Universität Stuttgart

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Contents

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Abstract

Ferroelectric materials are characterized by interaction-effects of mechanical and electrical fields due to different polarisation directions of the unit cells. The relations between polarisation and electric field and mechanical strain and electric field respectively can be described by hysteresis curves. Some models, which describe the ferroelectric material behaviour, e.g. [4], [10], rely on concepts close to elastoplasticity. We use these ideas and derive variational evolution inequalities analogously to elastoplastic models discussed in [2]. Based on these inequalities we formulate equivalent mathematical problems and get some existence results. The formulation of variational evolution inequalities is a good starting point for numerical methods similar to elastoplasticity.

Keywords: Ferroelectric hysteresis, Variational inequality, Principle of maximum dissipation

AMS Subject Classification:

1 Introduction

Piezoelectric materials are widely used in electromechanical sensors and actuators, e.g. in accustic devices as microphones, in ultrasonic transducers for medical imaging, in fuel injectors of diesel engines or in high-precision positioners. In particular, piezoceramics are very important for actuator applications, since they show short response times. Moreover, considerable forces can be induced by small electric fields due to the strong inverse piezoelectric effect. Barium titanate ($BaTiO_3$) and lead zirconate titanate (PZT) are the most prominent materials in this class; $BaTiO_3$ is mainly interesting for scientific research, PZT is commonly used for technical applications.

Piezoceramics belong to the class of ferroelectric materials. Hysteresis phenomena occur due to the fact that the polarisation in the unit cells can be influenced by an external electric field. For small fields this effect does not occur and the theory for linear piezoelectricity leads to good simulation results. For larger fields this is not true any more and because this cannot be neglected for a permanently growing range of applications, it becomes more and more important to study these phenomena.

The increasing economic relevance induced a lot of research activities in the last years. There are different approaches to model ferroelectric material behaviour. In microscopic models the switching behaviour of the polarization directions for polycrystals is investigated, see e.g. [3], [7]. The major drawback of these models is the computational effort required for the simulation of macroscopic devices. Another approach are thermodynamically consistent macroscopic models. There, a phenomenological description is favoured where hysteresis curves characterize the relations between polarisation and electric field and mechanical strain and electric field respectively. In [4] and [10], two similar models of this type are presented, which are based on concepts developed in the late 1980s. One can compare these models with the theory for elasto-plastic hysteresis phenomena since the basic ideas are very similar. Besides coupled field equations for the mechanical and electric fields evolution equations for internal variables occur. This mathematical structure resembles models in viscoplasticity, see [1].

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In this paper we follow ideas of elasto-plasticity, see [2], and formulate a class of ferroelectric models as variational inequality. The model of [10] is included. We use the principle of maximum dissipation for the mechanical and electric thermodynamic forces. Adding the resulting inequality to the weakly formulated field equations we derive variational inequalities for mechanical displacement and electric potential fields as well as for the remanent strain and polarisation fields. The resulting variational inequalities model the ferroelectric hysteresis as an evolution process and are suitable for numerical computations. We discuss the existence of solutions in appropriate function spaces for linear and nonlinear models which are given by different choices of the enthalpy function. In general, the problem is equivalent to a doubly nonlinear one. Problems of this type are investigated in [8], [11] and especially for the ferroelectric model in [5].

The paper is organised as follows: Section 2 explains shortly the physical background for piezo- and ferroelectricity and remind the reader of the linear model for piezoelectricity. Especially, we focus on the material structure of piezoceramics and discuss the hysteresis curves for the polarisation and the strain. Then, we present the model which was suggested in [10] and discuss in particular the special choice of the electric enthalpy functional. In section 3, our variational formulation is mathematically derived in detail. The problem is stated as variational inequality in appropriate function spaces. Section 4 treats the existence of solutions for our problem. We first consider the general case, which leads to a doubly nonlinear problem, before we turn to a simplified case where the electric enthalpy is a quadratic form.

2 A model for ferroelectric hysteresis

In this section, we derive a model for ferroelectric hysteresis phenomena, which is based on ideas that are used in elasto-plasticity. For the elasto-plastic theory, we refer to [2], the ferroelectric model was presented in [10], a similar one in [4]. But before we start to discuss the details, we will first have a look on the physical background, especially on the microstructure of ferroelectric materials. We refer to [4] where this is discussed more detailed.

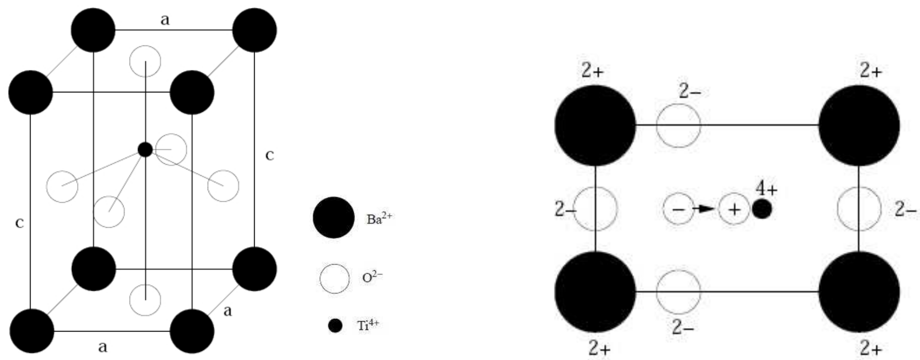
2.1 Physical background and coupled field equations

Ferroelectricity is, as well as piezoelectricity, an electromechanical coupling effect. The reason for the interaction between mechanical and electric fields lies in the microstructure of the material. Ferroelectric materials have a crystalline microstructure, where unit cells are positioned in a periodic lattice. Each unit cell consists of positively and negatively charged ions. Although the total electric charge of each unit cell is zero, the centers of positive and negative charges need not to be at the same place. The position of these centers with respect to each other is very important for the electromechanical properties of the material. If they can be shifted against each other by an external load, the material is called *polarisable*. A displacement of the centers of charges builds an electric dipole and if such a dipole exists without any external load, the unit cell posesses a *spontaneous polarisation*, see figure 1(b). This is the case for ferroelectric materials as for example barium titanate below the Curie temperature, see figure 1(a).

The asymmetry caused by the shift of the charges can be described by a *polar axis*, e.g. the z-axis in figure 1(a). A rotation by 180° with a rotation axis perpendicular to the polar axis leads to another configuration as the initial situation. If there exists such a polar axis in a polarisable material, an external mechanical load in the direction of the polar axis displaces the ions against each other and induces an electric field. This is the (direct) piezoelectric effect which was discovered by Pierre and Jacques Curie in 1880. The inverse effect also exists: an external electric field parallel to the polar axis causes a deformation of the unit cells: compression in one and dilatation in the opposite direction. Both, the direct and the inverse piezoelectric effect have many technical applications, especially as sensors and actuators.

The piezoelectric effect can be described by a well known linear model which was suggested by Woldemar Voigt in 1910, see [12]: As mechanical quantities, we consider the dispacement field u, the linearised strain tensor

$$\varepsilon = \frac{1}{2}\left(\nabla u + (\nabla u)^T\right),$$



(a) The unit cell of barium titanate below the Curie temperature

(b) Spontaneous polarisation of a unit cell

Figure 1: The structure of ferroelectric materials

and the Cauchy stress tensor σ. The electric quantities are the electric potential φ, the quasi-static electric field E given by

$$E = -\nabla\varphi,$$

and the dielectric displacement D. The piezoelectric effect is described by the force balance

$$-\operatorname{div}\sigma = f, \tag{2.1}$$

where f is a given external load, and by

$$\operatorname{div} D = 0, \tag{2.2}$$

which is one of Maxwell's equations. In general, the density of the free electric charges occurs on the right hand sight of equation (2.2), but here, we assume that the material is an ideal dielectric and thus, all electric charges are bound in the lattice. The model is completed by linear constitutive relations:

$$\sigma = \mathbf{c}\varepsilon - \mathbf{e}^\top E, \tag{2.3}$$

$$D = \mathbf{e}\varepsilon + \epsilon E. \tag{2.4}$$

$\mathbf{c}$ is the elastic tensor, ϵ the dielectric tensor and $\mathbf{e}$ the piezoelectric coupling tensor.

For many applications, this linear model turned out to be a very good description of the piezoelectric effect. But for piezoceramics as barium titanate and lead zirconate titanate ferroelectric hysteresis phenomena play an important role for technical applications and these effects are not covered by the linear model.

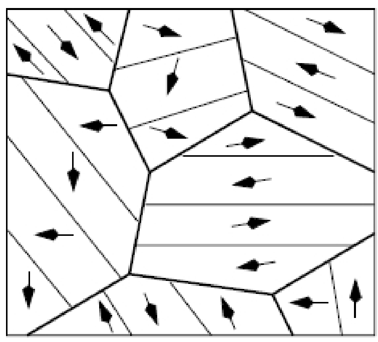


Figure 2: Domain structure in ferroelectric materials ([4], S.225)

In order to understand what happens with these materials we have to look again at the microstructure, but on a larger scale as before. Ferroelectrics are polycrystalline materials, that means that several unit cells

together build a *domain*, see figure 2. Inside one domain, the dipoles of the single unit cells point in the same direction. For completeness, it should be mentioned that several domains build a so-called *grain*, but this is not important at the moment. It is characteristic for ferroelectrics that the direction of the dipoles of the domains can be shifted by an external load. This process is partly irreversible and that is why hysteresis phenomena occur.
For technical applications which use the piezoelectric properties of a material, it is crucial that there exisists a macroscopic polar axis. In general, this it not the case for piezoceramics, since the orientations of the domains are randomly distributed, but a polar axis can be created by shifting the domains by an external field. As we can see, the dipoles of the unit cells play a very important role here and thus, we have to integrate that fact into the model. First, we define the dipole moment: Consider two electric charges $+q$ and $-q$ and the displacement vector $\overrightarrow{d}$, pointing from $-q$ to $+q$. Then, the dipole moment p is defined by

$$p = q\,\overrightarrow{d}\,.$$

The model in [4] and [10] is a macroscopic model and thus, the dipole moment is not a usefull quantity here, since we have one in every unit cell. Therefore, we assume the existence of a density function for the dipoles, the *polarisation* P, such that for every $\omega \subset \mathbb{R}^3$ the total dipole moment in ω is given by

$$p = \int_\omega P(x)\;dx.$$

As mentioned before, the orientation of the dipoles in the domains can be shifted by a sufficiently large external load, e.g. by an electric field. The polarisation follows a hysteresis curve, see figure 3. Here, the

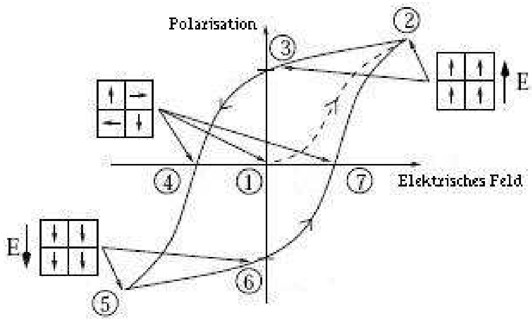


Figure 3: Hysteresis curve of the polarisation ([4], S.236)

electric field points in x_3-direction. Figure 3 shows the components E_3 and P_3 and means:

- Initial configuration (①): The orientations of the dipoles in the domains are randomly distributed such that there is no macroscopic dipole moment.
- If $|E|$ exceeds a critical value, the domains begin to switch until the polarisation in all domains points almost in the same direction as the external field and a saturation is reached (②). This process is partly irreversible.
- After turning off the external electric field, the *remanent polarisation* remains (③). This state is important for technical applications, since there is a macroscopic dipole moment in absence of an external field. For small loads, the behaviour of the material can be described by the linear model for the piezoelectric effect.
- Application of a sufficiently large electric field in the opposite direction causes the polarisation to vanish at (④) until it reaches a saturation again at (⑤).
- When turnig off the electric field, we can see that the remanent polarisation remains again, but in the other direction (⑥).

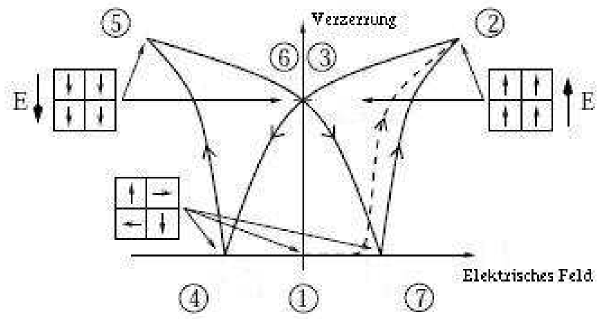


Figure 4: Butterfly hysteresis curve of the strain ([4], S.237)

Associated with the switching of the polarisation is a mechanical deformation. That is why the strain also follows a hysteresis loop during this process. Figure 4 shows the components ε_{33} of the strain tensor and E_3 of the electric field and can be interpreted as follows:

- The reference configuration (①): The displacement field and the strain vanish.
- As before, the domains begin to switch when $|E|$ reaches a critical value. The material expands until a saturation is reached, i.e. the polarisation in all domains points almost in the same direction as the external field (②). Again this process is partly irreversible.
- A remanent strain remains, if the electric field is turned off (③).
- After applying a sufficently large electric field in the opposite direction, the strain vanishes first (④) until it reaches a saturation again (⑤). In contrast to the polarisation the saturation of the strain is independent of the direction of the external field.
- The remanent strain remains again after turnig off E (⑥).

2.2 The model

The basic idea for the model is that both the strain ε and the polarisation P can be split additively into elastic parts ε^e, P^e and remanent parts ε^r, P^r:

$$\varepsilon = \varepsilon^e + \varepsilon^r,$$
$$P = P^e + P^r.$$

This leads to an additive splitting of D:

$$D = \epsilon_0 E + P = \underbrace{\epsilon_0 E + P^e}_{=:D^e} + P^r.$$

The remanent variables ε^r and P^r can be interpreted as inner variables. In order to derive evolution equations for ε^r and P^r, we consider the electric enthalpy H as a thermodynamic potential. As unkown variables we consider the mechanical displacement u and the electric potential φ, as it is often done in the linear piezoelectric model, and ε^r and P^r. Thus, H is assumed to be dependent of these unkowns, i.e.

$$H = H(\varepsilon, \varepsilon^r, E, P^r).$$

Due to the irreversibility of the processes, some energy gets lost (*dissipation*). We consider the second law of thermodynamics which leads here to the so-called *dissipation inequality*:

$$\mathcal{D} = \sigma : \dot{\varepsilon} - D \cdot \dot{E} - \dot{H} \geq 0. \tag{2.5}$$

A formal calculation of the time derivative $\dot{H}$ in (2.5) yields

$$\mathcal{D} = (\sigma - \frac{\partial H}{\partial \varepsilon}) : \dot{\varepsilon} - (D + \frac{\partial H}{\partial E}) \cdot \dot{E} - \frac{\partial H}{\partial \varepsilon^r} : \dot{\varepsilon}^r - \frac{\partial H}{\partial P^r} \cdot \dot{P}^r \geq 0. \tag{2.6}$$

Note that '$\cdot$' denotes the usual scalar product of vectors in $\mathbb{R}^n$, and ':' stands for the scalar product of matrices in $\mathbb{R}^{n \times n}$:

$$a \cdot b = \sum_{i=1}^{n} a_i b_i, \quad A : B = \sum_{i,j=1}^{n} a_{ij} b_{ij}.$$

Inequality (2.6) has to be satisfied for all possible processes, especially for reversible ones where $\varepsilon^r = 0$ and $P^r = 0$. But for these processes, the inversion is also allowed and thus the following constitutive relations hold true:

$$\sigma = \frac{\partial H}{\partial \varepsilon}, \tag{2.7}$$

$$D = -\frac{\partial H}{\partial E}. \tag{2.8}$$

As a condition for the electric enthalpy we assume that the elastic parts ε^e and D^e satisfy the linear constitutive equations (2.3) and (2.4), i.e.

$$\sigma = \mathbf{c}(\varepsilon - \varepsilon^r) - \mathbf{e}^T E, \tag{2.9}$$

$$D - P^r = \mathbf{e}(\varepsilon - \varepsilon^r) + \epsilon E. \tag{2.10}$$

Due to (2.6), (2.7) and (2.8) we get the reduced dissipation inequality

$$\mathcal{D} = \tilde{\sigma} : \dot{\varepsilon}^r + \tilde{E} \cdot \dot{P}^r \geq 0, \tag{2.11}$$

where

$$\tilde{\sigma} := -\frac{\partial H}{\partial \varepsilon^r}, \tag{2.12}$$

$$\tilde{E} := -\frac{\partial H}{\partial P^r} \tag{2.13}$$

denote the *thermodynamic forces*. We use $\tilde{\sigma}$ and $\tilde{E}$ to formulate a criterion to decide wether a process is irreversible or not. Again we orient ourselves by the elasto-plastic theory and define a yield function and a yield surface:

Definition 1 (Yield function und yield surface)**.** *Let $S \subset S^{3\times3} \times \mathbb{R}^3$ be a convex and closed set and $0 \in \mathrm{int}(S)$. We call the boundary ∂S* yield surface. *Furthermore, we assume that S can be described by a function $\phi : S^{3\times3} \times \mathbb{R}^3 \to \mathbb{R}$, the* yield function, *such that*

- $\mathrm{int}(S) = \{(\tilde{\sigma}, \tilde{E}) \in S^{3\times3} \times \mathbb{R}^3 : \phi(\tilde{\sigma}, \tilde{E}) < 0\}$,
- $\partial S = \{(\tilde{\sigma}, \tilde{E}) \in S^{3\times3} \times \mathbb{R}^3 : \phi(\tilde{\sigma}, \tilde{E}) = 0\}$.

The physical interpretation is the following:

- $\phi(\tilde{\sigma}, \tilde{E}) < 0$: The material behaviour is reversible.
- $\phi(\tilde{\sigma}, \tilde{E}) = 0$: The process is (partly) irreversible.
- $\phi(\tilde{\sigma}, \tilde{E}) > 0$: These states are not allowed.

It should be mentioned that the previous definition of the yield surface is given for fixed $x \in \Omega$ and $t \in [0, T]$. In particular, yield surface and yield function can vary in x and t.

We return to the reduced dissipation inequality (2.11). The expression on the left hand sight can interpreted as the rate of energy that gets lost during the process. In order to describe this in detail, we apply a well known principle, the *principle of maximum dissipation*, which reads as follows:
For fixed $\dot{\varepsilon}^r$ and $\dot{P}^r$, the thermodynamic forces are given in such a way that the expression

$$\tilde{\sigma} : \dot{\varepsilon}^r + \tilde{E} \cdot \dot{P}^r$$

of the right hand sight of (2.11) gets maximal, i.e.

$$\mathcal{D}(\dot{\varepsilon}^r, \dot{P}^r) = \tilde{\sigma}(\dot{\varepsilon}^r, \dot{P}^r) : \dot{\varepsilon}^r + \tilde{E}(\dot{\varepsilon}^r, \dot{P}^r) \cdot \dot{P}^r = \max_{(\tilde{\varsigma}, \tilde{\mathcal{E}}) \in S} \{\tilde{\varsigma} : \dot{\varepsilon}^r + \tilde{\mathcal{E}} \cdot \dot{P}^r\}. \tag{2.14}$$

Since the set S is defined pointwise for $x \in \Omega$, this principle has also to be understood pointwise. If S is bounded and thus compact, there exists a state $(\tilde{\sigma}, \tilde{E})$ which realise the maximum of the dissipation. We will later suppose, that the sets $S(x)$ are even uniformly bounded in Ω. In this case, there exist functions $\tilde{\sigma}(x), \tilde{E}(x) \in L^2(\Omega)$ such that the maximum above is realised for every $x \in \Omega$.
With the help of the principle of maximum dissipation it is possible to derive evolution equations:

Theorem 1. *Assume the principle of maximum dissipation (2.14) to hold. Furthermore, suppose that the set $S \subset S^{3\times 3} \times \mathbb{R}^3$ has a smooth boundary. Then the associated flow rules hold true:*

$$\dot{\varepsilon}^r = \tilde{\lambda} \frac{\partial \phi}{\partial \tilde{\sigma}} = \lambda \mathbf{n}, \tag{2.15}$$

$$\dot{P}^r = \tilde{\lambda} \frac{\partial \phi}{\partial \tilde{E}} = \lambda \mathbf{m}, \tag{2.16}$$

where $\lambda = \lambda(\tilde{\sigma}, \tilde{E})$ is a nonnegative factor and $(\mathbf{n}, \mathbf{m})$ an outer normal vector on ∂S.

Proof. (see e.g. [10])
We define the Lagrangian functional on S

$$\mathcal{L}(\tilde{\sigma}, \tilde{E}, \tilde{\lambda}) = -\mathcal{D}(\tilde{\sigma}, \tilde{E}) + \tilde{\lambda}\phi(\tilde{\sigma}, \tilde{E}) = -\tilde{\sigma} : \dot{\varepsilon}^r - \tilde{E} \cdot \dot{P}^r + \tilde{\lambda}\phi(\tilde{\sigma}, \tilde{E}),$$

where $\tilde{\lambda} \in \mathbb{R}$ is a nonnegative Lagrange multiplier. The method of Lagrange multipliers with the constraint $\phi(\tilde{\sigma}, \tilde{E}) \leq 0$ leads to the conditions

$$\frac{\partial \mathcal{L}}{\partial \tilde{\sigma}} = -\dot{\varepsilon}^r + \tilde{\lambda} \frac{\partial \phi}{\partial \tilde{\sigma}} = 0,$$
$$\frac{\partial \mathcal{L}}{\partial \tilde{E}} = -\dot{P}^r + \tilde{\lambda} \frac{\partial \phi}{\partial \tilde{E}} = 0,$$

and

$$\tilde{\lambda}\phi(\tilde{\sigma}, \tilde{E}) = 0.$$

Since ∂S is described by the equation $\phi(\tilde{\sigma}, \tilde{E}) = 0$ with a smooth function ϕ and since the gradient is perpendicular to level sets and points in the direction of the steepest slope, equations (2.15) and (2.16) hold true with a rescaled factor $\lambda(\tilde{\sigma}, \tilde{E})$. ☐

The conditions

- $\lambda \geq 0$,
- $\phi(\tilde{\sigma}, \tilde{E}) \leq 0$,
- $\lambda\phi(\tilde{\sigma}, \tilde{E}) = 0$,

from above are called *Karush-Kuhn-Tucker conditions*.

We summarise the model: We have the balance equations

$$-\operatorname{div}\sigma = f, \tag{2.17}$$

$$\operatorname{div} D = 0, \tag{2.18}$$

the evolution equations

$$\dot{\varepsilon}^r = \tilde{\lambda}\frac{\partial\phi}{\partial\tilde{\sigma}}, \tag{2.19}$$

$$\dot{P}^r = \tilde{\lambda}\frac{\partial\phi}{\partial\tilde{E}}, \tag{2.20}$$

the constitutive relations

$$\sigma = \frac{\partial H}{\partial\varepsilon} = \mathbf{c}(\varepsilon - \varepsilon^r) - \mathbf{e}^T E, \tag{2.21}$$

$$D = -\frac{\partial H}{\partial E} = \mathbf{e}(\varepsilon - \varepsilon^r) + \epsilon E + P^r, \tag{2.22}$$

and the relations

$$\tilde{\sigma} = -\frac{\partial H}{\partial\varepsilon^r}, \tag{2.23}$$

$$\tilde{E} = -\frac{\partial H}{\partial P^r}, \tag{2.24}$$

$$\varepsilon = \varepsilon^e + \varepsilon^r, \tag{2.25}$$

$$P = P^e + P^r. \tag{2.26}$$

2.3 A special choice for the electric enthalpy H and the yield function ϕ

As explained above, the electric enthalpy should satisfy the constitutive equations (2.7), (2.8), (2.9) and (2.10). In the simpliest case H is a quadratic form. In [10], Schröder/Romanowski choose the following form:

$$\begin{aligned} H =& H(\varepsilon, \varepsilon^r, E, P^r) \\ =& \frac{1}{2}\mathbf{c}(\varepsilon - \varepsilon^r) : (\varepsilon - \varepsilon^r) - \frac{1}{2}\epsilon E \cdot E - E \cdot \mathbf{e}(P^r)(\varepsilon - \varepsilon^r) - E \cdot P^r + f(P^r). \end{aligned} \tag{2.27}$$

Schröder/Romanowski suggest for the hardening term f that

$$f(P^r) = (P^r \cdot \mathbf{a}) \operatorname{Artanh}\left(\frac{P^r \cdot \mathbf{a}}{P_s}\right) + \frac{P_s}{2}\ln\left(1 - \left(\frac{P^r \cdot \mathbf{a}}{P_s}\right)^2\right).$$

Here, $P_s \in \mathbb{R}$ is a saturation for $|P^r|$ and $\mathbf{a} \in \mathbb{R}^3$ is the direction of the polar axis with $|a| = 1$. Note that f depends only on P^r and not on ε^r. The derivative

$$\frac{\partial f(P^r)}{\partial P^r} = \operatorname{Artanh}\left(\frac{P^r \cdot \mathbf{a}}{P_s}\right)\mathbf{a}$$

models the dependence between the effective electric field and the polarisation due to

$$\tilde{E} = -\frac{\partial H}{\partial P^r} = \frac{\partial}{\partial P^r}\left[E \cdot \mathbf{e}(P^r)(\varepsilon - \varepsilon^r)\right] + E - \frac{\partial f(P^r)}{\partial P^r}$$

which is equivalent to

$$\frac{\partial f(P^r)}{\partial P^r} = \frac{\partial}{\partial P^r}\left[E \cdot \mathbf{e}(P^r)(\varepsilon - \varepsilon^r)\right] + E - \tilde{E},$$

in agreement with figure 3.

Remark 1. *It should be mentioned here that the piezoelectric tensor* $\mathbf{e}$ *can depend on* P^r.

The yield function in [10] has the form (compare a von-Mises yield function in elasto-plasticity)

$$\phi(\tilde{\sigma}, \tilde{E}) = \tilde{E} \cdot \tilde{E} - E_c^2,$$

i.e. ϕ does not depend on $\tilde{\sigma}$. E_c is the coercive field strength, which is the critical value for $|E|$ at which the polarisation in the domains begin to switch.

But there are some problems with these choices for H and ϕ: There is no hardening term in H which models the butterfly hysteresis curve for the strain, see figure 4. Furthermore, the evolution equation (2.15) now reads

$$\dot{\varepsilon}^r = \tilde{\lambda} \frac{\partial \phi}{\partial \tilde{\sigma}} = 0,$$

due to the fact that ϕ is independent of $\tilde{\sigma}$. That implies, that the strain does not show any irreversible behaviour and that is not true. Following the ideas of [6] and [10], one can solve this problem by replacing the evolution equation (2.15) by a constitutive law of the form

$$\varepsilon^r = \frac{\varepsilon^r_{\mathbf{a}}}{P_s^2} \operatorname{dev}(P^r \otimes P^r),$$

where $\varepsilon^r_{\mathbf{a}}$ is the saturation for ε^r in the polarisation direction $\mathbf{a}$. Again, this modeling is not unquestioned and we refer to [6] for a more detailed discussion. However, some simulation results can be found in [10].

In the next section we will present a variational formulation for the model. We will not use the evolution equations (2.15) and (2.16), but the principle of maximum dissipation which led to these equations. Furthermore, we will allow a more general form for the electric enthalpy H which also contains hardening terms depending on ε^r.

3 Variational formulation

In this section we present a variational formulation to our model for ferroelectric hysteresis relying on ideas which model elasto-plastic behaviour of materials as variational inequalities, compare [2].

3.1 Function spaces

Let $\Omega \times [0, T] \subset \mathbb{R}^3 \times \mathbb{R}^+$ be a domain where Ω has a Lipschitz-boundary $\partial\Omega$. On this domain we consider the momentum balance equations

$$-\operatorname{div} \sigma(x, t) = f(x, t), \tag{3.1}$$

$$\operatorname{div} D(x, t) = 0, \tag{3.2}$$

where the vector function f is a given volume force density. The boundary $\partial\Omega$ is splitted into Dirichlet and Neumann parts, corresponding to mechanical $(i = 1)$ or electric loads $(i = 2)$:

$$\partial\Omega = \gamma_{N_i} \cup \gamma_{D_i},$$

where $\gamma_{N_i} \cap \gamma_{D_i} = \emptyset$ and $|\gamma_{D_i}| > 0$ for $i = 1, 2$. As unknown variables we have the mechanical displacement field u and the electric potential φ, which satisfy the boundary conditions

$$\begin{aligned} u(\cdot, t) &= 0 \quad \text{on } \gamma_{D_1}, \\ \sigma\mathbf{n} &= g_1 \quad \text{on } \gamma_{N_1}, \\ \varphi(\cdot, t) &= 0 \quad \text{on } \gamma_{D_2}, \\ D \cdot \mathbf{n} &= g_2 \quad \text{on } \gamma_{N_2}, \end{aligned}$$

where g_1 and g_2 are given. With respect to the space variable x we suppose for a fixed t

$$u(\cdot,t) \in V_1 := \{[H^1(\Omega)]^3 : u|_{\gamma_{D_1}} = 0\},$$
$$\varphi(\cdot,t) \in V_2 := \{H^1(\Omega) : \varphi|_{\gamma_{D_2}} = 0\}.$$

As before, the strain tensor and the electric field are defined by

$$\varepsilon(u) = \frac{1}{2}(\nabla u + (\nabla u)^T),$$
$$E(\varphi) = -\nabla\varphi,$$

and we assume an additive splitting of ε and P

$$\varepsilon = \varepsilon^e + \varepsilon^r,$$
$$P = P^e + P^r,$$

where the remanent quantities ε^r and P^r as well as their time derivatives $\dot{\varepsilon}^r$ and $\dot{P}^r$ belong for fixed t to the following spaces:

$$\varepsilon^r(\cdot,t), \dot{\varepsilon}^r(\cdot,t) \in Q_1 := [L^2(\Omega)]^{3\times 3},$$
$$P^r(\cdot,t), \dot{P}^r(\cdot,t) \in Q_2 := [L^2(\Omega)]^3.$$

In addition, we have the constitutive equations

$$\sigma = \frac{\partial H}{\partial \varepsilon} = \mathbf{c}(\varepsilon - \varepsilon^r) - \mathbf{e}^T E, \tag{3.3}$$
$$D = -\frac{\partial H}{\partial E} = \mathbf{e}(\varepsilon - \varepsilon^r) + \epsilon E + P^r. \tag{3.4}$$

For the components of the material tensors $\mathbf{c}, \mathbf{e}$ and ϵ we suppose that

$$c_{ijkl}, \epsilon_{ij}, e_{ijk} \in L^\infty(\Omega),$$

and that the tensors $\mathbf{c}$ and ϵ are positive definite, i.e. there exist constants $c_0 > 0, \epsilon_0 > 0$ such that

$$\mathbf{c}\varepsilon : \varepsilon \geq c_0|\varepsilon|^2, \qquad \forall \varepsilon \in S^{3\times 3},$$
$$\epsilon E \cdot E \geq \epsilon_0 |E|^2 \qquad \forall E \in \mathbb{R}^3.$$

Note that $\sigma \in Q_1,\ D \in Q_2$. Furthermore, we consider symmetric material tensors $\mathbf{c}$, ϵ and $\mathbf{e}$, that means

$$c_{ijkl} = c_{klij},\ c_{ijkl} = c_{jikl},\ e_{ijk} = e_{jik},\ \epsilon_{ij} = \epsilon_{ji}.$$

We define the space Z by

$$Z = V_1 \times V_2 \times Q_1 \times Q_2.$$

Z is a Hilbert space with the scalar product

$$(w,z)_Z = (u,v)_{V_1} + (\varphi,\vartheta)_{V_2} + (\varepsilon,q)_{Q_1} + (P,T)_{Q_2},$$

for $w = (u,\varphi,\varepsilon,P)$, $z = (v,\vartheta,q,T)$ and with the usual scalar products of the particular spaces on the right hand sight of the equation. Together with the space $H = [L^2(\Omega)]^3 \times L^2(\Omega) \times [L^2(\Omega)]^{3\times 3} \times [L^2(\Omega)]^3$, (Z,H,Z') is a Gelfand's triple. Here, Z' denotes the dual space. Taking the time into account, we assume w to be an element of $H^1([0,T],Z)$. As initial condition we suppose that

$$w(0) = 0.$$

3.2 Derivation of the variational inequality

We derive a variational inequality in appropriate function spaces, adding an inequality based on the principle of maximum dissipation to a weakly formulated boundary value problem.

We remind of the **principle of maximum dissipation** (2.14):
For fixed states $\dot{\varepsilon}^r, \dot{P}^r$ the thermodynamical forces $\tilde{\sigma}(\dot{\varepsilon}^r, \dot{P}^r), \tilde{E}(\dot{\varepsilon}^r, \dot{P}^r)$ are given by

$$\mathcal{D}(\dot{\varepsilon}^r, \dot{P}^r) = \tilde{\sigma}(\dot{\varepsilon}^r, \dot{P}^r) : \dot{\varepsilon}^r + \tilde{E}(\dot{\varepsilon}^r, \dot{P}^r) \cdot \dot{P}^r = \max_{(\tilde{\varsigma}, \tilde{\mathcal{E}}) \in S} \{\tilde{\varsigma} : \dot{\varepsilon}^r + \tilde{\mathcal{E}} \cdot \dot{P}^r\}.$$

For an arbitrary state $(q, T) \in Q_1 \times Q_2$ holds analogously

$$\mathcal{D}(q, T) = \tilde{\sigma}(q, T) : q + \tilde{E}(q, T) \cdot T = \max_{(\tilde{\varsigma}, \tilde{\mathcal{E}}) \in S} \{\tilde{\varsigma} : q + \tilde{\mathcal{E}} \cdot T\}.$$

It follows from the maximum-property that

$$\begin{aligned} \mathcal{D}(q, T) &= \tilde{\sigma}(q, T) : q + \tilde{E}(q, T) \cdot T \\ &= \max_{(\tilde{\varsigma}, \tilde{\mathcal{E}}) \in S} \{\tilde{\varsigma} : q + \tilde{\mathcal{E}} \cdot T\} \geq \tilde{\sigma}(\dot{\varepsilon}^r, \dot{P}^r) : q + \tilde{E}(\dot{\varepsilon}^r, \dot{P}^r) \cdot T. \end{aligned}$$

Adding and subtracting $\mathcal{D}(\dot{\varepsilon}^r, \dot{P}^r)$ we get finally

$$\mathcal{D}(q, T) \geq \mathcal{D}(\dot{\varepsilon}^r, \dot{P}^r) + \tilde{\sigma} : (q - \dot{\varepsilon}^r) + \tilde{E} \cdot (T - \dot{P}^r), \qquad \forall (q, T) \in Q_1 \times Q_2,$$

and after integration over Ω

$$\int_\Omega \mathcal{D}(q, T)\, dx \geq \int_\Omega \mathcal{D}(\dot{\varepsilon}^r, \dot{P}^r)\, dx + \int_\Omega \tilde{\sigma} : (q - \dot{\varepsilon}^r) + \tilde{E} \cdot (T - \dot{P}^r)\, dx. \tag{3.5}$$

Now, we consider a **weak formulation** of the momentum balance equation

$$-\operatorname{div} \sigma = f.$$

Taking the scalar product of this equation with $(v - \dot{u})$, where $v \in V_1$, and integrating over Ω we get

$$\begin{aligned} &\int_\Omega (\mathbf{c}(\varepsilon - \varepsilon^r) - \mathbf{e}^T E) : (\varepsilon(v) - \varepsilon(\dot{u}))\, dx \\ &\qquad = \int_\Omega f \cdot (v - \dot{u})\, dx + \int_{\gamma_{N_1}} g_1 \cdot (v - \dot{u})\, dx. \end{aligned} \tag{3.6}$$

Analogously we multiply the electric balance equation

$$\operatorname{div} D = 0$$

with $(\beta - \dot{\varphi})$, $\beta \in V_2$, and integrate over Ω

$$\int_\Omega (\mathbf{e}(\varepsilon - \varepsilon^r) + \epsilon E + P^r) \cdot (E(\beta) - E(\dot{\varphi}))\, dx = \int_{\gamma_{N_2}} g_2(\beta - \dot{\varphi})\, dx. \tag{3.7}$$

Adding (3.5), (3.6) and (3.7) we get the inequality

$$\begin{aligned} &\int_\Omega (\mathbf{c}(\varepsilon - \varepsilon^r) - \mathbf{e}^T E) : (\varepsilon(v) - \varepsilon(\dot{u}))\, dx \\ &+ \int_\Omega (\mathbf{e}(\varepsilon - \varepsilon^r) + \epsilon E + P^r) \cdot (E(\beta) - E(\dot{\varphi}))\, dx \\ &+ \int_\Omega \frac{\partial H}{\partial \varepsilon^r} : (q - \dot{\varepsilon}^r) + \frac{\partial H}{\partial P^r} \cdot (T - \dot{P}^r)\, dx \\ &+ \int_\Omega \mathcal{D}(q, T) - \mathcal{D}(\dot{\varepsilon}^r, \dot{P}^r)\, dx \\ &\geq \int_\Omega f \cdot (v - \dot{u})\, dx + \int_{\gamma_{N_1}} g_1 \cdot (v - \dot{u})\, da + \int_{\gamma_{N_2}} g_2(\beta - \dot{\varphi})\, da. \end{aligned} \tag{3.8}$$

We define for $w = (u, \varphi, \varepsilon^r, P^r)$ and $z = (v, \beta, q, T)$, and for fixed t,

$$\begin{aligned}
\langle Aw, z\rangle &= \int_\Omega (\mathbf{c}(\varepsilon(u) - \varepsilon^r) - \mathbf{e}^T E(\varphi)) : \varepsilon(v)\, dx \\
&\quad + \int_\Omega (\mathbf{e}(\varepsilon(u) - \varepsilon^r) + \epsilon E(\varphi) + P^r) \cdot E(\beta)\, dx \\
&\quad + \int_\Omega \frac{\partial H}{\partial \varepsilon^r} : q + \frac{\partial H}{\partial P^r} \cdot T\, dx, \qquad (3.9)\\
j(z) &= \int_\Omega \mathcal{D}(q, T)\, dx, \qquad (3.10)\\
\langle l(t), z\rangle &= \int_\Omega f(t) \cdot v\, dx + \int_{\gamma_{N_1}} g_1(t) \cdot v\, da + \int_{\gamma_{N_2}} g_2(t)\beta\, da. \qquad (3.11)
\end{aligned}$$

Let us make some remarks to the properties of the operators A, j and l.

- The operator $A : Z \to Z'$ consists of a linear part and a nonlinear one. The nonlinearity is generated by the enthalpy H.

- The functional $j : Q_1 \times Q_2 \subset Z \to \mathbb{R} \cup \{\pm\infty\}$ is positively homogeneous, that means $j(cz) = cj(z)$ for all $c > 0$. Furthermore, j is convex, that means, for $\lambda \in (0, 1)$ and all $(z_1, z_2) \in Q_1 \times Q_2$ holds

  $$j(\lambda z_1 + (1 - \lambda)z_2) \le \lambda j(z_1) + (1 - \lambda)j(z_2).$$

  This follows immediately from the principle of maximal dissipation, since for $z_i = (q_i, T_i), i = 1, 2,$ holds

  $$\begin{aligned}
  \mathcal{D}(\lambda z_1 + (1 - \lambda)z_2) &= \max_{(\tilde\varsigma,\tilde{\mathcal{E}})\in S} \{\tilde\varsigma : (\lambda q_1 + (1 - \lambda)q_2) + \tilde{\mathcal{E}} \cdot (\lambda T_1 + (1 - \lambda)T_2)\}\\
  &= \Pi_1 : (\lambda q_1 + (1 - \lambda)q_2) + \Pi_2 \cdot (\lambda T_1 + (1 - \lambda)T_2)\\
  &\le \lambda \mathcal{D}(q_1, T_1) + (1 - \lambda)\mathcal{D}(q_2, T_2).
  \end{aligned}$$

  Moreover, the functional j is lower semicontinuous, that means, if $z_n \to z$, then $\liminf_{n\to\infty} j(z_n) \ge j(z)$. Indeed, for $z_n = (q_n, T_n)$ we have

  $$\begin{aligned}
  \mathcal{D}(z_n) &= \max_{(\tilde\varsigma,\tilde{\mathcal{E}})\in S} \{\tilde\varsigma : q_n + \tilde{\mathcal{E}} \cdot T_n\}\\
  &= \Pi_{1,n} : q_n + \Pi_{2,n} \cdot T_n\\
  &\ge \Pi_1 : q_n + \Pi_2 \cdot T_n,
  \end{aligned}$$

  where (Π_1, Π_2) are the states which realize the maximum in $\mathcal{D}(z)$. Going to the limit, we get after integration the lower semicontinuity of j.

- If we assume that the sets $S(x)$ of all allowed states are uniformly bounded, i.e.

  $$S(x) \subset B_R(0_{S^{3\times 3}\times\mathbb{R}^3})$$

  with $R > 0$ independent of x, then j is Lipschitz continuous. We can proof this as follows:
  Let $z_1 = (v_1, \beta_1, q_1, T_1), z_2 = (v_2, \beta_2, q_2, T_2) \in Z$. As mentioned before, there exist functions $(s_1, E_1), (s_2, E_2)$, such that

  $$\begin{aligned}
  \mathcal{D}(s_1(x), E_1(x)) &= s_1(x) : q_1(x) + E_1(x) \cdot T_1(x),\\
  \mathcal{D}(s_2(x), E_2(x)) &= s_2(x) : q_2(x) + E_2(x) \cdot T_2(x),
  \end{aligned}$$

and $(s_i(x), E_i(x)) \in S(x)$, $i = 1, 2$. For fixed $x \in \Omega$, let be without loss of generality $\mathcal{D}(s_1(x), E_1(x)) \geq \mathcal{D}(s_2(x), E_2(x))$. It follows

$$\begin{aligned}
|s_1(x) : q_1(x) + E_1(x) \cdot T_1(x) - s_2(x) : q_2(x) - E_2(x) \cdot T_2(x)| \\
&\leq s_1(x) : q_1(x) + E_1(x) \cdot T_1(x) - s_1(x) : q_2(x) - E_1(x) \cdot T_2(x) \\
&\leq |(s_1(x), E_1(x))||(q_1(x), T_1(x)) - (q_2(x), T_2(x))| \\
&\leq R|(q_1(x), T_1(x)) - (q_2(x), T_2(x))|.
\end{aligned}$$

Here, $|\cdot|$ denotes the Euclidian norm on $S^{3\times 3} \times \mathbb{R}^3$. Since Ω is bounded, we have

$$\|(s_i, E_i)\|_{L^1(\Omega)} \leq C\|(s_i, E_i)\|_{L^2(\Omega)}.$$

It follows that

$$\begin{aligned}
|j(z_1) - j(z_2)| &\leq \int_\Omega |\mathcal{D}((s_1, E_1)(x)) - \mathcal{D}((s_2, E_2)(x))| \, dx \\
&\leq R \int_\Omega |(s_1(x), E_1(x)) - (s_2(x), E_2(x))| \, dx \\
&\leq RC \cdot \|(s_1, E_1) - (s_2, E_2)\|_{L^2(\Omega)} \\
&= RC \cdot \|z_1 - z_2\|_Z
\end{aligned}$$

and thus the Lipschitz-continuity.

- If we assume that for fixed time t the mechanical volume force density $f \in V_1'$ and that the mechanical and electric Neumann boundary data $g_1 \in [H^{-\frac{1}{2}}(\gamma_{N_1})]^3$ and $g_2 \in H^{-\frac{1}{2}}(\gamma_{N_2})$, then the mapping $l : V_1 \times V_2 \subset Z \to I\!R$ is linear and continuous and represents the exterior loads. Note, that we have to understand the integrals as dual pairing; usual integrals occur, if f, g_1, g_2 are L_2-functions on Ω or on γ_{N_i}, $i = 1, 2$, respectively.

Now, we formulate the **Variational inequality problem**:

Find $w = (u, \varphi, \varepsilon^r, P^r) \in H^1([0,T], Z)$ *with* $w(0) = 0$*, such that for all* $z \in Z$ *and almost all* $t \in [0,T]$ *holds:*

$$\langle Aw(t), z - \dot{w}(t)\rangle + j(z) - j(\dot{w}(t)) \geq \langle l(t), z - \dot{w}(t)\rangle. \tag{3.12}$$

3.3 Remarks to the choice of the enthalpy function

To ensure that the variational inequality is well-defined we assume

$$\frac{\partial H}{\partial P^r} \in [L^2(\Omega)]^3, \tag{3.13}$$

$$\frac{\partial H}{\partial \varepsilon^r} \in [L^2(\Omega)]^{3\times 3}. \tag{3.14}$$

If we consider an electric enthalpy of the form

$$H = H(\varepsilon, \varepsilon^r, E, P^r) = \frac{1}{2}\mathbf{c}(\varepsilon - \varepsilon^r) : (\varepsilon - \varepsilon^r) - \frac{1}{2}\epsilon E \cdot E - E \cdot P^r - E \cdot \mathbf{e}(P^r)(\varepsilon - \varepsilon^r) + f(P^r) + g(\varepsilon^r), \tag{3.15}$$

these conditions are equivalent to

$$\frac{\partial f}{\partial P^r} \in [L^2(\Omega)]^3, \tag{3.16}$$

$$\frac{\partial g}{\partial \varepsilon^r} \in [L^2(\Omega)]^{3\times 3}. \tag{3.17}$$

In this case the reversible parts $\sigma = \frac{\partial H}{\partial \varepsilon}$ and $D = -\frac{\partial H}{\partial E} + P^r$ satisfy the linear constitutive equations (2.9) and (2.10). The electric enthalpy considered by Schröder/Romanowski in [10] satisfies the condition (3.13), if

$$P^r \cdot \mathbf{a} \leq P_s - \delta, \text{a.e. in } \Omega \text{ for a fixed } \delta > 0.$$

The hysteresis curve of the polarisation, see figure 3, holds approximately in this case. In order to guarantee that the butterfly hysteresis curve of the strain, see figure 4, holds, too, we have to specify the quantities $\mathbf{e}(P^r), g(\varepsilon^r)$ and the yield function ϕ. As mentioned before, another possibility is to consider additional constitutive equations, e.g. as in [6].

4 Solvability of the variational inequality

In general, the variational inequality (3.12) is nonlinear in w and $\dot{w}$ and belongs to the class of doubly nonlinear problems. We will give some equivalent formulations, which facilitate the reading of the corresponding literature. For this we bring the definition of a subdifferential to mind:

Definition 2. *Let V be a real Banach space and $F : V \to [-\infty, \infty]$ a functional on V. An element $u^* \in V'$ is called subgradient of F at $u \in V$, if $F(u) \not\equiv \pm\infty$ and*

$$F(v) \geq F(u) + \langle u^*, v - u \rangle \quad \forall v \in V.$$

The set of all subgradients at u is called subdifferential and is denoted by $\partial F(u)$. If no subgradient exists at u, then we put $\partial F(u) = \emptyset$.

4.1 Equivalent formulations

Lemma 1. *Let be $A : Z \to Z'$, $j : Z \to I\!R$ and $l \to I\!R$ the operators defined by (3.9), (3.10) and (3.11). The following problems are equivalent*

1. *Find an element $w \in H^1([0,T], Z)$ with $w(0) = 0$, such that for almost all $t \in (0,T)$ holds:*

$$\langle Aw(t), z - \dot{w}(t) \rangle + j(z) - j(\dot{w}(t)) \geq \langle l(t), z - \dot{w}(t) \rangle, \quad \forall z \in Z.$$

2. *Find an element $w \in H^1([0,T], Z)$ with $w(0) = 0$ and an element $w^* \in H^1([0,T], Z')$, such that for almost all $t \in (0,T)$ holds:*

$$\langle Aw(t), z \rangle + \langle w^*(t), z \rangle = \langle l(t), z \rangle, \qquad \forall z \in Z,$$
$$w^*(t) \in \partial j(\dot{w}(t))$$

   or shorter

$$l(t) \in Aw(t) + \partial j(\dot{w}(t)).$$

3. *Find an element $w \in H^1([0,T], Z)$ with $w(0) = 0$ and an element $w^* \in H^1([0,T], Z')$, such that for almost all $t \in (0,T)$ holds:*

$$\langle Aw(t), z \rangle + \langle w^*(t), z \rangle = \langle l(t), z \rangle, \qquad \forall z \in Z,$$
$$\langle w^*(t), z \rangle \leq j(z), \qquad \forall z \in Z,$$
$$\langle w^*(t), \dot{w}(t) \rangle = j(\dot{w}(t)).$$

Proof. **First step** $1. \Rightarrow 2.$
We consider a solution $w \in H^1([0,T], Z)$ of problem 1., that means

$$\langle Aw(t), z - \dot{w}(t) \rangle + j(z) - j(\dot{w}(t)) \geq \langle l(t), z - \dot{w}(t) \rangle, \quad \forall z \in Z. \tag{4.1}$$

We define $w^*(t) \in H^1([0,T], Z')$ through

$$\langle w^*(t), z \rangle = -\langle Aw(t), z \rangle + \langle l(t), z \rangle.$$

From inequality (4.1) follows

$$\langle w^*(t), z - \dot{w}(t)\rangle \leq j(z) - j(\dot{w}(t)), \quad \forall z \in Z,$$

and therefore we have

$$w^*(t) \in \partial j(\dot{w}(t)).$$

The elements w und w^* satisfy problem 2.
Second step $2. \Rightarrow 3.$
Assume that $w \in H^1([0,T], Z)$ and $w^* \in H^1([0,T], Z')$ solve problem 2. Since $w^*(t) \in \partial j(\dot{w}(t))$ it holds

$$j(z) \geq j(\dot{w}(t)) + \langle w^*(t), z - \dot{w}(t)\rangle, \qquad \forall z \in Z. \tag{4.2}$$

We show by contradiction that

$$\langle w^*(t), \dot{w}(t)\rangle = j(\dot{w}(t)).$$

First, we assume

$$\langle w^*(t), \dot{w}(t)\rangle > j(\dot{w}(t)).$$

Then, it follows for almost all fixed $t \in [0,T]$ and for $z = 2\dot{w}(t)$ from (4.2) due to the positive homogenity of j

$$0 > j(\dot{w}(t)) - \langle w^*(t), \dot{w}(t)\rangle \geq 0,$$

what cannot be.
Now, we assume

$$\langle w^*(t), \dot{w}(t)\rangle < j(\dot{w}(t)).$$

Then we get for $z = 0$ from (4.2) that

$$0 \geq j(\dot{w}(t)) - \langle w^*(t), \dot{w}(t)\rangle > 0,$$

a contradiction, too. Here we have used that $j(0) = 0$. Therefore, we have

$$\langle w^*(t), \dot{w}(t)\rangle = j(\dot{w}(t)),$$

and consequently due to (4.2)

$$\langle w^*(t), z\rangle \leq j(z), \qquad \forall z \in Z.$$

Second step $3. \Rightarrow 1.$
Inserting $z - \dot{w}$ into the first equation of problem 3 instead of z and using both other conditions of problem 3 we get immediately that w is a solution of problem 1. ☐

4.2 Remarks to the solvability of the doubly nonlinear problem

As we have seen the variational inequality (3.12) can be equivalently rewritten as follows:
For $l \in H^1([0,T]), Z')$ find an element $w \in H^1([0,T], Z)$ with $w(0) = 0$, such that for almost all $t \in [0,T]$:

$$l(t) \in Aw(t) + \partial j(\dot{w}(t)), \tag{4.3}$$

where ∂j is the subdifferential of the functional j. Since (4.3) is nonlinear in w and $\dot{w}$, this is called a *doubly nonlinear problem*. In [8] one can find an existence theorem for a solution of the initial value problem

$$f(t) \in Aw(t) + \partial\Psi(\dot{w}(t)), \quad w(0) = w_0. \tag{4.4}$$

There the Rothe method is used, which we will explain shortly:
Let us consider an equidistant partition of $[0,T]$, namely, $0 = t_0 < t_1 < t_2 < \cdots < t_N = T$, $t_n - t_{n-1} = k$, $k = T/N$, $n = 1, \ldots N$. We set $f_n = \frac{1}{k}\int_{t_{n-1}}^{t_n} f(t)\,dt$. This discretisation in time leads to a semi-discrete recursive formulated problem for the unknowns w_n:

$$f_n \in Aw_n + \partial\Psi(\frac{w_n - w_{n-1}}{k}), \quad w(0) = w_0. \tag{4.5}$$

Rothe solutions w^k are defined by piecewise affine interpolation

$$w^k(t) = w_{n-1} + \delta w_n \cdot (t - t_{n-1}) \quad \text{for} \quad t_{n-1} < t \leq t_n, \tag{4.6}$$

with

$$\delta w_n = \frac{\triangle w_n}{k} = \frac{w_n - w_{n-1}}{k}. \tag{4.7}$$

The following theorem is proved in [8], pp. 322-326,

Theorem 2. *Let $V \subset H \subset V'$ be a Gelfand's tripel. Assume that the operator $A : V \to V'$ can be splitted as $A = A_1 + A_2$, where $A_1 : V \to V'$ is linear and selfadjoint, $\langle A_1 v, v\rangle \geq |v|_V^2$, and $A_2 : H \to H$ is Lipschitz continuous. Suppose that $\Psi : H \to I\!R \cup \{+\infty\}$ is uniformly convex on H in the sense*

$$\langle \xi_1 - \xi_2, v_1 - v_2\rangle \geq c\|v_1 - v_2\|^2, \quad \forall \xi_1 \in \partial\Psi(v_1), \forall \xi_2 \in \partial\Psi(v_2), \tag{4.8}$$

and that Ψ is lower semicontinuous on V, proper and $0 \in \partial\Psi(0)$. Furthermore, suppose that V is compactly imbedded in H. Moreover, let $f \in H^1([0,T], H)$ and $w_0 \in V$ be a steady state to $f(0)$ in the sense that $A(w_0) = f(0)$.

- *Then the Rothe functions w^k exist and belong to $C([0,T], V)$ and we have the estimates*

$$\|w^k\|_{W^{1,\infty}([0,T],V)} \leq C.$$

- *There is a subsequence such that $w^k \to w$ weakly* in $W^{1,\infty}([0,T], V)$ and every such w is a solution from $H^1([0,T], V)$ to the problem (4.4).*

Now, we discuss, whether the assumptions of theorem 2 are satisfied for the operators occuring in our problem (4.3).

The function spaces:

At the end of subsection 3.1 we have introduced the space

$$Z = V_1 \times V_2 \times Q_1 \times Q_2,$$

where

$$\begin{aligned} V_1 &:= \{[H^1(\Omega)]^3 : u|_{\gamma_{D_1}} = 0\}, \\ V_2 &:= \{H^1(\Omega) : \varphi|_{\gamma_{D_2}} = 0\}, \\ Q_1 &:= [L^2(\Omega)]^{3\times 3}, \\ Q_2 &:= [L^2(\Omega)]^3. \end{aligned}$$

Furthermore, it was

$$H = [L^2(\Omega)]^3 \times L^2(\Omega) \times [L^2(\Omega)]^{3\times 3} \times [L^2(\Omega)]^3.$$

Note that (Z, H, Z') is a Gelfand-triple. Now, we identify Z with V and see that the condition, V is compactly imbedded in H, is not satisfied. This can be repaired, if some additional regularity of the solutions can be guaranteed, see Lemma 4.

The operators:

The operator A was defined by (3.9) as a mapping from $Z \to Z'$: A is decomposed into a linear part and a nonlinear one, where the nonlinearity is generated by the electric enthalpy H. The linear part contains the selfadjoint operator

$$\langle A_1 w, z\rangle = \int_\Omega (\mathbf{c}\varepsilon(u) : \varepsilon(v)\; dx + \int_\Omega \epsilon E(\varphi) \cdot E(\beta)\; dx,$$

which is V-elliptic in Z, if the measures of the mechanical and electric boundary parts γ_{D_1} and γ_{D_2} are positive. The remainding part $A_2 = A - A_1 : H \to H$ has to be Lipschitz continuous what can be realized by a suitable choice of the electric enthalpy H.

The functional Ψ is identified with the dissipation functional j. As we have already discussed in subsection

3.2 the functional j is lower semicontinuous on V, proper and $0 \in \partial\Psi(0)$. Furthermore we have seen the convexity of j, but we could not show the uniform convexity (4.8).
In [5] existence and uniqueness results for a class of nonlinear hyteresis models for ferroelectric materials are derived using the theory of viscoplasticity developed in [1]. But, in general it is an open problem, for which class of electric enthalpies we will get the existence of a solution $w \in H^1([0,T],Z)$ for our variational inequality. We concentrate on the linear case in what follows.

4.3 Solvabilty of the linear problem

We consider a simple form of the hardening term $f(\varepsilon^r, P^r)$ in the electric enthalpy in (2.27), setting

$$\begin{aligned} H =& H(\varepsilon,\varepsilon^r,E,P^r) \\ =& \frac{1}{2}\mathbf{c}(\varepsilon-\varepsilon^r):(\varepsilon-\varepsilon^r) - \frac{1}{2}\epsilon E\cdot E - E\cdot \mathbf{e}(P^r)(\varepsilon-\varepsilon^r) - E\cdot P^r \\ &+ \tfrac{1}{2}H_1\varepsilon^r:\varepsilon^r + \tfrac{1}{2}H_2P^r\cdot P^r, \end{aligned} \tag{4.9}$$

where H_1 and H_2 are positive definite tensors. Then the corresponding operator A generates a bilinear form on $Z\times Z$:

$$\begin{aligned} \langle Aw,z\rangle = a(w,z) =& \int_\Omega \mathbf{c}(\varepsilon(u)-\varepsilon^r):(\varepsilon(v)-q) + \epsilon E(\varphi)\cdot E(\beta)\,dx \\ &+ \int_\Omega \mathbf{e}^\top E(\beta):(\varepsilon(u)-\varepsilon^r) - \mathbf{e}^\top E(\varphi):(\varepsilon(v)-q)\,dx \\ &+ \int_\Omega E(\beta)\cdot P^r - E(\varphi)\cdot T\,dx + \int_\Omega H_1\varepsilon^r:q + H_2P^r\cdot T\,dx. \end{aligned}$$

Note that the bilinear form $a(\cdot,\cdot)$ is not symmetric, that means $a(w,z)\neq a(z,w)$.
Analogously to (3.12) the simplified variational inequality reads:

For $l\in H^1([0,T],Z')$ find $w=(u,\varphi,\varepsilon^r,P^r)\in H^1([0,T],Z)$ with $w(0)=0$ such that for all $z\in Z$ and almost all $t\in[0,T]$ the following inequality is satisfied:

$$a(w(t),z-\dot{w}(t)) + j(z) - j(\dot{w}(t)) \geq \langle l(t), z-\dot{w}(t)\rangle. \tag{4.10}$$

A similar variational problem for elasto-plasticity is analysed in [2], chapter 7, with the help of the Rothe method. In [2] the elasto-plastic bilinear form is symmetric in contrast to our problem where a nonsymmetric bilinear form occurs. This makes the proof more complicated, but we can follow the steps of the proof of Theorem 7.3 in [2] in principle.

As before we start with an equidistant partition of $[0,T]$, $0=t_0<t_1<t_2<\cdots<t_N=T$, $t_n-t_{n-1}=k$, $k=T/N$ and $l_n=l(t_n)$, which is well defined due to the embedding $H^1([0,T],Z')\hookrightarrow C([0,T],Z')$. We consider the semi-discrete problem:

Find $\{w_n\}_{n=0,\dots,N}\subset Z$ with $w_0=0$ such that

$$a(w_n, z-\triangle w_n) + j(z) - j(\triangle w_n) \geq \langle l_n, z-\triangle w_n\rangle, \qquad \forall z\in Z. \tag{4.11}$$

Here, $\triangle w_n := w_n - w_{n-1}$ and $n=1,\dots,N$.
The existence of the set $\{w_n\}_{n=0,\dots,N}\subset Z$ and appropriate estimates can be proved analogously to [2], Lemma 7.1, p.160, by the following Lemma:

Lemma 2. *For every set $\{l_n\}_{n=0,\dots,N}\subset Z'$ with $l_0=0$ there exists a uniquely determined set of solutions of (4.11) $\{w_n\}_{n=0,\dots,N}\subset Z$ with $w_0=0$ such that*

1. *$j(\triangle w_n)<\infty$.*
2. *There exists a constant c independent of k with*

$$\|\triangle w_n\|_Z \leq c\|\triangle l_n\|_{Z'}. \tag{4.12}$$

Furthermore it holds, compare [2], Lemma 7.2, p.161:

Lemma 3. *Assume that $l \in H^1([0,T],Z')$ with $l(0) = 0$. Then the solution $\{w_n\}_{n=0,\dots,N}$ defined in Lemma 2 satisfies*

$$\max_{1\le n\le N} \|w_n\|_Z \le c\|\dot{l}\|_{L^1([0,T],Z')}, \tag{4.13}$$

$$\sum_{n=1}^{N} k\|\delta w_n\|_Z^2 \le \tilde{c}\|\dot{l}\|^2_{L^2([0,T],Z')}, \tag{4.14}$$

with $\delta w_n := \triangle w_n/k \quad \text{for } n = 1,\dots,N.$

Now, we can construct a Rothe sequence, defining on $[0,T]$ the piecewise linear function

$$w^k(t) = w_{n-1} + \delta w_n \cdot (t - t_{n-1}), \quad \text{for} \quad t_{n-1} \le t \le t_n, 1 \le n \le N. \tag{4.15}$$

It follows directly from (4.13) and (4.14)

$$\|w^k\|_{L^2([0,T],Z)} \le c_0\|w^k\|_{L^\infty([0,T],Z)} \le c, \tag{4.16}$$

$$\|\dot{w}^k\|_{L^2([0,T],Z)} \le c, \tag{4.17}$$

with a constant c , independent on k. Due to the fact that bounded sets in reflexive Banach spaces (here $H^1([0,T],Z)$) are weakly sequentially compact we get immediately the following corollary:

Corollary 1. *Assume that $l \in H^1([0,T],Z')$ with $l(0) = 0$. Then every sequence of time steps $(k_m)_{m\in\mathbb{N}} \subset \mathbb{R}$ with $k_m \to 0$ for $m \to \infty$ has a subsequence , also denoted by $(k_m)_{m\in\mathbb{N}}$, such that*

$$w^{k_m} \rightharpoonup w \quad \text{in } H^1([0,T],Z). \tag{4.18}$$

All considerations are valid for both symmetric and nonsymmetric bilinear forms until now. In order to show that the limit function w from (4.18) is indeed a solution of the variational inequality (4.10) we need the symmetry of the bilinear form as in [2] or an additional condition if the bilinear form is not symmetric. Moreover, the dissipation functional should satisfy some conditions.

Theorem 3. *Let $l \in H^1([0,T],Z')$ with $l(0) = 0$. Suppose the sets of admissible stresses $S = S(x)$ for points $x \in \Omega$ are uniformly bounded. Then, the dissipation functional in (4.10) $j : Z \to \mathbb{R} \cup \{\pm\infty\}$ is non-negative, positively homogeneous, convex, proper und Lipschitz-continuous. The bilinear form a is Z-elliptic, if $|\gamma_{D_i}| > 0, i = 1,2$. Furthermore, if we assume that*

$$\liminf_{m\to\infty} \int_0^T a(w^{k_m}(t), \dot{w}^{k_m}(t))\, dt \ge \int_0^T a(w(t), \dot{w}(t))\, dt \tag{4.19}$$

holds true, then the weak limit is a solution of problem (4.10).

Proof. The properties of the dissipation functional are proved in subsection 3.2.
Now, we adapt the proof of Theorem 7.3, p.166 in [2] to our case.

First step Introduction of step functions in Z.

We start with the discrete variational inequality (4.11).

$$a(w_n, \tilde{z} - \triangle w_n) + j(\tilde{z}) - j(\triangle w_n) \ge \langle l_n, \tilde{z} - \triangle w_n\rangle, \qquad \forall \tilde{z} \in Z. \tag{4.20}$$

We divide (4.20) by k and due to the positive homogeneity of j we get

$$a(w_n, z - \delta w_n) + j(z) - j(\delta w_n) \ge \langle l_n, z - \delta w_n\rangle, \qquad \forall z = \frac{\tilde{z}}{k} \in Z. \tag{4.21}$$

Now, we indroduce the following set of step functions $z(t)$: For any sequence $\{z_n\}_{n=1\ldots,N} \subset Z$ and $z_{N+1=0}$ we put

$$\begin{aligned} z(t) &= z_n \quad \text{for} \quad t_{n-1} \leq t < t_n;\ n = 1, \ldots, N-1, \\ z(t) &= z_N \quad \text{for} \quad t_{N-1} \leq t \leq t_N. \end{aligned} \tag{4.22}$$

Analogously we define the step function

$$\begin{aligned} z(t) &= \frac{z_n + z_{n+1}}{2} \quad \text{for} \quad t_{n-1} \leq t < t_n;\ n = 1, \ldots, N-1, \\ z(t) &= \frac{z_N}{2} \quad \text{for} \quad t_{N-1} \leq t \leq t_N. \end{aligned} \tag{4.23}$$

We insert (4.23) into (4.21), multiply by k and sum over n from 1 to N. Thus we get:

$$\begin{aligned} \sum_{n=1}^{N} ka(w_n, \frac{(z_n + z_{n+1})}{2} - \delta w_n) + \sum_{n=1}^{N} kj(\frac{(z_n + z_{n+1})}{2}) - \sum_{n=1}^{N} kj(\delta w_n) \\ \geq \sum_{n=1}^{N} k\langle l_n, \frac{(z_n + z_{n+1})}{2} - \delta w_n\rangle. \end{aligned} \tag{4.24}$$

Second step Estimates for the step functions.

We estimate the different terms in (4.24) by the Rothe interpolant $w^k(t)$, given by (4.15).
Integrating piecewise and merging the summands adequately we have for z, introduced by (4.22),

$$\sum_{n=1}^{N} ka(w_n, \frac{(z_n + z_{n+1})}{2}) = \int_0^T a(w^k(t), z(t))\ dt. \tag{4.25}$$

Moreover, exploiting the Z-ellipticity of the bilinear form $a(w, z)$, that means $a(z, z) \geq C\|z\|_Z^2$, we get

$$\sum_{n=1}^{N} ka(w_n, \delta w_n) \geq \int_0^T a(w^k(t), \dot{w}^k(t))\ dt. \tag{4.26}$$

Due to the convexity of j the second sum can be estimated

$$\sum_{n=1}^{N} kj(\frac{(z_n + z_{n+1})}{2}) \leq \sum_{n=1}^{N} \frac{k}{2}(j(z_n) + j(z_{n+1})) = \int_0^T j(z(t))\ dt - \frac{k}{2} j(z_1). \tag{4.27}$$

The third sum can be rewritten as

$$\sum_{n=1}^{N} kj(\delta w_n) = \int_0^T j(\dot{w}^k(t))\ dt. \tag{4.28}$$

It remains the estimate of the right hand side of (4.24). Analogously to (4.25) we get

$$\sum_{n=1}^{N} k\langle l_n, \frac{(z_n + z_{n+1})}{2}\rangle = \int_0^T \langle l^k(t), z(t)\rangle\ dt, \tag{4.29}$$

where $l^k(t)$ is the piecewise linear interpolant of $\{l_n\}_{n=0,\ldots,N}$. Using the estimate (4.12) we have

$$\sum_{n=1}^{N} k\langle l_n, \delta w_n\rangle = \int_0^T \langle l^k(t), \dot{w}^k(t)\rangle\ dt + \frac{1}{2}\sum_{n=1}^{N} \langle \triangle l_n, \triangle w_n\rangle \leq \int_0^T \langle l^k(t), \dot{w}^k(t)\rangle\ dt + \frac{c}{2}\|\triangle l_n\|_{Z'}^2.$$

Now, due to Schwarz' inequality it holds

$$\|\triangle l_n\|_{Z'}^2 \leq (\int_{t_{n-1}}^{t_n} 1 \cdot \|\dot{l}(\tau)\|_{Z'}\, d\tau)^2 \leq k \int_{t_{n-1}}^{t_n} \|\dot{l}(\tau)\|_{Z'}^2\, d\tau,$$

what leads finally to

$$\sum_{n=1}^{N} k\langle l_n, \delta w_n\rangle \leq \int_0^T \langle l^k(t), \dot{w}^k(t)\rangle\, dt + k \int_0^T \|\dot{l}(\tau)\|_{Z'}^2\, d\tau. \tag{4.30}$$

Using the estimates (4.25),..., (4.30) inequality (4.24) implies

$$\int_0^T a(w^k(t), z(t) - \dot{w}^k(t)) + j(z(t)) - j(\dot{w}^k(t)) - \langle l^k(t), z(t) - \dot{w}^k(t)\rangle\, dt$$
$$-\frac{1}{2}kj(z_1) + \frac{1}{2}ck \int_0^T \|\dot{l}(t)\|_{Z'}^2\, dt \geq 0. \tag{4.31}$$

Third step The limit inequality for $w^{k_m} \rightharpoonup w$.

Corollary 1 guarantees that a subsequence $\{w^{k_m}\}$ of $\{w^k\}$ exists which weakly converges in $H^1([0,T], Z)$ to the limit function w. We insert such a subsequence into (4.31)

$$\int_0^T a(w^{k_m}(t), z(t) - \dot{w}^{k_m}(t)) + j(z(t)) - j(\dot{w}^{k_m}(t)) - \langle l^{k_m}(t), z(t) - \dot{w}^{k_m}(t)\rangle\, dt$$
$$-\frac{1}{2}k_m j(z_1) + \frac{1}{2}ck_m \int_0^T \|\dot{l}(t)\|_{Z'}^2\, dt \geq 0. \tag{4.32}$$

It follows

$$\limsup_{m\to\infty} \left\{ \int_0^T a(w^{k_m}(t), z(t) - \dot{w}^{k_m}(t)) + j(z(t)) - j(\dot{w}^{k_m}(t)) - \langle l^{k_m}(t), z(t) - \dot{w}^{k_m}(t)\rangle\, dt \right\} \geq 0.$$

Due to the assumption (4.19), the weakly lower semicontinuity of j and the construction from l^{k_m} as Rothe sequence we get for any step function corresponding to the step sizes $k_m, m = 1, 2, \ldots$ the limit inequality

$$\int_0^T a(w(t), z(t) - \dot{w}(t)) + j(z(t)) - j(\dot{w}(t)) - \langle l(t), z(t) - \dot{w}(t)\rangle\, dt \geq 0. \tag{4.33}$$

Fourth step Estimation of the integrand of (4.33).

Consider an arbitrary $z \in L^2([0,T], Z)$. We can approximate z by its piecewise averaging step functions z^{k_m}, corresponding to the time step-size k_m. Using the Lipschitz-continuity of j, it follows that (4.33) holds for any $z \in L^2([0,T], Z)$. For $t_0 \in (0,T)$ and $h > 0$ with $t_0 + h < T$ we define for an arbitrary $z \in Z$

$$z(t) = \begin{cases} z & t_0 \leq t \leq t_0 + h, \\ \dot{w}(t) & \text{otherwise.} \end{cases}$$

We can see easily that $z(t) \in L^2([0,T], Z)$. Inserting in (4.33) implies that

$$\frac{1}{h} \int_{t_0}^{t_0+h} a(w(t), z - \dot{w}(t)) + j(z) - j(\dot{w}(t)) - \langle l(t), z - \dot{w}(t)\rangle\, dt \geq 0.$$

Applying the Lebesgue theorem, see [2], Thm. 5.21, p. 123, we get for $h \to 0$

$$a(w(t), z - \dot{w}(t)) + j(z) - j(\dot{w}(t)) - \langle l(t), z - \dot{w}(t)\rangle \geq 0,$$

which proves that w is a solution of the original problem (4.10). □

Remark 2. *If the bilinear form a is symmetric, estimate (4.19) is shown in [2] as follows:*

$$\liminf_{m\to\infty} \int_0^T a(w^{k_m}(t), \dot{w}^{k_m}(t))\, dt = \liminf_{m\to\infty} \int_0^T \tfrac{1}{2}\tfrac{d}{dt} a(w^{k_m}(t), w^{k_m}(t))\, dt$$
$$= \liminf_{m\to\infty} \tfrac{1}{2} a(w^{k_m}(T), w^{k_m}(T)) \geq \tfrac{1}{2} a(w(T), w(T)) = \int_0^T a(w(t), \dot{w}(t))\, dt.$$

Moreover, the uniqueness of the solution can be proved for symmetric bilinear forms, see [2], p.165.

If the solutions of the semi-discrete problem are sufficiently smooth with respect to x and if furthermore $\partial\Omega$, l and $\dot{l}$ are sufficiently smooth, then (4.19) is satisfied. We can proof the following Lemma:

Lemma 4. *Define for* $0 < \delta < 1$

$$Z^\delta := [H^{1+\delta}(\Omega)]^3 \times H^{1+\delta}(\Omega) \times [H^\delta(\Omega)]^{3\times 3}_{sym} \times [H^\delta(\Omega)]^3.$$

Assume that Ω has a smooth boundary. If there exists a constant c independent of k such that for one $0 < \delta < 1$ the estimates

$$\|w^k\|_{L^2([0,T],Z^\delta)} \leq c, \tag{4.34}$$

$$\|\dot{w}^k\|_{L^2([0,T],Z^\delta)} \leq c \tag{4.35}$$

hold true, estimate (4.19) is satisfied.

Proof. We have the compact imbedding

$$Z^\delta \hookrightarrow\hookrightarrow Z,$$

see e.g. [13], Thm. 7.9, p. 123. Thus, we know that

$$H^1([0,T], Z^\delta) \hookrightarrow\hookrightarrow L^2([0,T], Z),$$

see [9], Lemma 3.74 (Aubin, Lions), p. 121. Analogously to Corollary 1 it follows from (4.34) and (4.35) that there exists a subsequence $(k_m)_{m\in\mathbb{N}}$ of time steps and a function $w \in H^1([0,T], Z^\delta)$ such that

$$w^{k_m} \rightharpoonup w \quad \text{in } H^1([0,T], Z^\delta). \tag{4.36}$$

Due to the compact imbeddings, it follows that

$$w^{k_m} \to w \quad \text{in } L^2([0,T], Z). \tag{4.37}$$

Thus we get

$$\begin{aligned}\int_0^T a(w^{k_m}(t), \dot{w}^{k_m}(t))\, dt = &\int_0^T a(w^{k_m}(t) - w(t), \dot{w}^{k_m}(t))\, dt \\ &+ \int_0^T a(w(t), \dot{w}^{k_m}(t))\, dt\end{aligned} \tag{4.38}$$

and

$$\begin{aligned}\int_0^T a(w^{k_m}(t) - w(t), \dot{w}^{k_m}(t))\, dt &\leq c \int_0^T \|w^{k_m}(t) - w(t)\|_Z \|\dot{w}^{k_m}(t)\|_Z\, dt \\ &\leq c\|w^{k_m} - w\|_{L^2([0,T],Z)} \|\dot{w}^{k_m}\|_{L^2([0,T],Z)}.\end{aligned} \tag{4.39}$$

Then, (4.37), (4.38) and (4.39) imply

$$\lim_{m\to\infty} \int_0^T a(w^{k_m}(t), \dot{w}^{k_m}(t))\, dt = \int_0^T a(w(t), \dot{w}(t))\, dt,$$

and this implies (4.19). □

Remark 3. *The condition that Ω has a smooth boundary can be replaced by suitable cone properties.*

We underline, that in [5] a symmetric piezoelectric operator is considered. There is proved the existence and uniqueness of the linear problem. Whether this is indeed equivalent to our variatonal inequality should be investigated.

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