

Ferroelectric Polarization of bimorph piezoelectric plates - an accurate equivalent single-layer approach

Astrid Pechstein, Alexander Humer, Michael Krommer

Abstract. The aim of the current contribution is the derivation of an equivalent single layer formulation for the evolution of the electric polarization in ferroelectric bimorph plates. Plate or shell models and finite elements for layered piezoelectric devices operated in linear regime are available and prove to be highly accurate. The driving electric field relevant to the evolution of internal polarization, is sensitive to the local stress distribution in the layered medium. Plate or shell formulations, mostly rely on stress resultants such as membrane stress and bending moments. We propose a formulation within a thermodynamically consistent framework based on the Clausius-Duhem inequality. Different variants of reduction from continuum to plate elastic potentials are discussed, and the implications on the driving electric field are analyzed. Numerical examples give evidence of the suitability of a newly proposed variant.

Key words: ferroelectric polarization, Kirchhoff-Love plate, equivalent single layer, ferroelectric bimorph plates

1 INTRODUCTION

When polarizing thin, bimorph ferroelectric plates through the application of high electric fields in two layers independently, the reordering of ferroelectric domains and deformation of single crystals in the electric field leads to out-of-plane deformation of the initially plane structure. The phenomenological modeling of the ferroelectric polarization process using the concept of ferroelectric and piezoelectric strains in a continuum mechanics framework is well understood, see e.g. the extensive article by Kamlah [1], or the works by Miehe and Rosato developing a variational framework [2, 3]. Finite element methods implementing these models using volume elements have been developed simultaneously, see [4] or [3], although at considerable computational cost. Locking effects prevent the usage of flat elements when using classical finite element basis functions. This behavior is remedied in using mixed elements as were developed by Meindlhumer and Pechstein [5, 6], or extend elements from the family of

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smart solid shell elements (e.g. as proposed by [7, 8]) to ferroelectric hysteresis. However, the different layers still have to be resolved by layers of finite elements in such a setup.

Whenever thin structures are considered, a dimensional reduction achieved by a transition from continuum to plate or shell theories is of interest, as then thickness as limiting geometric dimension is avoided in discretizations. Plate models and finite elements for layered piezoelectric devices operated in linear regime have long been available and prove to be highly accurate, see e.g. [9, 10].

Ferroelectric polarization was modeled in a first order shear deformable plate consisting of a single layer [11], where limitations of the approach became apparent in cases where thickness deformation is essential. In a previous contribution [12], we found that as the evolution of ferroelectric polarization in layered plates is concerned, a straightforward reduction of the aforementioned phenomenological material models to a plate theory based on classical deformation measures such as membrane strains and curvature fails.

The present contribution aims at developing an equivalent single-layer plate model, which is capable of predicting the evolution of independent ferroelectric polarization in one or both of the layers, while employing classical Kirchhoff-Love plate theory for the mechanical response. Numerical results show accurate reproduction of the evolution of electric polarization when compared to fully three-dimensional computations at greatly reduced cost.

2 MODELING THE FERROELECTRIC POLARIZATION PROCESS

Let Ω denote the material domain of interest. Considering some material point $\mathcal{P}$, we use its coordinates $\mathbf{X} = X_i \mathbf{e}_i$ with respect to the inertial frame $(\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3)$. Throughout the manuscript, we adopt a notation for tensor analysis as described by Lebedev et al. [13], where the dot denotes the contraction operation, and no symbol is used for the tensor product. Displacement field $\mathbf{u}$ and electric potential φ denote the primary kinematic fields. The material derivative $\nabla = \partial/\partial X_i$ is used to define the deformation gradient $\mathbf{F}$, Green strain tensor $\boldsymbol{\varepsilon}$ and material electric field $\mathbf{E}$ through

$$\mathbf{F} = \mathbf{I} + (\nabla \mathbf{u})^T, \quad \boldsymbol{\varepsilon} = \frac{1}{2}(\mathbf{F}^T \cdot \mathbf{F} - \mathbf{I}), \quad \mathbf{E} = -\nabla \varphi. \quad (1)$$

In macroscopic models of the ferroelectric polarization process, it is common to introduce the *internal polarization* $\mathbf{P}_i$ as an additional independent unknown field.

In the following, we assume all strains to be small. In this case, an additive split of the total strain $\boldsymbol{\varepsilon}$ into an elastic contribution $\boldsymbol{\varepsilon}_e$ and an eigenstrain contribution $\boldsymbol{\varepsilon}^*$ is feasible, such that $\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}_e + \boldsymbol{\varepsilon}^*$. This eigenstrain again consists of two additive contributions: the ferroelectric polarization strain $\boldsymbol{\varepsilon}_f^*$ and the reversible piezoelectric strain $\boldsymbol{\varepsilon}_p^*$.

$$\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}_e + \boldsymbol{\varepsilon}^*, \quad \boldsymbol{\varepsilon}^* = \boldsymbol{\varepsilon}_f^* + \boldsymbol{\varepsilon}_p^*. \quad (2)$$

The ferroelectric polarization strain evolves with the internal polarization, similar to an electrostrictive strain. It is modeled in a volume-preserving manner, where saturation strain ε_{sat} and saturation polarization P_{sat} occur as material constants,

$$\varepsilon_f^* = \frac{\varepsilon_{\text{sat}}}{P_{\text{sat}}^2} \frac{3}{2} (\mathbf{P}_i \mathbf{P}_i - \frac{1}{3} (\mathbf{P}_i \cdot \mathbf{P}_i) \mathbf{I}). \quad (3)$$

The piezoelectric strain is modeled in such a way that it grows linearly with the electric field. In its definition, for non-zero internal polarization we use the polarization direction $e_P = \mathbf{P}_i / |\mathbf{P}_i|$, and the piezoelectric constants d_{33} , d_{31} and d_{15} ,

$$\varepsilon_p^* = \frac{1}{P_{\text{sat}}} (d_{33} (\mathbf{P}_i \cdot \mathbf{E}) e_P e_P + d_{31} (\mathbf{P}_i \cdot \mathbf{E}) (\mathbf{I} - e_P e_P) + d_{15} \text{sym}(\mathbf{E} \cdot (\mathbf{I} - e_P e_P) \cdot \mathbf{P}_i)). \quad (4)$$

To model the material behavior, we use an approach based on thermodynamics. Let $\mathbf{S}$ denote the second Piola-Kirchhoff stress tensor, and let $\mathbf{D}$ be the dielectric displacement vector. For ψ the thermodynamic potential density, the Clausius-Duhem inequality states non-negative dissipation,

$$\mathcal{D} = \mathbf{S} : \dot{\boldsymbol{\varepsilon}} - \mathbf{D} \cdot \dot{\mathbf{E}} - \dot{\psi} \geq 0, \quad (5)$$

see Eringen and Maugin [14]. In the current contribution, two contributions to the potential $\psi = \psi_{\text{me}} + \psi_{\text{el}}$ are considered; the mechanic free energy ψ_{me} depending on the elastic part of the strain $\boldsymbol{\varepsilon}_e$, and the electric potential ψ_{el} which is deduced from the electric Helmholtz free energy through an Legendre transformation,

$$\psi_{\text{me}} = \mu \boldsymbol{\varepsilon}_e : \boldsymbol{\varepsilon}_e + \frac{\lambda}{2} (\boldsymbol{\varepsilon}_e : \mathbf{I})^2, \quad \psi_{\text{el}} = \psi_p(|\mathbf{P}_i|) - \mathbf{P}_i \cdot \mathbf{E} - \frac{\epsilon}{2} \mathbf{E} \cdot \mathbf{E}. \quad (6)$$

Above, the mechanic potential is governed by the Lamé parameters λ and μ describing the isotropic elastic behavior according to a St. Venant-Kirchhoff law. In the electric potential, ϵ denotes the isotropic dielectric permittivity for small electric fields. The polarization potential ψ_p determines the evolution and saturation of the internal polarization $\mathbf{P}_i$, and depends only on its magnitude. In the current contribution, we present its derivative, characteristic parameters are the polarization susceptibility χ_i and, again, the saturation polarization P_{sat} ,

$$\psi_p'(p) = -\frac{P_{\text{sat}}}{2\chi_i} (\log(P_{\text{sat}} - p) - \log(P_{\text{sat}} + p)). \quad (7)$$

For modeling the dissipation, we use a dissipation function ϕ depending on the coercive electric field E_c as well as the rate of internal polarization $\dot{\mathbf{P}}_i$, such that

$$\mathcal{D} = \frac{\partial \phi}{\partial \dot{\mathbf{P}}_i} \cdot \dot{\mathbf{P}}_i, \quad \phi = E_c |\dot{\mathbf{P}}_i|. \quad (8)$$

Note that this definition holds in classical sense only for $\dot{\mathbf{P}}_i \neq \mathbf{0}$; otherwise sub-differentials must be considered instead of differentiation, which leads to a case distinction discussed in the end of this section (14).

For such a choice as (6) and (8), the Clausius-Duhem inequality (5) can be re-written in the form

$$\left(\mathbf{S} - \frac{\partial \psi}{\partial \boldsymbol{\varepsilon}}\right) \cdot \dot{\boldsymbol{\varepsilon}} - \left(\mathbf{D} + \frac{\partial \psi}{\partial \mathbf{E}}\right) \cdot \dot{\mathbf{E}} - \left(\frac{\partial \psi}{\partial \mathbf{P}_i} + \frac{\partial \phi}{\partial \dot{\mathbf{P}}_i}\right) \cdot \dot{\mathbf{P}}_i = 0. \quad (9)$$

This leads to the defining relations for the second Piola-Kirchhoff stress, the dielectric displacement vector and the driving electric field

$$\mathbf{S} = \frac{\partial \psi}{\partial \boldsymbol{\varepsilon}}, \quad \mathbf{D} = -\frac{\partial \psi}{\partial \mathbf{E}}, \quad \hat{\mathbf{E}} = -\frac{\partial \psi}{\partial \mathbf{P}_i}. \quad (10)$$

One can easily verify the explicit relation for the driving electric field, where it is noted that $\lim_{p \rightarrow 0} \psi'_p(p)/p < \infty$ is essential for the equation below to be well defined,

$$\hat{\mathbf{E}} = \mathbf{S} : \frac{\partial \boldsymbol{\varepsilon}^*}{\partial \mathbf{P}_i} - \psi'_p(|\mathbf{P}_i|) \frac{\mathbf{P}_i}{|\mathbf{P}_i|} + \mathbf{E}. \quad (11)$$

The last constitutive relation to be derived from (9) is Biot's equation (see [15] for the original reference, and Rosato and Miehe [3] for the application to ferroelectric media),

$$\hat{\mathbf{E}} = \frac{\partial \phi}{\partial \dot{\mathbf{P}}_i}. \quad (12)$$

As the dissipation function is not differentiable at $\dot{\mathbf{P}}_i = \mathbf{0}$, Biot's equation (12) has to be considered in the sense of sub-differentials, which leads to the classical evolution conditions for the internal polarization,

$$\text{if } |\dot{\mathbf{P}}_i| = 0 : \quad |\hat{\mathbf{E}}| \leq E_c, \quad (13)$$

$$\text{else if } |\dot{\mathbf{P}}_i| \neq 0 : \quad \hat{\mathbf{E}} = E_c \frac{\dot{\mathbf{P}}_i}{|\dot{\mathbf{P}}_i|}. \quad (14)$$

3 AN EQUIVALENT SINGLE-LAYER APPROACH FOR BIMORPH PLATES

We consider the case of a structurally symmetric bimorph plate, with two layers of equal thickness $\frac{t}{2}$ made from ferroelectric material. According to standard notations in plate theories, we assume that the plate mid-surface coincides with the $e_1 e_2$ plane, and e_3 is the thickness direction. Let Γ be the plate's mid-surface, which is considered as the two-dimensional reference domain in the plate formulation. We use $\mathbf{X}_2 = X_1 e_1 + X_2 e_2$ for points in Γ

and the alias $z = X_3$ for the thickness coordinate for the sake of readability. The two layers are defined on the respective domains $\Omega_{(+)} = \{\mathbf{X}_2 + z\mathbf{e}_3 : \mathbf{X}_2 \in \Gamma, z \in (0, \frac{t}{2})\}$ and $\Omega_{(-)} = \{\mathbf{X}_2 + z\mathbf{e}_3 : \mathbf{X}_2 \in \Gamma, z \in (-\frac{t}{2}, 0)\}$, external and center electrodes are located at Γ , $\Gamma_{(+)} = \Gamma + \frac{t}{2}\mathbf{e}_3$ and $\Gamma_{(-)} = \Gamma - \frac{t}{2}\mathbf{e}_3$, respectively. Throughout the following, we use (+) and (−) as an index to indicate that the respective quantity is associated to positions $z > 0$ or $z < 0$; e.g. we denote the voltage prescribed at electrodes by

$$\varphi = V_{(+)} \text{ on } \Gamma_{(+)}, \quad \varphi = V_{(-)} \text{ on } \Gamma_{(-)}, \quad \varphi = 0 \text{ on } \Gamma. \quad (15)$$

Thus, the center electrode is grounded.

Next, a kinematic reduction of the plate deformation according to Kirchhoff-Love assumptions is performed. A projection to the tangential plane is realized in defining $\mathbf{A} = \mathbf{I} - \mathbf{e}_3\mathbf{e}_3$. Introducing membrane strain $\mathbf{e}$ and curvature $\boldsymbol{\kappa}$, the in-plane component of the strain tensor $\boldsymbol{\varepsilon}_2 = \mathbf{A} \cdot \boldsymbol{\varepsilon} \cdot \mathbf{A}$ is approximated through

$$\boldsymbol{\varepsilon}_2 = \mathbf{e} + z\boldsymbol{\kappa}. \quad (16)$$

In each of the two layers, internal polarization $\mathbf{P}_i$ and electric field $\mathbf{E}$ are assumed constant and orientied in thickness direction. We introduce the scalar-valued electric field $E_{(+)}$ and $E_{(-)}$ as well as the according internal polarization $P_{i,(+)}$ and $P_{i,(-)}$ such that

$$\mathbf{E} = E_{(\pm)}\mathbf{e}_3 = \mp \frac{2V_{(\pm)}}{t}\mathbf{e}_3 \quad \text{and} \quad \mathbf{P}_i = P_{i,(\pm)}\mathbf{e}_3 \quad \text{in } \Omega_{(\pm)}. \quad (17)$$

Inserting this assumption into the definition of the eigenstrain component $\boldsymbol{\varepsilon}_2^* = \mathbf{A} \cdot \boldsymbol{\varepsilon}^* \cdot \mathbf{A}$ implies a constant tensor in each layer,

$$\boldsymbol{\varepsilon}_2^* = \boldsymbol{\varepsilon}_{(\pm)}^* \mathbf{A} \quad \text{in } \Omega_{(\pm)}, \quad \text{with} \quad \boldsymbol{\varepsilon}_{(\pm)}^* = -\frac{\varepsilon_{\text{sat}}}{2P_{\text{sat}}^2} P_{i,(\pm)}^2 + d_{31} P_{i,(\pm)} E_{(\pm)}. \quad (18)$$

Thermodynamic potential and dissipation function for the plate formulation are often gained by through-the-thickness integration. For the electric contribution to the potential ψ_{el} and the dissipation function ϕ , one directly obtains surface potentials,

$$\psi_{\text{el},\Gamma} = \int_{-t/2}^{t/2} \psi_{\text{el}} dz = \frac{t}{2} \sum_{* \in \{+, -\}} \left(\psi_p(|P_{i,*}|) - P_{i,*} E_{(*)} - \frac{\epsilon}{2} (E_{(*)})^2 \right), \quad (19)$$

$$\phi_\Gamma = \int_{-t/2}^{t/2} \phi dz = \frac{t}{2} \sum_{* \in \{+, -\}} E_c |\dot{P}_{i,*}|. \quad (20)$$

The kinematic assumptions of Kirchhoff-Love theory do not consider an independent thickness deformation. We use the St. Venant-Kirchhoff elastic energy based on plane stress assumptions, which is defined in terms of the in-plane elastic strain $\boldsymbol{\varepsilon}_{e,2}$

$$\hat{\psi}_{\text{me}} = \frac{E}{2(1+\nu)} \boldsymbol{\varepsilon}_{e,2} : \boldsymbol{\varepsilon}_{e,2} + \frac{E\nu}{2(1-\nu^2)} (\boldsymbol{\varepsilon}_{e,2} : \mathbf{A})^2. \quad (21)$$

Regarding the treatment of eigenstrains in a plate formulation, a common possibility is to reduce the eigenstrain component ε_2^* to inelastic strain measures. Inelastic membrane strain and curvature can be deduced as mean value and first moment of ε_2^* ,

$$\mathbf{e}^* = e^* \mathbf{A}, \quad e^* = \frac{1}{2}(\varepsilon_{(+)}^* + \varepsilon_{(-)}^*), \quad (22)$$

$$\boldsymbol{\kappa}^* = \kappa^* \mathbf{A}, \quad \kappa^* = \frac{3}{2t}(\varepsilon_{(+)}^* - \varepsilon_{(-)}^*). \quad (23)$$

Accordingly, we define elastic membrane strain and curvature

$$\mathbf{e}_e = \mathbf{e} - \mathbf{e}^*, \quad \boldsymbol{\kappa}_e = \boldsymbol{\kappa} - \boldsymbol{\kappa}^*. \quad (24)$$

Reduction of St. Venant-Kirchhoff energy density (21) to plate kinematics for an assumed linear distribution of the elastic strain $\boldsymbol{\varepsilon}_{e,2} = \mathbf{e}_e + z\boldsymbol{\kappa}_e$ yields

$$\psi_{\text{me},\Gamma}^{\text{plate}} = \int_{-t/2}^{t/2} \hat{\psi}_{\text{me}}(\mathbf{e}_e + z\boldsymbol{\kappa}_e) dz = t\hat{\psi}_{\text{me}}(\mathbf{e}_e) + \frac{t^3}{12}\hat{\psi}_{\text{me}}(\boldsymbol{\kappa}_e). \quad (25)$$

We observe that the evolution of internal polarization is not caught correctly in a simulation based on such a plate formulation. To assess the reason for this failure, we define membrane stress $\mathbf{s}$ and moment tensor $\mathbf{m}$ as dual to the plate strain measures $\mathbf{e}$ and $\boldsymbol{\kappa}$, respectively:

$$\mathbf{s} = \frac{\partial \psi_{\text{me},\Gamma}^{\text{plate}}}{\partial \mathbf{e}} = - \frac{\partial \psi_{\text{me},\Gamma}^{\text{plate}}}{\partial \mathbf{e}^*} \quad (26)$$

$$\mathbf{m} = \frac{\partial \psi_{\text{me},\Gamma}^{\text{plate}}}{\partial \boldsymbol{\kappa}} = - \frac{\partial \psi_{\text{me},\Gamma}^{\text{plate}}}{\partial \boldsymbol{\kappa}^*} \quad (27)$$

The driving electric field, or rather voltage, in each layer is formally defined as

$$\begin{aligned} \frac{t}{2} \hat{E}_{(\pm)}^{\text{plate}} &= - \frac{\partial(\psi_{\text{me},\Gamma}^{\text{plate}} + \psi_{\text{el},\Gamma})}{\partial P_{i,(\pm)}} = \mathbf{s} : \mathbf{A} \frac{\partial e^*}{\partial P_{i,(\pm)}} + \mathbf{m} : \mathbf{A} \frac{\partial \kappa^*}{\partial P_{i,(\pm)}} - \frac{\partial \psi_{\text{el},\Gamma}}{\partial P_{i,(\pm)}} \\ &= \left(\frac{1}{2} \mathbf{s} \pm \frac{3}{2t} \mathbf{m} \right) : \mathbf{A} \frac{\partial \varepsilon_{(\pm)}^*}{\partial P_{i,(\pm)}} - \frac{\partial \psi_{\text{el},\Gamma}}{\partial P_{i,(\pm)}}. \end{aligned} \quad (28)$$

From the above expression we finally obtain the driving field, which we furnish with an additional index *plate* to distinguish it from other choices later,

$$\hat{E}_{(\pm)}^{\text{plate}} = \left(\frac{1}{t} \mathbf{s} \pm \frac{3}{t^2} \mathbf{m} \right) : \mathbf{A} \frac{\partial \varepsilon_{(\pm)}^*}{\partial P_{i,(\pm)}} - \partial \psi_p'(|P_{i,(\pm)}|) \frac{P_{i,(\pm)}}{|P_{i,(\pm)}|} + E_{(\pm)}. \quad (29)$$

We compare this expression to the continuum definition of driving electric field in the continuum model (11). Observe that, instead of the second Piola-Kirchhoff tensor $\mathbf{S}$, membrane stress $\mathbf{s}$ and moment tensor $\mathbf{m}$ influence the driving field.

4 AN AUGMENTED EQUIVALENT SINGLE-LAYER APPROACH

The aim is to obtain a more locally relevant approximation of the driving electric field.

In the present case of a constant internal polarization and electric field, we observe that the internal strain ε^* can be represented exactly through the thickness by three parameters, including inelastic membrane strain e^* , curvature κ^* and a further component ξ^* ,

$$\varepsilon^*(z) = \begin{cases} \varepsilon_{(+)}^* = e^* + z\kappa^* + (z - t/3)\xi^* & \text{if } z > 0, \\ \varepsilon_{(-)}^* = e^* + z\kappa^* + (z + t/3)\xi^* & \text{if } z < 0. \end{cases} \quad (30)$$

Let us use $(z \mp t/3)$ as a shorthand notation for the piecewise defined function $z \mapsto z - t/3$ if $z > 0$ and $z \mapsto z + t/3$ if $z < 0$. We observe that these thickness distributions 1, z and $(z \mp t/3)$ are orthogonal in the sense that

$$\int_{-t/2}^{t/2} z = 0, \quad \int_{-t/2}^{t/2} (z \mp t/3) = 0, \quad \int_{-t/2}^{t/2} z(z \mp t/3) = 0. \quad (31)$$

This implies that ξ^* above can be seen as a generalized higher moment of the distribution ε^* . Its defining equation reads

$$\int_{-t/2}^{t/2} (z \mp t/3)^2 \xi^* dz = \int_{-t/2}^{t/2} (z \mp t/3) \varepsilon^* dz. \quad (32)$$

For our special choice with two layers of constant inelastic strain, we obtain that the value of the generalized moment ξ^* equals the negative value of curvature,

$$\xi^* = -\kappa^*. \quad (33)$$

One can formally reduce the plane stress elastic energy density taking the additional inelastic strain component into account

$$\psi_{\text{me},\Gamma}^{\text{full}} = \int_{-t/2}^{t/2} \hat{\psi}_{\text{me}}(\mathbf{e} + z\boldsymbol{\kappa} - (e^* + z\kappa^* + (z \mp t/3)\xi^*)\mathbf{A}) dz \quad (34)$$

$$= \psi_{\text{me},\Gamma}^{\text{plate}}(\mathbf{e} - \mathbf{e}^*, \boldsymbol{\kappa} - \boldsymbol{\kappa}^*) + \psi_{\text{me},\text{aug},\Gamma}(\xi^*). \quad (35)$$

The splitting above is exact for quadratic potentials such as the plane-stress St. Venant-Kirchhoff energy due to the orthogonality relations (31). The augmentation potential computes as

$$\psi_{\text{me},\text{aug},\Gamma}(\xi^*) = \int_{-t/2}^{t/2} \hat{\psi}_{\text{me}}((z \mp t/3)\xi^* \mathbf{A}) dz = \frac{t^3}{36} \hat{\psi}_{\text{me}}(\xi^* \mathbf{A}). \quad (36)$$

Using such an augmentation term in a plate formulation is equivalent to exact integration through the thickness, and an exact representation of the in-plane stress distribution through the thickness.

We observe that there is some flexibility in the choice of the augmentation term. The first formulation neglecting any contribution from the higher moment ξ^* is equivalent to choosing an augmentation potential $\psi_{\text{me, aug}, \Gamma}^{\text{plate}}$ as zero,

$$\psi_{\text{me, aug}, \Gamma}^{\text{plate}} = 0. \quad (37)$$

The second formulation regarding the additional contribution stemming from ξ^* exactly re-uses the plane stress potential for the definition of the augmentation potential,

$$\psi_{\text{me, aug}, \Gamma}^{\text{full}} = \frac{t^3}{36} \hat{\psi}_{\text{me}}(\xi^* \mathbf{A}). \quad (38)$$

We propose a third variant, which performs well in simulations. For the augmentation potential, we propose to use the St. Venant-Kirchhoff model for uni-axial stress states, or Poisson ratio $\nu = 0$. This leads to

$$\psi_{\text{me, aug}, \Gamma}^{\text{new}} = \frac{t^3}{36} \frac{E}{2} (\xi^*)^2 \mathbf{A} : \mathbf{A}. \quad (39)$$

For all three variants, we use shorthand notation for the total potential including mechanic and electric contribution as well as the augmentation term,

$$\psi_{\Gamma}^{\text{variant}} = \psi_{\text{me}, \Gamma}^{\text{plate}} + \psi_{\text{me, aug}, \Gamma}^{\text{variant}} + \psi_{\text{el}, \Gamma} \quad \text{for variant either plate, full or new.} \quad (40)$$

5 IMPLICATIONS ON STRESS AND DRIVING ELECTRIC FIELD

The stress resultants $\mathbf{s}$ and $\mathbf{m}$ are independent of the choice of the augmentation potential, as these quantities depend solely on $\psi_{\text{me}, \Gamma}$. As neither the augmentation potential nor the electric contribution contain membrane strain or curvature, one verifies for variant either `plate`, `full` or `new`

$$\mathbf{s} = \frac{\partial \psi_{\Gamma}^{\text{variant}}}{\partial \mathbf{e}} = \frac{\partial \psi_{\text{me}, \Gamma}^{\text{plate}}}{\partial \mathbf{e}}, \quad \mathbf{m} = \frac{\partial \psi_{\Gamma}^{\text{variant}}}{\partial \boldsymbol{\kappa}} = \frac{\partial \psi_{\text{me}, \Gamma}^{\text{plate}}}{\partial \boldsymbol{\kappa}}. \quad (41)$$

Thus, the elastic behavior of the plate is independent of the choice of the augmentation potential; only the evolution of internal polarization, and thereby the inelastic strains, is affected.

The evolution equation in the form of Biot's law (12), or the definition of the driving electric field $\hat{\mathbf{E}}$ changes for different variants of augmentation. Let us review the impact of the choice of $\psi_{\text{me, aug}, \Gamma}$ on the driving electric field.

In case of the direct plate formulation without augmentation $\psi_{\text{me, aug}, \Gamma}^{\text{plate}}$, the driving electric field $\hat{E}_{(\pm)}^{\text{plate}}$ has been deduced to include membrane stress $\mathbf{s}$ and moment tensor $\mathbf{m}$, see (29).

Let us now consider the case of the augmentation energy density obeying the original elastic material law, characterized in $\psi_{\text{me, aug}, \Gamma}^{\text{full}}$. Then, in view of the exact representation of $\varepsilon^* = e^* + z\kappa^* + (z \mp t/3)\xi^*$ and (34),

$$\frac{t}{2}\hat{E}_{(\pm)}^{\text{full}} = -\frac{\partial\psi_{\Gamma}^{\text{full}}}{\partial P_{i,(\pm)}} \quad (42)$$

$$= \int_{-t/2}^0 \left(\frac{\partial\hat{\psi}_{\text{me}}}{\partial \varepsilon} \frac{\partial \varepsilon^*}{\partial P_{i,(-)}} - \frac{\partial\psi_{\text{el}}}{\partial P_{i,(-)}} \right) dz + \int_0^{t/2} \left(\frac{\partial\hat{\psi}_{\text{me}}}{\partial \varepsilon} \frac{\partial \varepsilon^*}{\partial P_{i,(+)}} + \frac{\partial\psi_{\text{el}}}{\partial P_{i,(+)}} \right) dz. \quad (43)$$

As $\partial \varepsilon^* / \partial P_{i,(\pm)}$ is constant in each layer and zero in the respective non-relevant domain, we see that in each layer integration through the thickness can be replaced by using the respective mean value $\mathbf{S}_{(\pm)}$ of $\mathbf{S}$,

$$\int_0^{t/2} \frac{\partial\hat{\psi}_{\text{me}}}{\partial \varepsilon} \frac{\partial \varepsilon^*}{\partial P_{i,(+)}} dz = \int_0^{t/2} \mathbf{S} : \frac{\partial \varepsilon^*}{\partial P_{i,(+)}} dz = \frac{t}{2} (\mathbf{S}_{(+)} : \mathbf{A}) \frac{\partial \varepsilon^*}{\partial P_{i,(+)}} , \quad (44)$$

$$\int_{-t/2}^0 \frac{\partial\hat{\psi}_{\text{me}}}{\partial \varepsilon} \frac{\partial \varepsilon^*}{\partial P_{i,(-)}} dz = \int_{-t/2}^0 \mathbf{S} : \frac{\partial \varepsilon^*}{\partial P_{i,(-)}} dz = \frac{t}{2} (\mathbf{S}_{(-)} : \mathbf{A}) \frac{\partial \varepsilon^*}{\partial P_{i,(-)}} . \quad (45)$$

This implies for the driving field when prescribing the full potential $\psi_{\Gamma}^{\text{full}}$

$$\hat{E}_{(\pm)}^{\text{full}} = (\mathbf{S}_{(\pm)} : \mathbf{A}) \frac{\partial \varepsilon_{(\pm)}^*}{\partial P_{i,(\pm)}} - \psi'_{\text{p}}(|P_{i,(\pm)}|) \frac{P_{i,(\pm)}}{|P_{i,(\pm)}|} + E_{(\pm)}. \quad (46)$$

This indicates a localized driving field using the mean value of in-plane stress through the respective layer. Numerical evidence implies that using the mean stress is not ideal to use in evolution of constant polarization.

For the proposed augmentation term $\psi_{\text{me, aug}, \Gamma}^{\text{new}}$, the driving electric field within the two different layers reads

$$\hat{E}_{(\pm)}^{\text{new}} = \left(\frac{1}{t} \mathbf{s} \pm \frac{3}{t^2} \mathbf{m} \right) : \mathbf{A} \frac{\partial \varepsilon_{(\pm)}^*}{\partial P_{i,(\pm)}} + \frac{2}{t} \frac{\partial \psi_{\text{me, aug}, \Gamma}^{\text{new}}}{\partial P_{i,(\pm)}} - \partial \psi'_{\text{p}}(|P_{i,(\pm)}|) \frac{P_{i,(\pm)}}{|P_{i,(\pm)}|} + E_{(\pm)}. \quad (47)$$

Deriving the potential $\psi_{\text{me, aug}, \Gamma}^{\text{new}}$ explicitly in each layer, we see that due to $\xi^* = -\kappa^*$,

$$\frac{\partial \psi_{\text{me, aug}, \Gamma}^{\text{new}}}{\partial P_{i,(\pm)}} = \frac{t^3}{36} E \kappa^* (\mathbf{A} : \mathbf{A}) \frac{\partial \kappa^*}{\partial P_{i,(\pm)}}. \quad (48)$$

Inserting the definition of κ^* in terms of the eigenstrain values in both layers $\varepsilon_{(+)}^*$ and $\varepsilon_{(-)}^*$ yields

$$\frac{\partial \psi_{\text{me, aug}, \Gamma}^{\text{new}}}{\partial P_{i, (\pm)}} = \pm \frac{Et^2}{24} \kappa^* \mathbf{A} : \mathbf{A} \frac{\partial \varepsilon_{(\pm)}^*}{\partial P_{i, (\pm)}}. \quad (49)$$

This implies for the driving field

$$\hat{E}_{(\pm)}^{\text{new}} = \left(\frac{1}{t} \mathbf{s} \pm \frac{3}{t^2} \mathbf{m} \pm \frac{t}{12} E \kappa^* \right) : \mathbf{A} \frac{\partial \varepsilon_{(\pm)}^*}{\partial P_{i, (\pm)}} - \partial \psi'_p(|P_{i, (\pm)}|) \frac{P_{i, (\pm)}}{|P_{i, (\pm)}|} + E_{(\pm)}. \quad (50)$$

In comparison, for $\psi_{\text{me, aug}, \Gamma}^{\text{full}}$, we get

$$\hat{E}_{(\pm)}^{\text{full}} = \left(\frac{1}{t} \mathbf{s} \pm \frac{3}{t^2} \mathbf{m} \pm \frac{t}{12} \frac{E}{1 - \nu} \kappa^* \right) : \mathbf{A} \frac{\partial \varepsilon_{(\pm)}^*}{\partial P_{i, (\pm)}} - \partial \psi'_p(|P_{i, (\pm)}|) \frac{P_{i, (\pm)}}{|P_{i, (\pm)}|} + E_{(\pm)}. \quad (51)$$

Numerical examples presented in the next section reveal that the proposed method employing the driving field (50) yields superior results, where the additional stress contribution $Et/12\kappa^*$ is considered independent of the Poisson ratio.

6 COMPUTATIONAL RESULTS

We consider a circular bimorph plate made from two equally thick layers of PZT. Plate radius and thickness are chosen as $R = 10$ mm and $t = 0.1$ mm, respectively. Material constants are taken from [16]. As elastic constants we use Young's modulus $E = 61$ GPa and Poisson ratio $\nu = 0.31$. Piezoelectric constants $d_{31} = -2.74 \times 10^{-10}$ C N $^{-1}$, $d_{33} = 5.48 \times 10^{-10}$ C N $^{-1}$ are used, the d_{15} effect is neglected in the current contribution. The electric permittivity is given by $\epsilon = 2.77 \times 10^{-8}$ C V $^{-1}$ m $^{-1}$, and the susceptibility relevant for the internal polarization is $\chi_i = 1.40 \times 10^{-6}$ C V $^{-1}$ m $^{-1}$. Saturation polarization and saturation strain are assumed as $P_{\text{sat}} = 0.24$ C m $^{-2}$ and $\varepsilon_{\text{sat}} = 9.3 \times 10^{-3}$. Last, the coercive electric field is $E_c = 820 \times 10^3$ V m $^{-1}$.

The circular plate is supported in such a manner that rigid body deformations are constrained in a stress-free manner, the central axis of the disk points in direction of $\mathbf{e}_3$ and the central point of the disk is fixed in space. We consider two cases: in a first analysis, cyclic polarization of a single layer is performed, such that hysteresis loops can be detected. In a second, independent analysis, the two layers are polarized in an alternating manner.

In both cases, the internal electrode is grounded, while voltage profiles $V_{(+)}$ and $V_{(-)}$ over time are prescribed at the top and bottom electrode. The mean value of polarization through the two layers is measured. Additionally, the deformation is monitored by tracking the relative vertical displacement of the center point and the outer circumference of the disc. The relevant quantities are

$$P_{i, (\pm)} = \frac{2}{R^2 t \pi} \int_{\Omega_{(\pm)}} \mathbf{P}_i \cdot \mathbf{e}_3 dV, \quad w = \frac{1}{2 R t \pi} \int_{r=R} \mathbf{u} \cdot \mathbf{e}_3 dA. \quad (52)$$

All simulations are conducted within the open source finite element software package Netgen/NGSolve (see ngsolve.org). For comparisons, the axisymmetric problem is solved on a two-dimensional mesh consisting of 1596 second order triangular elements in cylindric coordinates; these results are marked as 3d. The corresponding plate problem is solved employing low-regularity shell elements introduced by Neunteufel and Schöberl [17, 18] and extended to ferroelectric materials by the authors in [19]. Here, a quarter of the circular plate is resolved by 38 third order elements. The results corresponding to the various choices of augmentation potential are labelled `plate`, `full` and `new`, respectively.

6.1 Polarization of one layer

In the first scenario, only the upper layer is subject to electric loading. The voltage on the top electrode is varied within a range of $V_{(+)} \in [-250 \text{ V}, 250 \text{ V}]$. The corresponding applied electric field amounts to approximately three times the coercive field strength. This gives rise to hysteretic behavior; in Figure 1 the mean value of internal polarization in the top layer $P_{i,(+)}$ is shown, while Figure 2 holds the deflection of the disk's rim w over the applied voltage. All three variants $\psi_{\text{me, aug}, \Gamma}^{\text{plate}}$, $\psi_{\text{me, aug}, \Gamma}^{\text{full}}$ and $\psi_{\text{me, aug}, \Gamma}^{\text{new}}$ for the augmentation term are compared, and labeled accordingly. Classic ferroelectric and butterfly hysteresis behavior are observed. It is observed that when resorting to a classical plate formulation relying on stress resultants only (case `plate`), internal polarization evolves too fast and deflection is overestimated. On the other hand, when using stress mean values in the definition of the driving electric field (case `full`), the evolution of internal polarization is prohibited and deflections are underestimated. For the proposed variant, we get satisfactory results in the dielectric and the butterfly hysteresis loop.

6.2 Alternating polarization of both layers

In the second scenario, both layers are polarized in an alternating manner. The voltage is increased up to 100 V and then reduced back to zero in the top and bottom layer consecutively. The corresponding electric field of $E_{(\pm)} = 1000 \text{ V mm}^{-1}$ is slightly above the coercive field strength of $E_c = 820 \text{ V mm}^{-1}$. In a second and third cycle, the voltages are raised up to 150 V and 200 V in the same manner. Figure 3 holds the evolution of the observed mean internal polarization in both layers $P_{i,(\pm)}$ over load steps. Clearly, only the proposed variant using $\psi_{\text{me, aug}, \Gamma}^{\text{new}}$ is capable of reproducing the evolution of charges in a satisfying manner in this more complex scenario. The same observation is drawn from the evolution of the rim deflection w provided in Figure 4.

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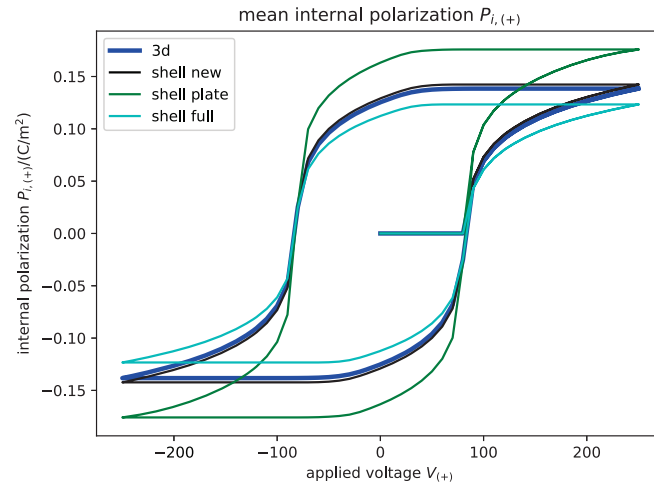


Figure 1: Polarization of one layer: mean internal polarization in layer $P_{i,(+)}$ over applied voltage $V_{(+)}$.

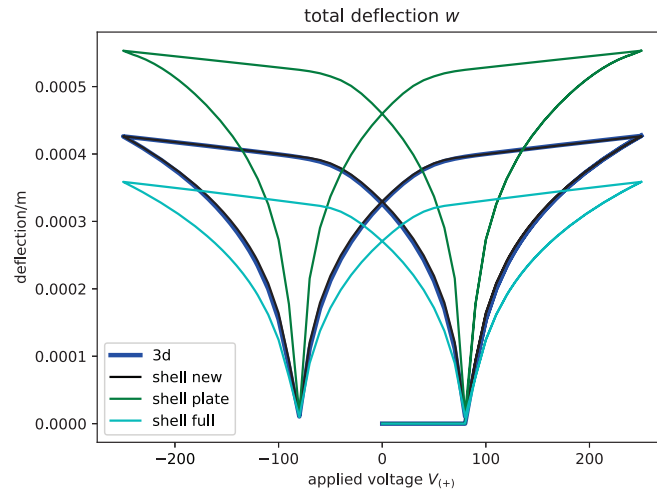


Figure 2: Polarization of one layer: deflection w over applied voltage $V_{(+)}$.

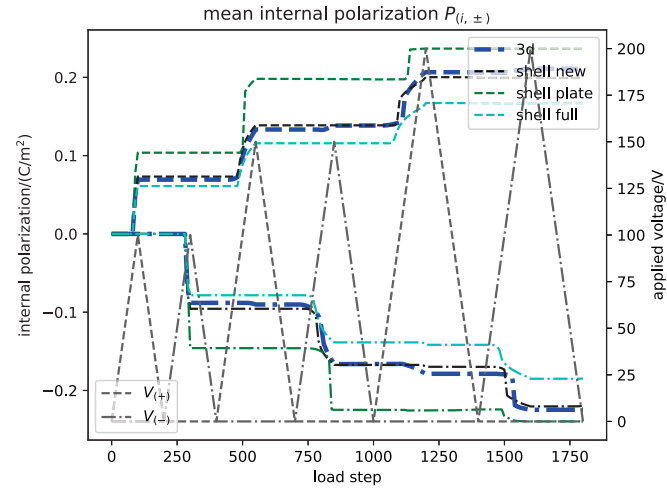


Figure 3: Alternating polarization of both layers: evolution of mean internal polarization in both layers $P_{(i, \pm)}$.

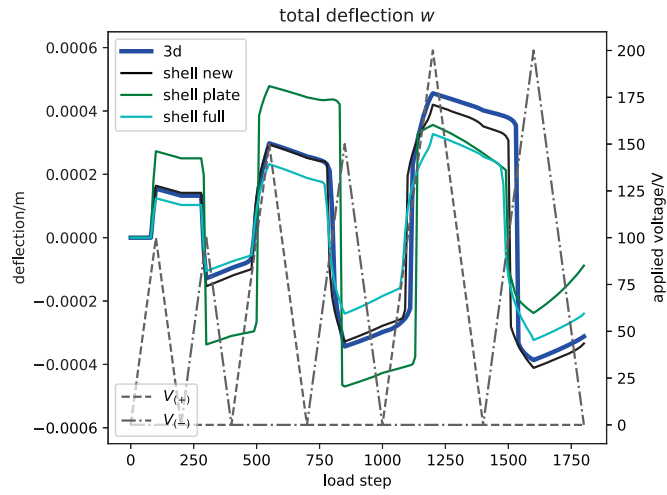


Figure 4: Alternating polarization of both layers: evolution of deflection w .

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