Modeling electro-elastic coupling phenomena in electrostrictive polymers in the context of structural mechanics

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Bringing into focus the design aspect of thin film electro-active polymer actuators justifies the deployment of a structural mechanics framework. We propose a physically consistent constitutive model for such actuators, which is valid for plates and shells as material surfaces within a complete direct formulation. To this end, we use the principle of virtual work to deduce the general form of the constitutive law from an augmented Helmholtz free energy, as a function of the structural Green-Lagrange type strain measures and of the material electric field, without the need of a\textit{priori} assumptions concerning the state of strain and stress.

Mechanical deformations of thin film devices - e.g. made of polyurethane - under the action of an external electric field, are caused by two different sources. On the one hand, the applied electric field causes a dielectric polarization of the polymer matrix, yielding to corresponding attractive electrostatic forces between the electrode surfaces resulting into a squeezing of the film. On the other hand, crystalline graft units with a certain natural, but arbitrarily directed polarization, embedded in between the polymer chains, have to align in the direction of the applied electric field such that a rotation of the whole crystal unit takes place. This rotation results in an additional macroscopic thickness squeeze - known as the electrostrictive effect.

We treat both electromechanical coupling phenomena separately, where it turns out, that the electrostatic forces can be accounted for by an electrical contribution to the augmented free energy, whereas, the electrostrictive effect is taken into account in the elastic part of the augmented free energy by virtue of a hybrid multiplicative and additive decomposition of the plate/shell deformation measures.

Benefiting from the structural mechanics formulation, we gain a lower - two-dimensional - formulation, which provides a clear physical insight into the nature of the deformation process initiated by the external electric field. E.g. for the linearised problem, a comparison to the literature on thermoelastic plates and shells uncovers the action of the electric field as a combined source of self-stresses. In order to solve particular problems, the constitutive relation of the geometrically and physically nonlinear formulation is implemented into our in-house finite element code. The computed results, which were tested against results from the literature as well as against test problems of our previous work (where numerical integration of the three dimensional plate/shell augmented free energy through the thickness was employed), show a very good agreement.

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1 Introduction

Dielectric elastomers (DEs) promise similar opportunities for sensing and actuation tasks currently offered only by piezoelectric ceramics. But DEs provide different qualities, at the foremost the soft polymer material enables large deformations at finite strains. The growing interest for DEs has led to a vast amount of literature within three-dimensional numerical modeling approaches; different multi-field problems e.g. electro-thermo-viscoelasticity [1] as well as micro-mechanically motivated models to resolve the polymer chain interactions applying homogenization techniques [2] have been presented. In order to effectively use DEs within a structurally integrated framework their design is typically very thin to ensure easy integration and embodiment. Such specifically thin devices are most efficiently modeled using a structural mechanics approach capable to resolve all relevant geometric and physical nonlinearities at reduced complexity. The present paper is devoted to the efficient modeling of electro-elastic coupled 2D manifolds, considering plates as a material surface. A special highlight is the excellent accuracy combined with the inherent efficiency demonstrated by the finite element results.

2 Electro-elastic coupling in thin plates

Thin structures, undergoing large deformations, are well described using the notion of material surfaces. In case of a plane reference state, the configuration is completely defined by the first metric tensor $I$ and a vanishing second metric tensor $B = 0$. For the actual state, the first and second metric are defined by $a = \nabla r = I_n - n n$ and $b = b^T = -\nabla n$, where the position vector $r$, the unit normal vector $n$ and the differential operator $\nabla$ refer to the actual state. Mapping between the configurations is performed by virtue of the deformation gradient tensor $F = (\nabla r)^T$ where $\nabla r$ refers to the differential operator with respect to the reference state. Finalizing the kinematic description, the strain measures

\begin{equation}
\varepsilon = 1/2(F^T \cdot a \cdot F - I); \quad \kappa = F^T \cdot b \cdot F
\end{equation}

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shall be introduced, which relate the metric tensors of both configuration using simple transformations by $F$. Both strains remain constant at rigid body motions, and it shall be emphasized that the unit normal vector remains normal to the surface throughout the deformation, rendering the definition of a Kirchhoff plate theory.

### 2.1 Variational principle

Analogous to the three dimensional case, an electro- mechanically extended variational principle is used to deduce the balance equations and stress measures conjugate to the discussed strain measures,

$$\int_{A_0} (\delta A^t + (p \cdot \delta r + m \times n \cdot \delta n - \sigma \delta V))dA_0 + \delta A^{ext} = 0. \quad (2)$$

One should notice the electric surface energy is accounted for by means of $\sigma \delta V$ in the integral over the reference surface $A_0$, with the external surface charges $\sigma$ and the voltage $V$. $p$ and $m$ account for pure mechanical external body forces and moments acting in the surface, while corresponding entities coming from the boundary, belong to the virtual work of external forces and moments $\delta A^{ext}$. Within $\delta A^{ext}$, quantities of both, mechanical and electrical origin are incorporated. The strain measures $\varepsilon$ and $\kappa$, as well as contributions from ponderomotive origin remain hidden in the variation of internal forces and moments $\delta A^t$. At a rigid body motion, the internal quantities produce no work, hence $\delta A^t = 0$, $\delta \varepsilon = 0$, and $\delta \kappa = 0$ hold, provided the voltage remains constant $\delta V = 0$. Since we discuss the kinematic relations within a Kirchhoff plate theory, variation of the unit normal vector are restricted $\delta n + \nabla \delta r \cdot n = 0$ as well. Each constraint is accounted for by virtue of correspondingly ranked Lagrange multipliers in the form $-\tau \cdot \delta \varepsilon - \mu \cdot \delta \kappa + q \delta V + q \cdot (\delta n + \nabla \delta r \cdot n)$ and reinserting into the variational principle yields

$$\int_{A_0} (\tau \cdot \delta \varepsilon + \mu \cdot \delta \kappa - q \cdot (\delta n + \nabla \delta r \cdot n) - p \cdot \delta r + m \times n \cdot \delta n)dA_0 - \int_{A_0} (q - \sigma)\delta V dA_0 + \delta A^{ext} = 0. \quad (3)$$

Omitting details on simple, but lengthy mathematical procedures, upon collection of all tensor valued relations to a resultant stress tensor $T = \tau \cdot F^T + (\mu \cdot F^T) \cdot b + F^{-1} \cdot qn$, we obtain formally identical balance equations to the three dimensional case referring to the reference surface

$$\nabla_0 \cdot T + p = 0, \quad \nabla_0 \cdot \mu \cdot a + F \cdot \tilde{q} - m \times n = 0. \quad (4)$$

$\tau$ and $\mu$ denote second Piola-Kirchhoff type stress measures of force and moment couple, and $\tilde{q} = F^{-1} \cdot q$ the transverse shear force vector. At constant voltage, the total internal charge per unit reference area $Q^{int} = \int_{A_0} qdA_0$ and the external charges $Q^{ext} = \int_{A_0} \sigma dA_0$ are balanced, $Q^{ext} - Q^{int} = 0$. We can now write the specific form of the virtual work of internal sources

$$-\delta A^t = \delta \Omega = \tau \cdot \delta \varepsilon + \mu \cdot \delta \kappa - q\delta V, \quad (5)$$

where the newly introduced augmented free energy $\Omega = \Omega(\varepsilon, \kappa, V)$ shall provide the constitutive relations upon application of the variational principle which defines the stress measures $\tau = \partial \Omega / \partial \varepsilon$, $\mu = \partial \Omega / \partial \kappa$ and $q = -\partial \Omega / \partial V$.

### 2.2 Direct approach for the constitutive relation

To close the set of equations, it remains to provide the specific form of the augmented free energy for the case of a dielectric elastomer plate as a material surface. To this end, we recall the polar decomposition of the deformation gradient tensor $F = R \cdot U$ and use the right Cauchy-Green tensor $C = F^T \cdot F = 2\varepsilon + I$. $R = R^T$ is the orthogonal tensor of rotation and $U = U^T$ is the symmetric stretch tensor of the material surface. The stretching part $U$ does not contribute to bending deformations which remain solely the task of the rotatory path $R$.

Given $n = R \cdot N$, bending, which is measured by the strain tensor $\kappa = U \cdot R^T \cdot b \cdot R \cdot U$, enters in the polar decomposition on top of the membrane path, starting from an unphysical intermediate configuration for which an intermediate curvature strain tensor

$$K = U^{-1} \cdot \kappa \cdot U^{-1} = R^T \cdot b \cdot R \quad (6)$$

can be defined. In consequence, all in-plane deformations remain solely task of the stretching path, such that $C = U^2$ holds. Another consequence we can draw from the polar decomposition is the associated additive decomposition of the strain energy, which we separate into a membrane and a bending part $\eta_0 \psi_m(C, K) = \eta_0 \psi_m(C) + \eta_0 \psi_b(C, K)$. 

**Fig. 1:** Deformation path split by $F = R \cdot U$ and corresponding parts of the augmented free energy.
The connection between the polar decomposition, pure mechanical strain energy and the previously introduced augmented free energy is, as well, coming from an additive decomposition, \( \Omega(C, K, V) = \eta_0 (C_m(C, K) + \eta_0 (C, K, V) \). We begin with the definition of the mechanical part, and start with the membrane energy, for which we use a hyperelastic neo-Hookean energy, as suggested in [5]. In the cited work, a three dimensional energy \( \psi(C_2, \tilde{C}_3, \tilde{\varepsilon}_3) \) has been specified to the case of plane stress using an incompressibility constraint such \( C_{33} = \det C_2^{-1} \) holds, to find \( \psi(C_2, \tilde{C}_3, \tilde{\varepsilon}_3) \equiv \psi_{me}(C_2, \tilde{\varepsilon}_3) \). We adapt this formulation by means of replacing the plane part of the three dimensional right Cauchy-Green tensor \( C_2 \), by our purely plane stretch right Cauchy-Green \( C = U^2 \) which yields the neo-Hookean type membrane energy

\[
\eta_0 \psi_m = \frac{1}{2} A (\text{tr} C + \det C^{-1} - 3).
\]

(7)

\( A = Y h/(1 - \nu^2) = 4\mu h \) is the extensional stiffness, using the Lame parameter \( \nu = 0.5 \) and \( Y = 3\mu \).

By now, no bending actions were involved such that we conclude the intermediate configuration is free from any bending stress see Fig. 1. As well, the bending energy must not depend on the stretch tensor, posing the curvature stain tensor \( \kappa \) as proper measure getting underway with a geometric nonlinear extension of the well proven Kirchhoff plate bending energy \( \eta_0 \psi_b = 1 / 2 D (\text{tr} K^2 - \det K) \). Yet, the material surface of the intermediate configuration has already experienced some area change measured by \( J = \det U = \det F \) which has to be regarded in the mass per unit area \( \tilde{\eta} = J^{-1} \eta_0 \), and in the definition of the bending stiffness \( D = J^{-2} D \), both get transformed back into the reference configuration. The relation between \( D \) and \( \tilde{D} \) follows from the three dimensional incompressibility condition, \( J_3 = 1 = J F_{33} \) with \( \lambda_3 = U_{33} \equiv F_{33} = J^{-1} \). \( J \) represents as well the area change into the actual configuration and by setting \( \nu = 0.5 \), the classical plate bending stiffness \( D = Y h^3 / 12 (1 - \nu^2)^{-1} \), becomes \( D = \mu h^3 / 3 \), such that we can finally write the bending energy

\[
\eta_0 \psi_b = \frac{1}{2} \det C^{-1} D (\text{tr} K^2 - \det K).
\]

(8)

Before we proceed to the electrical part, the specific choice of constitutive relation deserves some discussion. When considering a homogeneous dielectric elastomer under the action of an electric field, it primarily exerts extensional deformations, where the hyperelastic behavior is ensured. For the bending energy, we take the standpoint that the curvature tensor is sufficiently small, such that the incompressible Saint-Venant Kirchhoff bending energy \( \psi_b \) is justified. Moving on to the electro-mechanical contribution, a homogeneous dielectric elastomer plate is modeled as a capacitor, whose free energy is given by \( 2 \eta_0 \psi_{el} = \tilde{c} V^2 \), provided the electric field is homogeneous through the thickness. \( V \) is the voltage, \( \tilde{c} = J c \) denotes the capacity and \( \eta_0 \) the mass per unit area; both are defined in the deformed configuration. Since we have the same \( \eta_0 \) in the intermediate configuration \( J^2 = \det U^2 \) holds, such that the electrical energy defined in the reference configuration becomes \( \eta_0 \psi_{el} = -1 / 2 \epsilon_0 V^2 \det C \). Summation over all constituent parts renders the augmented free energy for an isotropic, elastically homogeneous and incompressible single layer neo-Hookean plate under the action of a homogeneous electric field

\[
\Omega(C, K, V) = \frac{1}{2} A (\text{tr} C + \det C^{-1} - 3) + \frac{1}{2} \det C^{-1} D (\text{tr} K^2 - \det K) - \frac{1}{2} \epsilon_0 V^2 \det C.
\]

(9)

### 2.3 Linearized equations - small strain regime

Up till now, the discussed constitutive relation holds for arbitrary large strains, but of particular interest is the question if the classical relations of a linear elastic Kirchhoff plate obeying St. Venant-Kirchhoff behavior can be retrieved? In order to deduce the linearized version of the augmented free energy, we formally enclose the strain tensors \( \varepsilon \) and \( \kappa \) with the small parameter \( \lambda \) and perform a series expansion about this small parameter. Hence, the two dimensional right Cauchy-Green tensor gets \( C = 2 \lambda \varepsilon + I \), and the curvature tensor is \( \kappa \). The square of the voltage is of order \( \lambda V^2 \). Upon series expansion in the vicinity of \( \lambda = 0 \), the principle term \( \lambda^3 \) remain independent from any deformation measure, such that the leading order is found to be \( \lambda^2 \). The membrane energy turns to the classical St.Venant Kirchhoff relation, using the identity \( (\text{tr} \varepsilon)^2 - \det \varepsilon = 1 / 2 ((\text{tr} \varepsilon)^2 + \varepsilon : \varepsilon) \). Claiming small curvature strains \( (\kappa \equiv K) \) holds, such that the bending energy remains formally unchanged, and the linearized electrical contribution simply changes to \(-2 \epsilon_0 V^2 \text{tr} \varepsilon \). Then, the linear augmented free energy of a homogeneous, incompressible single layered plate reads

\[
\eta_0 \Omega^{lin} = \frac{1}{2} (A (\text{tr} \varepsilon)^2 - \det \varepsilon - 2 \epsilon_0 V^2 \text{tr} \varepsilon) + \frac{1}{2} (D ((\text{tr} \kappa)^2 - \det \kappa)).
\]

(10)

Which is exactly the classical linear Kirchhoff plate relation under the action of membrane sources of self-stress, in the form \( \tau^* = -2 \epsilon_0 V^2 \text{tr} \varepsilon \). It remains to notice, the in the current formulation no sources of self-stress couples arise, since the voltage is assumed homogeneous through the thickness of the plate.

### 3 Finite element representation

For the numerical validation, the presented modern version of the Kirchhoff-Love plate theory is implemented into our in-house finite element code ShellFE. The presented theory requires a \( C^1 \) continuous approximation, which is achieved using a four-node finite element and an approximation scheme which features 16 shape-functions for each component of the spatial position vector capable to exactly represent any bi-cubic polynomial. Each isoparametric element has 48 mechanical degrees
of freedom, the prescribed voltage serves as load factor, such that we have no electrical degree of freedom, see [4] for the implementation details. Seeking for a static equilibrium position, we assemble the total energy functional \( \Sigma = \Sigma(\varepsilon, \kappa, V, p) \) as the sum of the plate augmented free energy and the potential energy of external forces

\[
\Sigma = \Sigma^\Omega + \Sigma^{\text{ext}} = \int_{A_0} (\Omega(\varepsilon, \kappa, V) - p \cdot r) dA_0;
\]

no external moments are applied in the domain and no external forces or moments act at the boundary. Solving for a stationary value of the total energy functional yields a nonlinear algebraic system of equations which can be solved numerically by employing Newton’s method. It remains to emphasize that in case the functional obeys linear elastic behavior instead of a hyperelastic one, the above variational formulation is equivalent to Koiter’s nonlinear plate model [3].

### 3.1 Buckling Actuator

As an example problem, we study a bifurcation problem, composed of a single dielectric plate with the size \( a \times b \times h = 4\text{mm} \times 2\text{mm} \times 0.01\text{mm} \) and the Lame parameter \( \mu = 20698\text{Pa} \) and the capacity \( c = \varepsilon_0 \varepsilon_r \varepsilon^{-1} = 4.16138 \times 10^{-6} \text{A}^2\text{V}^{-1}\text{m}^{-2} \). The plate is clamped at both ends \((x = 0 \text{ and } x = a)\), but translations in the direction parallel to the clamped edge remain unconstraint see Fig. 2 left. Upon application of a voltage, the plate exerts extensional deformation which is hindered by the clamped support, such that compressional forces yield to an out of plane buckling of the plate. At first, the critical buckling voltage is computed; converged solutions were obtained using \( 16 \times 8 \) elements and by solving an accompanied eigenvalue problem the critical voltage \( V_{\text{crit, buckling}} = 2.700\text{V} \) was identified. For the sake of comparison, the same example problem has been solved in the open-source multi-purpose finite element code Netgen/NGSolve featuring solid prism elements, which yields the critical voltage \( V_{\text{crit, NGSolve}} = 2.632\text{V} \), which means a difference of 6.8% to the shell solution, the difference in the results is caused by a slight difference in the boundary condition since in NGSolve the displacements in thickness direction were fixed as well in the clamped support.

To investigate the post-buckling behavior, a small geometrical pre-deformation, at the size \( w_{\text{mid, init}} h^{-1} = 0.01 \), is applied, and the out-of-plane mid-point deflection \( w_{\text{mid}} h^{-1} \) of the center point of the plate is plotted, see Fig. 2 right. Starting at 0V, the voltage is increased, till the electromechanical breakdown material electric field \( V_{\text{breakdown}} = 0.687\sqrt{\mu/c} = 153.215\text{V} \), is attained. The same breakdown voltage has been derived analytically in [5], and reported in [6] where a solid shell finite element scheme and an Ogden type material has been used. Finally, we mention the encouraging agreement with the results from NGSolve, up to the voltage of \( V = 95.4\text{V} \), at which the volume elements did not converge any more, whereas in the presented shell solution no problems were observed. In view of efficiency and accuracy the holistic direct approach fulfills all requested demands excellently, and strengthens our confidence to incorporate further effects, e.g. electrostriction.

![Fig. 2: Left deformed configuration at 153.5V, right comparison of the mid-point deflection between ShellFE (continuous line) and NGSolve (black marker).](image-url)

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