} P_{{\rm rem}\,j}) P_{{\rm rem}\,k} \\ & + \tfrac{d_{=}}{2}\big[(|P_{\rm rem}|^2\delta_{ki} - P_{{\rm rem}\,k} P_{{\rm rem}\,i}) P_{{\rm rem}\,j} + (|P_{\rm rem}|^2\delta_{kj} - P_{{\rm rem}\,k} P_{{\rm rem}\,j}) P_{{\rm rem}\,i}\big]\Big). \end{aligned} \tag{2.9}$$

with material parameters $d_{||}, d_{\perp}$ and $d_{=}$ and some functional dependence $P_{\rm rem} = \widehat{P}(Q)$. The hardening contribution $W_{\rm hard}$ is used to confine Q into reasonable bounds. In a system of uni-axial polarization the hardening contribution $W_{\rm hard}$ may be chosen to depend on $P_a = Q{\cdot}a$ for a given direction a with $|a| = 1$ only. Well-established choices are

$$\begin{aligned} W_{\rm hard}(Q) &= hP_{\rm sat}^2\left[\ln\left(1 - \tfrac{P_a}{P_{\rm sat}}\right) + \tfrac{P_a}{P_{\rm sat}}\right] \quad \text{or} \\ W_{\rm hard}(Q) &= h\left[P_a\, \mathrm{Artanh}(P_a/P_{\rm sat}) + \tfrac{P_{\rm sat}}{2}\ln(1 - (P_a/P_{\rm sat})^2)\right]. \end{aligned} \tag{2.10}$$

cf. [HF01, ML02] or [RS04], respectively. Note that these choices imply $|P_a| < P_{\rm sat}$.

In the papers [KJ98, Kam01, KW03] the choices are quite different an motivated by microscopic distributions of polarization directions. The simplest model assumes

$$Q = (\beta, \gamma) \in \mathbb{R}^2, \quad \varepsilon_{\rm rem}(Q) = \frac{\beta - \beta_{\rm ref}}{1 - \beta_{\rm ref}}\varepsilon_{\rm sat} \quad \text{and } P_{\rm rem} = \gamma P_{\rm sat},$$

where $P_{\rm sat} \in \mathbb{R}^d$ and $\varepsilon_{\rm sat} \in \mathbb{R}^{d\times d}$ are fixed and (β, γ) is restricted to the set $G = \{\,(\beta, \gamma) \in \mathbb{R}^2 \;:\; 0 \le |\gamma| \le \beta \le 1\,\}$ by adding a suitable constraint to the function $W_{\rm hard}$. More elaborate multi-axial versions are discussed in [KW03].

None of the models mentioned so far, include the nonlocal term $\int_\Omega \alpha(x, \nabla Q)\,\mathrm{d}x$, which penalizes formation of fast changes in the internal parameters. However, as is indicated in [SB01, Dav01] these contributions may be important to avoid the possible formation of microstructure. Thus, this part is used to limit the smallness of spatial scales and thus prevents the formation of microstructure. In fact, it is well known that rate-independent material models like for shape-memory alloys or for finite-strain elastoplasticity may not have solutions because of formation of microstructure, see [OR99, CHM02, Mie04a]. Thus, we include the regularizing term which is a crucial term to provide the desired compactness for the construction of solutions, see [FM04].

All the papers use very simple switching functions Φ and thus dissipation potentials, namely

$$\Phi(x,X)=|X|^2-X_0(x)^2 \quad \Longleftrightarrow \quad R(x,\dot{Q})=r(x)|\dot{Q}| \text{ with } r(x)=1/X_0(x).$$

3 Existence of solutions in the general case

Here we obtain the existence of energetic solutions for our mathematical problem. We next recall the concept of *energetic solution*. For more details see [Mie04b, Mai05, FM04, MM05].

Consider the set $\mathcal{Y}=\mathcal{F}\times\mathcal{Z}$ as the basic state space. Whenever possible we will write y instead of (φ,z) to shorten notation. Note that the splitting is done such that changes in z involve dissipation whereas those of φ do not. In the section above (u,D) takes the rôle of φ and Q is the internal variable z.

The state space $\mathcal{Y}$ is equipped with a Hausdorff topology $\mathcal{T}=\mathcal{T}_\mathcal{F}\times\mathcal{T}_\mathcal{Z}$ and we denote by $y_k \overset{\mathcal{Y}}{\to} y$, $\varphi_k \overset{\mathcal{F}}{\to} \varphi$ and $z_k \overset{\mathcal{Z}}{\to} z$ the corresponding convergence of sequences.

The first ingredient of the energetic formulation is the *dissipation distance* $\mathcal{D}:\mathcal{Z}\times\mathcal{Z}\to[0,\infty]$, which is a semi-distance (see (A1) below). For a given curve $z:[0,T]\to\mathcal{Z}$ we define the total dissipation on $[s,t]$ via

$$\mathrm{Diss}_\mathcal{D}(z;[s,t])=\sup\{\textstyle\sum_1^N \mathcal{D}(z(\tau_{j-1}),z(\tau_j)) \ : \ N{\in}\mathbb{N}, s{=}\tau_0{<}\tau_1{<}\cdots{<}\tau_N{=}t\,\}. \tag{3.1}$$

The second ingredient is the energy-storage functional $\mathcal{E}:[0,T]\times\mathcal{Y}\to\mathbb{R}_\infty:=\mathbb{R}\cup\{\infty\}$. Here $t\in[0,T]$ plays the rôle of a (very slow) process time which changes the underlying system via changing loading conditions. We assume that for all y_* with $\mathcal{E}(t,y_*)<\infty$, the function $\mathbb{R}\ni t\mapsto\mathcal{E}(t,y_*)\in\mathbb{R}$ is differentiable.

Definition 3.1 *A curve $y=(\varphi,z):[0,T]\to\mathcal{Y}=\mathcal{F}\times\mathcal{Z}$ is called an **energetic solution** of the rate-independent system associated with $(\mathcal{D},\mathcal{E})$, if $t\mapsto\partial_t\mathcal{E}(t,y(t))$ is integrable and if the **global stability*** **(S)** *and the **energy balance*** **(E)** *hold for all $t\in[0,T]$:*

(S) *For all $\widehat{y}=(\widehat{\varphi},\widehat{z})\in\mathcal{Y}$ we have $\mathcal{E}(t,y(t))\le\mathcal{E}(t,\widehat{y})+\mathcal{D}(z(t),\widehat{z})$.*

(E) $\mathcal{E}(t,y(t))+\mathrm{Diss}_\mathcal{D}(z;[0,t])=\mathcal{E}(0,y(0))+\int_0^t\partial_t\mathcal{E}(\tau,y(\tau))\,\mathrm{d}\tau$.

The definition of solutions of (S) & (E) is such that it implies the two natural requirements for evolutionary problems, namely that *restrictions* and *concatenations* of solutions remain solutions. To be more precise, for any solution $y:[0,T]\to\mathcal{Y}$ and any subinterval $[s,t]\subset[0,T]$, the restriction $y|_{[s,t]}$ solves (S) & (E) with initial datum $y(s)$. Moreover, if $y_1:[0,t_*]\to\mathcal{Y}$ and $y_2:[t_*,T]\to\mathcal{Y}$ solve (S) & (E) on the respective intervals and if $y_1(t_*)=y_2(t_*)$, then the concatenation $y:[0,T]\to\mathcal{Y}$ solves (S) & (E) as well.

To prove our existence result we impose the conditions (A1), (A2) and (A3) on the dissipation distance $\mathcal{D}$:

$$\begin{aligned}&\text{(i)} \quad \forall\, z_1,z_2\in\mathcal{Z}:\ \mathcal{D}(z_1,z_2)=0 \quad\Longleftrightarrow\quad z_1=z_2,\\ &\text{(ii)} \quad \forall\, z_1,z_2,z_3\in\mathcal{Z}:\ \mathcal{D}(z_1,z_3)\le\mathcal{D}(z_1,z_2)+\mathcal{D}(z_2,z_3).\end{aligned} \tag{A1}$$

Here (i) is the classical positivity of a distance and (ii) the triangle inequality. Note that we allow the value ∞ and that we do not enforce symmetry, i.e., $\mathcal{D}(z_1, z_2) \neq \mathcal{D}(z_2, z_1)$ is allowed, as this is needed in many applications.

$$\begin{array}{l}\text{For any sequence } (z_k)_k \text{ and any } z \text{ in } \mathcal{Z} \text{ we have:}\\ \min\{\mathcal{D}(z_k, z), \mathcal{D}(z, z_k)\} \to 0 \text{ for } k \to \infty \quad \Longrightarrow \quad z_k \overset{\mathcal{Z}}{\to} z \text{ for } k \to \infty.\end{array} \tag{A2}$$

$$\mathcal{D} : \mathcal{Z} \times \mathcal{Z} \to [0, \infty] \quad \text{is continuous.} \tag{A3}$$

For the energy functional $\mathcal{E}$ we impose the conditions (A4), (A5) and (A6):

$$\mathcal{E}(t, \cdot) : \mathcal{Y} \to \mathbb{R}_\infty \text{ has compact sublevels } \forall t \in [0, T]. \tag{A4}$$

Here the sublevels $L_{t,e}$ of $\mathcal{E}(t, \cdot)$ are defined as usual by $L_{t,e} := \{\, y \in \mathcal{Y} \,:\, \mathcal{E}(t, y) \leq e \,\}$. A classical fact is that compactness of sublevels implies lower semi-continuity and coercivity.

$$\begin{array}{l}\text{There exist } c_E^{(1)}, c_E^{(0)} > 0 \text{ such that for all } y_* \in \mathcal{Y} :\\ \text{If } \mathcal{E}(t, y_*) < \infty, \text{ then } \partial_t \mathcal{E}(\cdot, y_*) : [0, T] \to \mathbb{R} \text{ is measurable}\\ \qquad\qquad\qquad \text{and } |\partial_t \mathcal{E}(t, y_*)| \leq c_E^{(1)}(\mathcal{E}(t, y_*) + c_E^{(0)}).\end{array} \tag{A5}$$

$$\begin{array}{l}\forall\, E^* > 0\ \forall\, \varepsilon > 0\ \exists\, \delta > 0 : \ \ \mathcal{E}(t, y) \leq E^* \text{ and } |t - s| \leq \delta\\ \qquad\qquad\qquad\qquad\quad \Longrightarrow \quad |\partial_t \mathcal{E}(t, y) - \partial_t \mathcal{E}(s, y)| < \varepsilon.\end{array} \tag{A6}$$

The following existence result is proved in [FM04, Mie04b].

Theorem 3.2 *Assume that $\mathcal{E}$ and $\mathcal{D}$ satisfy the hypotheses* (A1)–(A6) *and that the initial datum $y_0 \in \mathcal{Y}$ is stable (i.e., y_0 satisfies* (S) *at $t = 0$), then there exists a solution $y = (\varphi, z) : [0, T] \to \mathcal{Y}$ of* (S) & (E) *with $y(0) = y_0$.*

Moreover, any solution of (S) & (E) *with $y(0) = y_0$ satisfies the a priori estimates*

$$\left.\begin{array}{r}\mathcal{E}(t, y(t)) \leq (c_E^{(0)} + \mathcal{E}(0, y_0))\, \mathrm{e}^{c_E^{(1)} t} - c_E^{(0)}\\ \mathrm{Diss}_{\mathcal{D}}(y; [0, t]) \leq (c_E^{(0)} + \mathcal{E}(0, y_0))\, \mathrm{e}^{c_E^{(1)} t}\end{array}\right\} \quad \textit{for } t \in [0, T].$$

4 Existence for ferroelectric models

To apply abstract theory of the previous section we need the following standard result in linearized elasticity. It allows us to obtain the desired coercivity of the energy functional which is used to establish condition (A4).

Proposition 4.1 (Korn's inequality) *Let $\Omega \subset \mathbb{R}^d$ be a nonempty connected open bounded set, with Lipschitz boundary Γ, and let Γ_{Dir} be a measurable subset of Γ, such that $\int_{\Gamma_{\mathrm{Dir}}} 1 \, \mathrm{d}a > 0$. Given a function $u \in \mathrm{H}^1(\Omega, \mathbb{R}^d)$, the linearized strain tensor $\boldsymbol{\varepsilon}$ is defined by* (2.2)*. Then, there exists a constant $k > 0$, such that*

$$\|u\|_{\mathrm{H}^1}^2 \leq k \int_\Omega |\boldsymbol{\varepsilon}(u)|^2 \, \mathrm{d}x \quad \textit{for all } u \in \mathrm{H}^1_{\Gamma_{\mathrm{Dir}}}(\Omega, \mathbb{R}^d) := \{\, v \in \mathrm{H}^1(\Omega, \mathbb{R}^d) \,:\, v|_{\Gamma_{\mathrm{Dir}}} \equiv 0 \,\}. \tag{4.1}$$

We now provide conditions on the constitutive functions W, α and R, such that he above abstract theory can be applied for our ferroelectricity model defined via the energy functional $\mathcal{E}$ in (2.1) and the dissipation potential $\mathcal{R}$ in (2.3).

The first assumption concerns the domain and the Dirichlet boundary:

$$\Omega \text{ and } \Gamma_{\mathrm{Dir}} \text{ satisfy the assumptions of Proposition 4.1.} \tag{B0}$$

The function $R : \Omega \times \mathbb{R}^{d_Q} \to [0, \infty)$ satisfies

$$R \in \mathrm{C}^0(\overline{\Omega} \times \mathbb{R}^{d_Q}) \quad \text{and} \quad \exists\, c_R, C_R > 0\ \forall V \in \mathbb{R}^{d_Q} :\ c_R|V| \leq R(x, V) \leq C_R|V|. \tag{B1}$$

$$\forall\, x \in \Omega :\ R(x, \cdot) : \mathbb{R}^{d_Q} \to [0, \infty) \text{ is 1-homogeneous and convex.} \tag{B2}$$

The functions W and α have to fulfill the following three conditions:

$$\begin{aligned} &W : \Omega \times \mathbb{R}^{d\times d}_{\mathrm{sym}} \times \mathbb{R}^d \times \mathbb{R}^{d_Q} \to [0, \infty] \text{ is a Caratheodory function,} \\ &\alpha : \Omega \times \mathbb{R}^{d_Q \times d} \to [0, \infty] \text{ is a Caratheodory function,} \end{aligned} \tag{B3}$$

which means for W that for each $(\boldsymbol{\varepsilon}, D, Q)$ the function $W(\cdot, \boldsymbol{\varepsilon}, D, Q)$ is measurable on Ω and for a.e. $x \in \Omega$ the mapping $W(x, \cdot, \cdot, \cdot)$ is continuous on $\mathbb{R}^{d\times d}_{\mathrm{sym}} \times \mathbb{R}^d \times \mathbb{R}^{d_Q}$ and similarly for α. Further we need coercivity and convexity assumptions:

$$\begin{aligned} &\exists\, c_{\mathcal{E}}, C_{\mathcal{E}} > 0,\ q > 1\ \forall\, (x, \boldsymbol{\varepsilon}, D, Q, V) \in \mathbb{R}^{d\times d}_{\mathrm{sym}} \times \mathbb{R}^d \times \mathbb{R}^{d_Q} \times \mathbb{R}^{d_Q\times d} : \\ &W(x, \boldsymbol{\varepsilon}, D, Q) + \alpha(x, V) \geq c_{\mathcal{E}}(|\boldsymbol{\varepsilon}|^2 + |D|^2 + |Q|^q + |V|^q) - C_{\mathcal{E}}. \end{aligned} \tag{B4}$$

$$\begin{aligned} &\forall\, (x, Q) \in \Omega \times \mathbb{R}^{d_Q} :\ W(x, \cdot, \cdot, Q) : \mathbb{R}^{d\times d}_{\mathrm{sym}} \times \mathbb{R}^d \to [0, \infty] \text{ is convex,} \\ &\forall\, x \in \Omega :\ \alpha(x, \cdot) : \mathbb{R}^{d_Q\times d} \to [0, \infty] \text{ is convex} \end{aligned} \tag{B5}$$

The fact that convexity in the variable Q is not needed is the basis for the ability to model the ferroelectric effect, since the choices of W presented in Section 2 certain are not convex in Q.

For the external loading $\ell(t)$ we assume

$$\ell \in \mathrm{C}^1([0, T], (\mathrm{H}^1_{\Gamma_{\mathrm{Dir}}}(\Omega; \mathbb{R}^d))^* \times \mathrm{L}^2_{\mathrm{div}}(\mathbb{R}^d)^*). \tag{B6}$$

We now relate the concrete ferroelectric model to the abstract one by choosing the function spaces first:

$$\mathcal{F} = \mathrm{H}^1_{\Gamma_{\mathrm{Dir}}}(\Omega, \mathbb{R}^d)_{\mathrm{weak}} \times \mathrm{L}^2_{\mathrm{div}}(\mathbb{R}^d)_{\mathrm{weak}} \quad \text{and} \quad \mathcal{Z} = \mathrm{L}^1(\Omega, \mathbb{R}^{d_Q})_{\mathrm{strong}}.$$

Here the subscripts "weak" and "strong" indicate whether we use the weak or the strong (norm) topology in the corresponding Banach spaces. The dissipation distance $\mathcal{D}$ is related to $\mathcal{R}$ by

$$\mathcal{D}(Q_0, Q_1) = \mathcal{R}(Q_1 - Q_0) = \int_\Omega R(x, Q_1(x) - Q_0(x))\,\mathrm{d}x. \tag{4.2}$$

The functional $\mathcal{E}$ is defined on $[0, T] \times \mathcal{F} \times \mathcal{Z}$ via (2.1) where $\mathcal{E}(t, u, D, Q)$ takes the value $+\infty$, if $Q \notin \mathrm{W}^{1,q}(\Omega; \mathbb{R}^{d_Q})$ or if the integrand is not in $\mathrm{L}^1(\Omega)$. With these choices the abstract energetic problem of Definition 3.1 leads us exactly to the energetic problem (S) & (E) for the ferroelectric model as defined in (2.7).

Thus, our first main result will be proved by checking the assumptions of the abstract existence theorem 3.2 from above.

Theorem 4.2 (Existence theorem)
If the assumptions (B0)–(B6) *hold, then for each stable initial condition* $(u_0, D_0, Q_0) \in \mathcal{F} \times \mathcal{Z}$ *the energetic problem* (S) & (E) *in* (2.7) *has a solution* $(u, D, Q) : [0, T] \to \mathcal{F} \times \mathcal{Z}$ *with* $(u(0), D(0), Q(0)) = (u_0, D_0, Q_0)$, *which satisfies*

$$(u, D, Q) \in \mathrm{L}^\infty([0, T], \mathrm{H}^1_{\Gamma_{\mathrm{Dir}}}(\Omega; \mathbb{R}^d) \times \mathrm{L}^2_{\mathrm{div}}(\mathbb{R}^d) \times \mathrm{W}^{1,q}(\Omega; \mathbb{R}^{d_Q})).$$

We have divided the proof into three lemmas, and we start with the properties of $\mathcal{D}$.

Lemma 4.3 *If* (B1) *and* (B2) *hold, then* $\mathcal{D}$, *defined in* (4.2), *satisfies*

$$c_R\|z_2 - z_1\|_{\mathrm{L}^1} \le \mathcal{D}(z_1, z_2) \le C_R\|z_2 - z_1\|_{\mathrm{L}^1} \ \forall z_1, z_2 \in \mathcal{Z}, \tag{4.3}$$

and consequently, (A1), (A2), (A3) *hold.*

Proof: It is easily seen that (4.3) follows from (B1).

ad (A1): R is subadditive, since it is convex and positively homogeneous. By (4.2), the triangle inequality for $\mathcal{D}$ becomes clear. Now let z_1, $z_2 \in \mathcal{Z}$, such that $\mathcal{D}(z_1, z_2) = 0$. By the left inequality from (4.3) we get $z_1 = z_2$. This completes the proof of (A1).

ad (A3): By (4.2) we see that $\mathcal{D}$ is continuous, if and only if so is the partial map $\mathcal{D}(\cdot, 0)$. As R is subadditive, so is $\mathcal{D}$. This together with the right inequality from (4.3) yields the continuity of $\mathcal{D}(\cdot, 0)$, and hence that of $\mathcal{D}$.

ad (A2): Let $(z_k)_k$ and z in $\mathcal{Z}$, such that $\min\{\mathcal{D}(z_k, z), \mathcal{D}(z, z_k)\} \to 0$ for $k \to \infty$. By the left inequality from (4.3) we obtain $c_R\|z_k - z\|_{\mathrm{L}^1} \le \min\{\mathcal{D}(z_k, z), \mathcal{D}(z, z_k)\}$, and hence $z_k \xrightarrow{\mathcal{Z}} z$ for $k \to \infty$, which proves (A2). ■

The second condition concerns the coercivity and the weak lower semi-continuity of the energy functional $\mathcal{E}$.

Lemma 4.4 *Let* (B0) *and* (B3)–(B5). *Then, the functionals* $\mathcal{E}(t, \cdot) : \mathcal{F} \times \mathcal{Z} \to \mathbb{R}_\infty$ *are sequentially lower semicontinuous (in the given topology of* $\mathcal{F} \times \mathcal{Z}$*) and there exist constants* $c_0, C_0 > 0$ *such the functional* $\mathcal{E}(t, \cdot)$ *satisfies the coercivity estimate*

$$\mathcal{E}(t, u, D, Q) \ge c_0(\|u\|^2_{\mathrm{H}^1} + \|D\|^2_{\mathrm{L}^2} + \|Q\|^q_{\mathrm{W}^{1,q}}) - \|\ell(t)\|_*\|(u, D)\|_{\mathrm{H}^1\times\mathrm{L}^2} - C_0. \tag{4.4}$$

In particular, the sublevels $L_{t,e}$ *are sequentially compact, i.e.,* (A4) *holds.*

Proof: We first establish the coercivity estimate. Using (B0) and (B4) we find

$$\begin{aligned} \mathcal{E}(t, u, D, Q) &\ge \int_\Omega c_\mathcal{E}(|\varepsilon(u)|^2 + |D|^2 + |Q|^q + |\nabla Q|^q) - C_\mathcal{E}\,\mathrm{d}x - \|\ell(t)\|_*\|(u, D)\|_{\mathrm{H}^1\times\mathrm{L}^2} \\ &\ge \tfrac{c_\mathcal{E}}{k}\|u\|^2_{\mathrm{H}^1} + c_\mathcal{E}(\|D\|^2_{\mathrm{L}^2} + \|Q\|^q_{\mathrm{W}^{1,q}}) - C_\mathcal{E}\mathrm{vol}(\Omega) - \|\ell(t)\|_*\|(u, D)\|_{\mathrm{H}^1\times\mathrm{L}^2}, \end{aligned}$$

where we have used Korn's inequality from Proposition 4.1. This gives the desired estimate (4.4) and we conclude that all sublevels $L_{t,e} = \{ y \in \mathcal{Y} : \mathcal{E}(t, y) \le e \}$ are bounded in $\mathcal{Y}_q := \mathrm{H}^1_{\Gamma_{\mathrm{Dir}}}(\Omega; \mathbb{R}^d) \times \mathrm{L}^2_{\mathrm{div}}(\mathbb{R}^d) \times \mathrm{W}^{1,q}(\Omega; \mathbb{R}^{d_Q}) \subset \mathcal{F} \times \mathcal{Z}$.

Next we show that the sublevels $L_{t,e}$ are sequentially compact in $\mathcal{Y}$. Let $(y_k)_{k\in\mathrm{N}} \subset L_{t,e}$ be given. Hence the sequence is bounded in $\mathcal{Y}_q$, which is a reflexive Banach space. Hence there exists a weakly convergent subsequence, which we do not relabel. Hence, we may assume $(u_k, D_k) \rightharpoonup (u, D)$ in $\mathrm{H}^1(\Omega; \mathbb{R}^d) \times \mathrm{L}^2(\mathbb{R}^d; \mathbb{R}^d)$ (weakly) and $Q_k \rightharpoonup Q$ in $\mathrm{W}^{1,q}(\Omega; \mathbb{R}^{d_Q})$. By the compact embedding of $\mathrm{W}^1 1, q(\Omega; \mathbb{R}^{d_Q})$ into $\mathrm{L}^1(\Omega; \mathbb{R}^{d_Q})$ we conclude

$Q_k \to Q$ in $\mathrm{L}^1(\Omega;\mathbb{R}^{d_Q})$ (strongly). This implies convergence in $\mathcal{Y}$. It remains to be shown that $y=(u,D,Q)$ lies in $L_{t,e}$.

Using the weak convergence of the sequence $y_k=(u_k,D_k,Q_k)$ in the $\mathcal{Y}_q$ we can employ a classical result from the theory for the direct method in the calculus of variations (see e.g., [Dac89, Thm. 3.4]), namely that $\mathcal{E}(t,\cdot):\mathcal{Y}_q\to\mathbb{R}_\infty$ is sequentially weakly lower semi-continuous, i.e.,

$$(u_k,D_k,Q_k)\rightharpoonup(u,D,Q) \quad\Longrightarrow\quad \mathcal{E}(t,u,D,Q)\le\liminf_{k\to\infty}\mathcal{E}(t,u_k,D_k,Q_k).$$

For this we use that our condition (B5) provides the sufficient convexity conditions for the weakly converging parts $(\boldsymbol{\varepsilon}_k,D_k,\nabla Q_k)$. Using $\mathcal{E}(t,u_k,D_k,Q_k)\le e$ we conclude $\mathcal{E}(t,u,D,Q)\le e$ and obtain $y=(u,D,Q)\in L_{t,e}$.

Standard arguments in the calculus of variations show that compactness of the sublevels implies lower semicontinuity. ∎

Finally we control the power of the external forces $\partial_t\mathcal{E}(t,u,D,Q)$.

Lemma 4.5 *If $\mathcal{E}$ satisfies the coercivity* (4.4) *and if the loading satisfies* (B6) *hold, then $\mathcal{E}$ and ∂_t satisfy* (A5) *and* (A6).

Proof: We first note that $\ell\in\mathrm{C}^1([0,T],\mathcal{Y}^*)$ implies

$$\partial_t\mathcal{E}(t,u,D,Q)=\langle\dot{\ell}(t),(u,D)\rangle \quad\Longrightarrow\quad |\partial_t\mathcal{E}(t,u,D,Q)|\le K_1\|(u,D)\|_{\mathrm{H}^1\times\mathrm{L}^2},$$

where $K_1=\max_{t\in[0,T]}\|\dot{\ell}(t)\|_*$. Letting $K_0=\max_{t\in[0,T]}\|\ell(t)\|_*$ and using the coercivity (4.4) of $\mathcal{E}$ we obtain

$$|\partial_t\mathcal{E}(t,y)|\le K_1\|(u,D)\|_{\mathrm{H}^1\times\mathrm{L}^2}\le c_0\|(u,D)\|^2_{\mathrm{H}^1\times\mathrm{L}^2}-C_0-K_0\|(u,D)\|_{\mathrm{H}^1\times\mathrm{L}^2}+M\le\mathcal{E}(t,y)+M,$$

where $M=C_0+(K_0+K_1)^2/(4c_0)$. Hence, (A5) holds with $c_E^{(0)}=M$ and $c_E^{(1)}=1$.

Since $\dot{\ell}$ is uniformly continuous on the compact interval $[0,T]$, the uniform boundedness of the sublevels $L_{t,e}$ for $t\in[0,T]$ shows condition (A6). ∎

Proof of Theorem 4.2: The above three lemmas show that the assumptions (B0)–(B6) of Theorem 4.2 imply that all hypotheses (A1)–(A6) of the abstract Theorem 3.2 are verified. We thus obtain the existence of an energetic solution $(u,D,Q):[0,T]\to\mathcal{Y}=\mathrm{H}^1_{\Gamma_{\mathrm{Dir}}}(\Omega;\mathbb{R}^d)\times\mathrm{L}^2_{\mathrm{div}}(\mathbb{R}^d)\times\mathrm{L}^1(\Omega;\mathbb{R}^{d_Q})$ of the rate-independent, energetic formulation (S) & (E) associated with $\mathcal{D}$ and $\mathcal{E}$ defined in (4.2) and (2.1), respectively.

The a priori bounds $\mathcal{E}(t,u(t),D(t),Q(t))\le E_T$ and $\int_0^T\mathcal{R}(\dot{Q}(s))\,\mathrm{d}s\le E_T$ provided at the end of Theorem 3.2 imply together with (4.4) that the function $t\mapsto(u(t),D(t),Q(t))\in\mathrm{H}^1_{\Gamma_{\mathrm{Dir}}}(\Omega;\mathbb{R}^d)\times\mathrm{L}^2_{\mathrm{div}}(\mathbb{R}^d)\times\mathrm{W}^{1,q}(\Omega;\mathbb{R}^{d_Q})$ is also bounded.

From $\int_0^T\mathcal{R}(\dot{Q}(s))\,\mathrm{d}s<\infty$ it follows that $t\mapsto Q(t)\in\mathrm{L}^1(\Omega)$ has total variation, which implies that it is continuous except for an at most countable set of jump points. Combining this with the boundedness in $\mathrm{W}^{1,q}$ we conclude weak measurability of $t\mapsto Q(t)\in\mathrm{W}^{1,q}$. However, in the reflexive, separable Banach space $\mathrm{W}^{1,q}$ weak and strong measurability coincide (see [Yos68, Ch. V.4]) and we conclude $Q\in\mathrm{L}^\infty([0,T],\mathrm{W}^{1,q}(\Omega;\mathbb{R}^{d_Q}))$.

Similar arguments do not apply for the bounded map $t\mapsto(u(t),D(t))\in\mathrm{H}^1_{\Gamma_{\mathrm{Dir}}}(\Omega;\mathbb{R}^d)\times\mathrm{L}^2_{\mathrm{div}}(\mathbb{R}^d)$. The measurability here has to be obtained by a intricate choice of the approximating functions in the construction of the solution and cannot be restored afterwards, see [Mai05]. ∎

We may now relate our conditions (B0)–(B6) to the special choices of W and R which are used in the engineering models mentioned in Section 2. Conditions (B0)–(B3) are easily satisfied and the same for the loading condition (B6). Moreover, the convexity condition (B5) holds if we choose $\alpha(x, \nabla Q) = \frac{\kappa}{2}|\nabla Q|^2$ and assume that W has the form given in (2.8). For convexity, we only have to guarantee that the combined tensor $\left(\begin{smallmatrix} A & -B \\ -B^\mathsf{T} & C \end{smallmatrix}\right)$ is positive semi-definite for all Q. Additionally the tensors A, B, C and the functions $\varepsilon_{\text{rem}}, P_{\text{rem}}$ and W_{hard} have to be continuous in Q, which is the case in the examples (2.9) and (2.10) given above.

Important is still the coercivity condition (B4). For W in the form (2.8) this holds if the tensor $\left(\begin{smallmatrix} A & -B \\ -B^\mathsf{T} & C \end{smallmatrix}\right)$ is uniformly strictly positive definite for all Q with $W_{\text{hard}}(Q) < \infty$ and if the hardening function W_{hard} is coercive as well, i.e., $W_{\text{hard}}(Q) \geq c_W|Q|^q - C_W$ for all Q. In fact, most engineering models let $W_{\text{hard}}(Q) = +\infty$ for $|\widehat{P}(Q)| \geq P_{\text{sat}}$ and thus coercivity in Q follows.

5 Uniqueness of solutions

Uniqueness results in rate-independent hysteresis models are rather exceptional, as they need strong assumptions on the nonlinearities, see [MT04, BKS04, MR04] and the survey in [Mie04b]. Building on the results in [MT04, Sect. 7] we now show that suitable restrictions on our ferroelectric model leads to uniqueness of solutions. However, it is unclear whether these restrictions are still compatible with models which are useful in practice.

First of all the theory has to be restricted to a Hilbert space setting and we let

$$\mathcal{Y}_2 = \mathrm{H}^1_{\Gamma_{\text{Dir}}}(\Omega;\mathbb{R}^d) \times \mathrm{L}^2_{\text{div}}(\mathbb{R}^d) \times \mathrm{H}^1(\Omega;\mathbb{R}^{d_Q}).$$

We still assume that the conditions (B0)–(B6) hold, but now with $q = 2$. We will add further condition below, such that we are able to apply the following abstract result [MT04, Thm. 7.4].

It is formulated on a general Hilbert space $\mathcal{Y}_H$ with functionals $\mathcal{E} : [0, T] \times Y_H \to \mathbb{R}$ and $\mathcal{R} : \mathcal{Y}_H \to \mathbb{R}$. The following conditions are imposed:

$$\mathcal{R} : \mathcal{Y}_H \to [0, \infty) \text{ is continuous, convex and 1-homogeneous.} \tag{C1}$$

$$\begin{aligned} &\mathcal{E} \in \mathrm{C}^{2,\text{Lip}}_{\text{loc}}([0,T] \times \mathcal{Y}_H, \mathbb{R}) \text{ and} \\ &\forall\, e_0\ \exists\, C > 0\ \forall\, y_j \text{ with } \mathcal{E}(0, y_j) \leq e_0 : \ \ \|\mathrm{D}\mathcal{E}(t, y_1)\|, \|\mathrm{D}^2\mathcal{E}(t, y_1)\| \leq C, \\ &\qquad\qquad\qquad\qquad\qquad\qquad\qquad\quad \|\mathrm{D}^2\mathcal{E}(t, y_1) - \mathrm{D}^2\mathcal{E}(t, y_2)\| \leq C\|y_1 - y_2\|. \end{aligned} \tag{C2}$$

$$\exists\, \alpha > 0\ \forall\, v, y \in \mathcal{Y}_H : \ \langle \mathrm{D}^2\mathcal{E}(t, y)v, v\rangle \geq \alpha\|v\|^2. \tag{C3}$$

The last condition is a uniform convexity condition which seems to be crucial for uniqueness results. Condition (C2) is a regularity conditions which cannot be avoided at present. The following existence and uniqueness result works totally without compactness assumptions, in contrast to the more general existence theory in Section 3.

Theorem 5.1 *If the conditions* (C1)–(C3) *and* (A5) *hold, then the energetic problem* (S) & (E) *has for each stable initial datum* $y_0 \in \mathcal{Y}_H$ *a unique solution* $y : [0, T] \to \mathcal{Y}_H$ *with* $y(0) = y_0$. *This solution satisfies* $y \in \mathrm{C}^{\text{Lip}}([0, T]; \mathcal{Y}_H)$ *and depends Lipschitz continuously on the initial data. Moreover, these solutions satisfy the* ***differential inclusion***

$$0 \in \partial\mathcal{R}(\dot{y}(t)) + \mathrm{D}\mathcal{E}(t, y(t)) \quad \textit{for a.e. } t \in [0, T],$$

which is equivalent to the ***quasi-variational inequality***

$$\Big(\forall\, v \in \mathcal{Y}_H: \ \langle \mathrm{D}\mathcal{E}(t,y(t)), v-\dot y(t)\rangle + \mathcal{R}(\dot y(t)) \geq 0 \Big) \qquad \textit{for a.e. } t \in [0,T].$$

The proof of this theorem is the content of [MT04, Sect. 7]. There the condition $\mathcal{E} \in \mathrm{C}^3$ is imposed, but a check of the calculations there reveals that only Lipschitz continuity of the second derivative is needed. Having added condition (A5), we have the usual a priori estimate show energetic boundedness of solutions and all approximate solutions used in the proof. Thus our boundedness assumptions in (C2), which are only on sublevels, are sufficient as well.

We now have to discuss how the new assumptions (C1)–(C3) can be satisfied in our ferroelectric model. Condition (C1) on the dissipation potential $\mathcal{R}$ is a direct consequence of the previous assumptions (B1) and (B2).

The conditions on the energy-storage functional $\mathcal{E}$ are more critical. First, the differentiability of functionals needs that the integrands W and α have the same order of differentiability. However, there is an additional constraint concerning the Lebesgue integrability. For instance, a functional

$$\mathcal{I}: \mathrm{L}^p(\Omega) \to \mathbb{R}; \phi \mapsto \int_\Omega f(x,\phi(x))\,\mathrm{d}x,$$

is in $\mathrm{C}^{k,\mathrm{Lip}}(\mathrm{L}^p(\Omega);\mathbb{R})$ if and only if $f \in \mathrm{C}^k(\mathbb{R};\mathbb{R})$, $p \geq k{+}1$ and

$$\exists\, C>0\ \forall\, u_1,u_2 \in \mathbb{R}: \ |f^{(k)}(u_1) - f^{(k)}(u_2)| \leq C\big[1+(|u_1|+|u_2|)^{p-k-1}\big]\,|u_1-u_2| \text{ a.e. on } \Omega.$$

This is easily seen when using the formula

$$\mathrm{D}^k\mathcal{I}(\phi)[\phi_1,\dots,\phi_k] = \int_\Omega f^{(k)}(\phi(x))\phi_1(x)\cdots\phi_k(x)\,\mathrm{d}x$$

and Hölder's inequality. There is only one exception which allows for $p<k{+}1$, namely if $f^{(k)} \equiv \text{const}$.

As we are forced into the Hilbert space setting with $q=2$ but need a functional which is $\mathrm{C}^{2,\mathrm{Lip}}$ we conclude that only quadratic terms may appear:

$$\alpha(x,\nabla Q) = \frac{1}{2}\langle A_Q(x)\nabla Q, \nabla Q\rangle \quad \text{with } a_0\mathbf{1} \leq A_Q(x) \leq a_1\mathbf{1} \text{ a.e. on } \Omega, \tag{5.1}$$

where $a_1 \geq a_0 > 0$. The same problem occurs in the Helmholtz free energy W, which must be quadratic in the variables $(\boldsymbol{\varepsilon}, D)$ as the corresponding function space is $\mathrm{L}^2(\Omega;\mathbb{R}^{d\times d}_{\mathrm{sym}}) \times \mathrm{L}^2_{\mathrm{div}}(\mathbb{R}^d)$. Thus, we conclude that assumption (C2) can be satisfied only if W has the quadratic form given in (2.8).

However, we obtain further restrictions concerning the dependence on Q. Note that $\mathrm{H}^1(\Omega;\mathbb{R}^{d_Q})$ embeds continuously into $\mathrm{C}^0(\overline{\Omega};\mathbb{R}^{d_Q})$ for $d=1$, into any $\mathrm{L}^q(\Omega;\mathbb{R}^{d_Q})$, $q\geq 1$, for $d=2$ and into $\mathrm{L}^{p_d}(\Omega;\mathbb{R}^{d_Q})$ with $p_d = 2d/(d{-}2)$ for $d \geq 3$. To avoid notational inconveniences for the case $d=2$, we choose p_2 as a very big fixed number (e.g., $p=1000$).

The case $d=1$ is trivial, as the electric displacement D always vanishes because of $D \in \mathrm{L}^2$ and $\operatorname{div} D = 0$. Thus, we consider only the cases $d \geq 2$, where $\mathrm{H}^1(\Omega;\mathbb{R}^{d_Q})$ does not embed into $\mathrm{C}^0(\overline{\Omega};\mathbb{R}^{d_Q})$ but only into $\mathrm{L}^{p_d}(\overline{\Omega};\mathbb{R}^{d_Q})$. Clearly, $\mathcal{E}\in\mathrm{C}^2$ implies that the stress mapping

$$(\varepsilon,D,Q)\mapsto\begin{pmatrix}\sigma\\E\end{pmatrix}=\begin{pmatrix}A(Q)&-B(Q)\\-B^\mathsf{T}(Q)&C(Q)\end{pmatrix}\begin{pmatrix}\varepsilon\\D\end{pmatrix}$$

is a C^1 mapping from $\mathrm{L}^2(\Omega;\mathbb{R}^{d\times d}_{\mathrm{sym}}\times\mathbb{R}^d)\times\mathrm{H}^1(\Omega;\mathbb{R}^{d_Q})$ into $\mathrm{L}^2(\Omega;\mathbb{R}^{d\times d}_{\mathrm{sym}}\times\mathbb{R}^d)$. This implies that no dependence on Q is allowed in the whole tensor $\left(\begin{smallmatrix}A&-B\\-B^\mathsf{T}&C\end{smallmatrix}\right)$.

Thus, we now restrict the form of W as follows:

$$W(x,\varepsilon,D,Q)=\frac{1}{2}\langle\mathbb{A}(x)\begin{pmatrix}\varepsilon-\varepsilon_{\mathrm{rem}}(x,Q)\\D-P_{\mathrm{rem}}(x,Q)\end{pmatrix},\begin{pmatrix}\varepsilon-\varepsilon_{\mathrm{rem}}(x,Q)\\D-P_{\mathrm{rem}}(x,Q)\end{pmatrix}\rangle+W_{\mathrm{hard}}(x,P_{\mathrm{rem}}),\tag{5.2}$$

where $\mathbb{A}(x)=\left(\begin{smallmatrix}A(x)&-B(x)\\-B^\mathsf{T}(x)&C(x)\end{smallmatrix}\right)$ is assumed to be bounded and uniformly positive definite on $\mathbb{R}^{d\times d}_{\mathrm{sym}}\times\mathbb{R}^d$.

The conditions on the function W_{hard} follow as indicated on the functional $\mathcal{I}$ above, by replacing f through W_{hard}:

$$W_{\mathrm{hard}}\in\mathrm{L}^\infty(\Omega;\mathrm{C}^3(\mathbb{R}^{d_Q})\text{ and }\exists\,C>0\ \forall\,x,Q:|\mathrm{D}^3_QW(x,Q)|\le C(1+|Q|)^{p_d-3}.\tag{5.3}$$

The restriction for the functions $\varepsilon_{\mathrm{rem}}$ and P_{rem} are more severe, as the mapping $Q\mapsto(\varepsilon_{\mathrm{rem}}(Q),P_{\mathrm{rem}}(Q))$ must map smoothly from $\mathrm{L}^{q_d}(\Omega;\mathbb{R}^{d_Q})$ into L^2. We impose

$$\begin{aligned}&(\varepsilon_{\mathrm{rem}},P_{\mathrm{rem}})\in\mathrm{L}^\infty(\Omega;\mathrm{C}^3(\mathbb{R}^{d_Q};\mathbb{R}^{d\times d}_{\mathrm{sym}}\times\mathbb{R}^d)),\quad p_d\ge 6\text{ and}\\&\exists\,C>0\ \forall x,Q:\ |\mathrm{D}^3_Q\varepsilon_{\mathrm{rem}}(x,Q)|,|\mathrm{D}^3_QP_{\mathrm{rem}}(x,Q)|\le C(1+|Q|)^{(p_d-6)/2}.\end{aligned}\tag{5.4}$$

Note that the restriction $p_d=2d/(d-2)\ge 6$ leads to the restriction $d\le 3$.

The above discussion provides the following result.

Proposition 5.2 *If $\ell\in\mathrm{C}^{2,\mathrm{Lip}}([0,T];\mathrm{H}^1_{\Gamma_{\mathrm{Dir}}}(\Omega;\mathbb{R}^d))^*\times\mathrm{L}^2_{\mathrm{div}}(\mathbb{R}^d)^*)$ and if W and α satisfy* (5.1)–(5.4) *and* (B4) *with $q=2$, then $\mathcal{E}$ satisfies* (C2).

The final condition to be added is a uniform convexity on the sum of W and α:

$$\exists\,c_0>0\ \forall x,\varepsilon,D,Q:\ \mathrm{D}^2_{\varepsilon,D,Q}W(x,\varepsilon,D,Q)\ge c_0\mathbf{1}.\tag{5.5}$$

Note that this condition is stronger than (B5) where convexity in Q was not needed.

Together with the convexity of α from (5.1) we immediately find the desired condition (C3). Thus, we conclude with the second main result, which is now a direct application of Theorem 5.1.

Theorem 5.3 *Assume $d\in\{2,3\}$ and $\ell\in\mathrm{C}^2([0,T];\mathrm{H}^1_{\Gamma_{\mathrm{Dir}}}(\Omega;\mathbb{R}^d))^*\times\mathrm{L}^2_{\mathrm{div}}(\mathbb{R}^d)^*)$. Moreover, let the conditions* (B0)–(B4) *with $q=2$ and the conditions* (5.1)–(5.5) *be satisfied. Then, the energetic formulation* (S) & (E) *has for each stable initial datum $y_0=(u_0,D_0,Q_0)$ a unique solution $y=(u,D,Q):[0,T]\to\mathcal{Y}_2=\mathrm{H}^1_{\Gamma_{\mathrm{Dir}}}(\Omega;\mathbb{R}^d)\times\mathrm{L}^2_{\mathrm{div}}(\mathbb{R}^d)\times\mathrm{H}^1(\Omega;\mathbb{R}^{d_Q})$.*

Moreover, other conclusions of Theorem 5.1 hold as well.

We finally show that there are constitutive laws which satisfy all these assumptions. As in Section 2 we let

$$P_{\mathrm{rem}} = Q, \quad \varepsilon_{\mathrm{rem}}(Q) = c_0 \,\mathrm{dev}(Q\otimes Q) \quad \text{and } W_{\mathrm{hard}}(Q) = \frac{w_1}{2}|Q|^2 + \frac{w_2}{q}|Q|^q, \text{ with } q \in [4,6],$$

and choose a fixed positive definite tensor $\mathbb{A} = \left(\begin{smallmatrix} A & -B \\ -B^{\mathsf{T}} & C \end{smallmatrix}\right)$ in (2.8). The only condition to be checked is the uniform convexity of W. For this we use the explicit form of the second derivative

$$\begin{aligned} &\mathrm{D}^2 W(\varepsilon, D, Q)[(\widehat{\varepsilon}, \widehat{D}, \widehat{Q}), (\widehat{\varepsilon}, \widehat{D}, \widehat{Q})] \\ &= \langle \mathbb{A}\left(\begin{smallmatrix} \widehat{\varepsilon} - M_Q \widehat{Q} \\ \widehat{D} - \widehat{Q} \end{smallmatrix}\right), \left(\begin{smallmatrix} \widehat{\varepsilon} - M_Q \widehat{Q} \\ \widehat{D} - \widehat{Q} \end{smallmatrix}\right)\rangle + 2\langle \mathbb{A}\left(\begin{smallmatrix} \varepsilon - \varepsilon_{\mathrm{rem}}(Q) \\ D - Q \end{smallmatrix}\right), \left(\begin{smallmatrix} -c_0 \,\mathrm{dev}(\widehat{Q}\otimes\widehat{Q}) \\ 0 \end{smallmatrix}\right)\rangle \\ &\quad + w_1 |\widehat{Q}|^2 + w_2 |Q|^{q-4}\big(|Q|^2|\widehat{Q}|^2 + (q-2)(Q\cdot\widehat{Q})^2\big), \end{aligned}$$

where $M_Q \widehat{Q} = c_0 \,\mathrm{dev}(Q\otimes\widehat{Q} + \widehat{Q}\otimes Q)$. Because of the linear terms in ε and D, it is easy to see that uniform positive definiteness can only be achieved for $c_0 = 0$. But then making w_1 and w_2 sufficiently large gives the desired definiteness.

As a general rule, the functions $\varepsilon_{\mathrm{rem}}(Q)$ and $P_{\mathrm{rem}}(Q)$ have to be linear and all nonlinearity has to be moved into W_{hard}.

As a conclusion we may say that it is possible to prove existence results for slight modifications of the engineering models. However, for the presently developed uniqueness theory the conditions are very restrictive and seem to contradict most useful models.

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