A model for elastic flexoelectric materials including strain gradient effects

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Abstract. A constitutive model for elastic flexoelectric materials under small deformation based on second gradient continuum theory is developed, using a Toupin-like variational formulation to simultaneously obtain constitutive relations, balance equations and boundary conditions. The model includes three different electromechanical "stresses": a higher order stress, an extended local electric force, and a generalized Cauchy stress tensor. The constitutive equations of the model are obtained by postulating an internal energy density function which depends on both the strain and its gradient as well as the polarization. Finally, as an application of the model, we derive the explicit analytical expressions of the polarization and displacement vector fields for the problem of the polarization induced over a thin spherical shell subjected to hydrostatic loading conditions.

Keywords. Flexoelectric materials, Second gradient theory, Constitutive equations, thin shell, electromechnical couplings.

1. Introduction

Flexoelectricity is a physical phenomenon that was first theoretically predicted for crystalline dielectrics by Maskevich and Tolpygo [25], and later observed and described from a phenomenological standpoint by Kogan [34] some decades ago. Lately, an increasing in the interest for this subject has occurred, the origin of which mainly comes from two sources.

First of all, there is the need to develop novel methodologies to design and manufacture materials showing connection between mechanical and electrical behavior (as the well established piezoelectric composites do) with environmentally friendly industrial processes. Indeed, while the current methods used for the manufacturing of piezoelectrics in industries are complicated

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and expensive, flexoelectric effects can be exploited just relying on the properties of a very large class materials (Foussek and Cross [19]). Another reason for the rapid growth of interest for flexoelectricity is that, unlike piezoelectric effects, flexoelectricity is not limited to non-centrosymmetric materials.

Currently, flexoelectric effects are well established for several dielectrics and semi-conductors and can thus be very useful for many practical applications. However, due to the novelty of this research line, there are still few available theoretical and experimental works in the field. Among these works, let us mention those of (i) Bursian and Trunov [2] where the flexoelectric phenomena were observed during the bending of crystal plates and (ii) Catalan et al. [4] where flexoelectricity was demonstrated during measurements on thin films. A comprehensive review of experimental works that demonstrate the role of flexoelectricity in crystalline materials, liquid crystals, and biomembranes can be found in Sharma et al. [40].

On theoretical grounds, most of the works in the field use constitutive relations based on a strain gradient approach. This approach originates from the seminal works by Lord Kelvin, the Cosserat brothers and before them by the (maybe not so universally known) Italian mathematician Gabrio Piola, and has recently (mainly due to the increase of the power of the computers) been object of intensive study in the works of Sciarra et al. [39] , Sedov [37], Madeo et al. [30, 29], Rosi et al. [36], Pideri and Seppecher[32], Placidi et al. [33], dell'Isola et al. [10] to mention a few. In particular, higher order continuum theories such as micropolar and micromorphic theories of Eringen [13] and Eringen and Suburi [14, 15] can be applied to model flexoelectric effects, as shown for instance in Chen [5] and Romeo [35].

Several other authors have used strain gradient continuum theory to derive the constitutive equations for elastic flexoelectric solids. Among them let us mention the works of Mao and Purohit [23] where the governing equations for elastic flexoelectric solids were derived using a Toupin [42]-like variational principle in the context of small strain approximation. The Navier-Cauchy equations obtained in the work of Mao and Purohit are similar to those of Mindlin[26, 27] strain gradient elasticity theory. Toupin's variational principle was also used by Sharma et al.[40] to develop a slightly different model for elastic flexoelectric solids. The internal energy density employed in the works of Sharma et al. is inspired by a previous paper by Sahin and Dost [38]; it contains both the second gradient of the displacement and the polarization. The constitutive relations these authors obtained neglect the contributions of higher order terms (fifth and higher order tensors) in the internal energy. These approximations were conceived in order to obtain simplified constitutive models (with reduced number of internal parameters) for flexoelectric solids for practical applications. However, the refining of these assumptions, which could include a more detailed physic description, is by now required by both theoretical and applicative reasons. In the present work, we shall follow up the development of constitutive laws for elastic flexoelectric materials as well as their applications to boundary value problems of either theoretical or practical interests. Namely, we propose a new model for elastic flexolectric materials based on an internal energy density function which depends on the strain, its gradient and the polarization. This density function generalizes the one suggested by Mao and Purohit [23] by accounting for a fifth-order tensor coupling between first and second order effects (as a general rule these effects exist in all non-centrosymmetric materials) as proposed by dell'Isola et al. [6, 8, 7, 9] and recently studied by Enakoutsa [16]. Also, the density function proposed in this work does not depend on the polarization gradient as it is the case in Sharma et al. [40]. This simplification will allow us to perform explicit calculation which would be much more complex with assumptions similar to those of Sharma et al., where both the polarization due to the strain gradient and the gradient of the polarization were accounted for. A variational principle, which is inspired by those developed by Toupin[42] and Gao and Park [20], based on our proposed internal energy density function is used to find both the balance equations and the boundary conditions. The plan of the paper is the following.

- In Section 2 we present the governing equations of the model proposed for elastic flexoelectric materials. They consist of three different constitutive relations, each of them defining some electromechanical "stress". These stresses are deduced from a postulated internal energy density function, which is also presented in this section. The same section includes a variational formulation used to determine both the balance equations and the boundary conditions.

- Section 3 provides an application of our model for flexoelectric solids; namely, we derive an explicit analytical solution of the problem of the polarization induced by a thin spherical shell subjected to hydrostatic loading conditions. The solution of this simple problem offers not only a direct comparison to classical elasticity and strain gradient elasticity but also some insights into the polarization fields near point defects in flexoelectric materials.

- A discussion of the analytical solution is provided in Section 3.2. Namely, a comparison between the displacement field here found and those obtained with classical elasticity and strain gradient elasticity are provided.

2. Governing equations

This section presents the derivation of the governing equations for elastic flexoelectric materials. Flexoelectric effects are observed in a large class of materials, characterized by diverse elastic behaviors. Anyway, since well consolidated experimental data show appreciable flexoelectric effects in case of small deformation, our proposed model aims to describe flexoelectric effects in the linear elastic regime of materials. We thus do not consider in the present paper dissipative mechanical phenomena, whose investigation will be of course of great interest in the future.

2.1. Internal energy density function

We postulate an internal energy density function $\mathcal{W}$ which depends on the strain, the gradient of the strain, and the polarization. This last assumption is to us very natural, since the polarization, just like the strain and its gradient, is of course measurable, traceable, independent from other descriptors and it has a well defined initial state. This density function, which is inspired by the one proposed by Sahin and Dost[38] and studied by Sharma et al.[40], is defined by

$$\begin{aligned} \mathcal{W}\left(D_{ij}, D_{ij,k}, P_i\right) \quad &:= \quad \frac{1}{2}C_{ijkl}D_{ij}D_{kl} + \frac{1}{2}H_{ijklmn}D_{ij,k}D_{lm,n} + \frac{1}{2}\chi_{ij}P_iP_j \\ &+ \quad e_{ijk}P_iD_{jk} + G_{ijklm}D_{ij}D_{kl,m} + K_{ijkl}P_iD_{jk,l} \end{aligned} \tag{2.1}$$

where

- the tensor $C_{ijkl,1\leq i,j,k,l\leq 3}$ is the usual fourth-rank elasticity tensor;
- the tensor $e_{ijk,1\leq i,j,k\leq 3}$ represents the third-rank piezoelectric tensor;
- the tensor $H_{ijklmn,1\leq i,j,k,l,m,n\leq 3}$ and $G_{ijklm,1\leq i,j,k,l,m\leq 3}$ denote the sixth-rank and fifth-rank generalized second gradient elastic constants as suggested by dell'Isola et al.[6, 8, 7, 9];
- the tensor $K_{ijkl,1\leq i,j,k,l\leq 3}$ is the fourth-rank flexoelectricity tensor;
- the tensor $\chi_{ij,1\leq i,j\leq 3}$ is the familiar second order reciprocal dielectric susceptibility tensor;
- the tensor $D_{ij,1\leq i,j\leq 3}$ is the second-rank symmetric strain tensor which is defined as

$$D_{ij} = 1/2\left(u_{i,j} + u_{j,i}\right) \tag{2.2}$$

  assuming small deformation approximation;
- the vector $P_{i,1\leq i\leq 3}$ is the polarization vector field;
- the comma denotes the differentiation with respect to spatial variables

Also, in Eq.(2.1) the tensors **C, H**, and **G** obey the following symmetry properties

$$\begin{cases} C_{ijkl} &= \quad C_{klij} \\ H_{ijklp} &= \quad H_{lpijkl} \\ G_{ijklpq} &= \quad G_{lpqijk}. \end{cases} \tag{2.3}$$

The symmetry properties of the strain tensor $\mathbf{D}$ enforces the following additional symmetry properties:

$$\left\{\begin{array}{lcl} C_{ijkl} & = & C_{ijlk} = C_{jikl} \\ H_{ijklp} & = & H_{jiklp} = H_{ijkpl} \\ G_{ijklpq} & = & G_{jiklpq} = G_{ijkplq}. \end{array}\right. \tag{2.4}$$

Note that the internal energy density function Eq.(2.1) is a modified version of the one proposed by Mindlin [28]. This density function is an extension of the one suggested by Mao and Purohit [23]; it does not include the gradient of the polarization as it is the case in the works of Maranganti et al.[22] and Sharma et al.[40]. Also, it does not include a remaining part as suggested by Toupin[42]; finally, it differs from the one used in classical theory for piezoelectric materials and includes nonlocal effects.

2.2. Variational formulation

From the definition of the internal energy density function Eq.(2.1), we get the internal energy $\mathcal{E}^i$ of the (deformed) flexoelectric materials as

$$\mathcal{E}^i = \int_\Omega \mathcal{W} dv = \frac{1}{2}\int_\Omega \left(\Sigma_{ij} D_{ij} + M_{ijk} D_{ij,k} - E_i P_i\right) dv \tag{2.5}$$

where the components of the Cauchy stress, Σ_{ij}, the hyperstress, M_{ijk}, the strain gradient $D_{ij,k}$, and the local electric vector field E are given by

$$\left\{\begin{array}{lcl} \Sigma_{ij} & = & \dfrac{\partial \mathcal{W}}{\partial D_{ij}} = C_{ijkl} D_{jk} + G_{ijklm} D_{kl,m} + e_{ijk} P_l \\ \\ M_{ijk} & = & \dfrac{\partial \mathcal{W}}{\partial D_{ij,k}} = G_{ijklp} D_{lp} + H_{ijklpq} D_{lp,q} + K_{ijkl} P_l \\ \\ E_i & = & -\dfrac{\partial \mathcal{W}}{\partial P_i} = e_{ijk} D_{jk} + K_{ijkl} D_{jk,l} + \chi_{ij} P_j, \end{array}\right. \tag{2.6}$$

with

$$D_{ij,k} = \frac{1}{2}\left(u_{i,jk} + u_{j,ik}\right). \tag{2.7}$$

In Eq.(2.7) $u_{i,1\leq i\leq 3}$ is the displacement vector field. Strictly speaking the internal energy $\mathcal{U}$ in the integral over the body domain of the internal energy density function Eq.(2.1) should include the additional terms $\frac{1}{2}\psi_{,i}\psi_{,i} + \psi_{,i}P_i$ in the integrand of the internal energy $\mathcal{U}$ (where ψ is an electrical potential) to be consistent with Toupin[42]'s variational principle. However, they are omitted here because they are not needed in the derivation of the electromechanical forces.

The work done by the external forces $\mathcal{E}^e$ is defined as

$$\mathcal{E}^e = \int_\Omega \left(f_i u_i + E_i^0 P_i\right) dv + \int_{\partial\Omega} \left(t_i u_i + q_i dDu_i\right) da \tag{2.8}$$

where

- f_i is the external body force;
- E_i^0 denotes the external electric field;
- t_i is the Cauchy traction vector;
- q_i is the double stress traction vector;
- $\partial\Omega$ is the closed smooth bounding surface of Ω;
- Du_i is the normal (directional) derivative of the displacement component u_i defined by
$$Du_i = n_l u_{i,l} \tag{2.9}$$
with n_l being the outward unit normal to the surface $\partial\Omega$

Using Toupin [42]-like variational approach under the assumption of quasi-static analyses[1]
$$\delta\mathcal{E}^i - \delta\mathcal{E}^e = 0, \tag{2.10}$$

along with a double integration by parts, and the divergence theorem, we find the balance equations

$$\left\{ \begin{array}{lcl} \Sigma_{ij,j} - M_{ijk,jk} + f_i & = & 0 \\ \\ E_i + E_i^0 & = & 0 \end{array} \right. \tag{2.11}$$

and the boundary conditions

$$\left\{ \begin{array}{lcl} \Sigma_{ij} n_j - (M_{ijk} n_k)_{,j} + (M_{ijk} n_k n_j)_{,l} n_j & = & t_i \\ \\ M_{ijk} n_j n_k & = & q_i \end{array} \right. \tag{2.12}$$

Let us mention that, formally speaking Eq.$(2.11)_1$ are similar to those found in [31, 18, 1, 21, 11, 12, 16]; however, our definition of the third-rank tensor M_{ijk}, work conjugate of the strain gradient $D_{ij,k}$, differs from those obtained in the works mentioned above. The balance equations (2.11), the boundary conditions (2.12) along with the relations (2.6) represent our proposed governing equations of elastic flexoelectric materials under small deformation.

2.3. Centrosymmetric materials

For centrosymmetric materials, the piezoelectricity coefficients tensor $e_{ijk,1\leq i,j,k\leq 3}$ as well as the fifth rank strain gradient tensor $G_{ijklmn,1\leq i,j,k,l,m,m\leq 3}$ vanish. Thus, the constitutive relations (2.6) reduce to

$$\left\{ \begin{array}{lcl} \Sigma_{ij} & = & C_{ijkl} D_{jk} \\ \\ M_{ijk} & = & H_{ijklpq} D_{lp,q} + K_{ijkl} P_l \\ \\ E_i & = & K_{ijkl} D_{jk,l} + \chi_{ij} P_j \end{array} \right. \tag{2.13}$$

[1] In Eq.(2.10) the term δX denotes the variation of the parameter X.

For isotropic linear elastic materials, dell'Isola et al.[6], using some material symmetry arguments previously developed by Suiker et al. [41], have shown that

$$\left\{\begin{array}{lcl} C_{ijkl} & = & \lambda\delta_{ij}\delta_{kl}+\mu\left(\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk}\right) \\ \\ H_{ijklp} & = & 0 \end{array}\right. \tag{2.14}$$

and

$$\left\{\begin{array}{lcl} H_{ijklpq} & = & c_1\left(\delta_{ij}\delta_{kl}\delta_{pq}+\delta_{ij}\delta_{kp}\delta_{lq}+\delta_{ik}\delta_{jq}\delta_{lp}+\delta_{iq}\delta_{jk}\delta_{lp}\right) \\ & + & c_3\left(\delta_{ik}\delta_{jl}\delta_{pq}+\delta_{ik}\delta_{jp}\delta_{lq}+\delta_{il}\delta_{jk}\delta_{pq}+\delta_{ip}\delta_{jk}\delta_{lq}\right) \\ & + & c_5\left(\delta_{il}\delta_{jq}\delta_{kp}+\delta_{ip}\delta_{jq}\delta_{kl}+\delta_{iq}\delta_{jl}\delta_{kp}+\delta_{iq}\delta_{jp}\delta_{kl}\right) \\ & + & c_2\delta_{ij}\delta_{kq}\delta_{lp}+c_4(\delta_{il}\delta_{jp}\delta_{kq}+\delta_{ip}\delta_{jl}\delta_{kq}) \end{array}\right. \tag{2.15}$$

where δ_{ij} denotes the Kronecker delta symbol and c_i some strain gradient elastic material constants that are characteristic of different materials.

Also, Mason [24] and Maranganti et al. [22] have shown that, for linear isotropic centrosymmetric materials the tensors $\chi_{ij,1\leq i,j\leq 3}$ and $K_{ijkl,1\leq i,j,k,l\leq 3}$ reduce

$$\left\{\begin{array}{lcl} K_{ijkl} & = & k_{12}\delta_{ij}\delta_{kl}+k_{44}\left(\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk}\right) \\ \\ \chi_{ij} & = & a\delta_{ij}. \end{array}\right. \tag{2.16}$$

Thus, from Eqs.(2.13), (2.14), (2.15) and (2.16) we get

$$\left\{\begin{array}{lcl} \Sigma_{ij} & = & \lambda D_{kk}\delta_{ij}+2\mu D_{ij} \\ \\ M_{ijk} & = & 2c_1D_{kp,p}\delta_{ij}+c_1D_{pp,j}\delta_{ik}+c_1D_{pp,i}\delta_{jk}+c_2D_{ll,k}\delta_{ij} \\ \\ & + & 2c_3(D_{jq,q}\delta_{ik}+D_{iq,q}\delta_{jk})+2c_4D_{ij,k}+2c_5(D_{ik,j}+D_{jk,i}) \\ \\ & + & \delta_{ij}k_{12}P_k+k_{44}\left(\delta_{ik}P_j+\delta_{jk}P_i\right) \\ \\ E_i & = & k_{12}D_{ik,k}+k_{44}\left(D_{ji,j}+D_{jj,i}\right)+aP_i \end{array}\right. \tag{2.17}$$

The relations (2.17) involve ten constitutive constants: two of them represent the usual Lame's elastic coefficients, λ and μ; the remaining eight constants (five strain gradient elasticity constants, two flexoelectricity constants and one second-order reciprocal dielectric susceptibility constant) are needed. To illustrate the potential of the proposed constitutive relations, we shall use them to model the matrix material in the solution of the polarization of a thin spherical shell subjected to axisymmetric loading conditions.

3. Polarization of a thin spherical shell

This section is devoted to the solution of a polarization problem for a thin walled spherical shell deformed under axisymmetric loading conditions problem, the deformation being inhomogeneous. The aim in introducing this simple problem is twofold. On one hand, our analytical solution could provide insights into nanoscale experiments based on flexoelectric solids. Besides, this solution could be used as a benchmark solution to assess computational tools (based on the constitutive model developed in this paper) for flexoelectric materials. The model problem is illustrated in Figures (1, 2).

3.1. Problem description

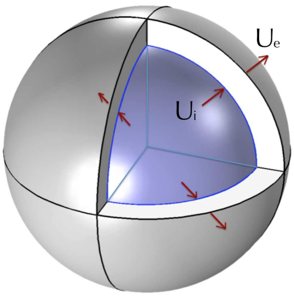

FIGURE 1. Polarization of a thin spherical shell undergoing axisymmetric loading model problem

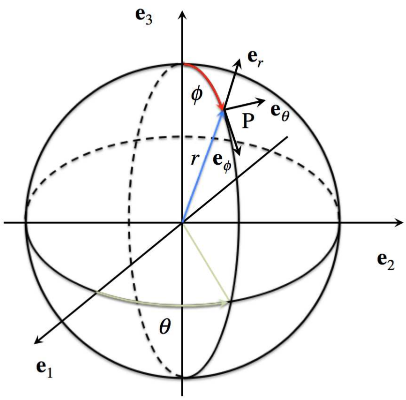

FIGURE 2. Polar coordinates associated with the problem model

The internal radius of the spherical shell is denoted by r_i, while the external radius is r_e. The matrix of the shell is supposed to be linear elastic, obeying the constitutive relations (2.17). Use will be made of the classical spherical coordinates r, θ and ϕ and the corresponding orthogonal basis

e_r, e_θ, e_ϕ. Closely related boundary value problems (BVPs) were considered in Enakoutsa[12, 16], Collina et al.[3] and Gao et al. [21] but in the context of another strain gradient elasticity theory. The problem under consideration involves spherical symmetries, hence the displacement and polarization vector fields (denoted here by $\mathbf{U} \equiv U_r$ and $\mathbf{P} \equiv P_r$, respectively) in the spherical shell are radial.

During the solution of the model problem use will be made of the vector field $\mathbf{W} = \Delta\mathbf{U}$ (the symbol Δ stands here for the Laplacian operator) which satisfies the following mathematical properties

$$W_{i,hh} = W_{h,hi} \tag{3.1}$$

thanks to the facts that $\mathbf{W}$ is a radial vector and that the *curl* of a gradient is zero. As a consequence, considering the definitions of the strain tensor $\mathbf{D}$ and of the vector $\mathbf{W}$, we have

$$D_{hh,i} = U_{h,hi} = W_i \quad \text{and} \quad D_{ih,h} = \frac{1}{2}(U_{i,hh} + U_{h,ih}) = U_{i,hh} = \Delta U_i, \tag{3.2}$$

and so,

$$D_{hh,i} = D_{ih,h} = W_i. \tag{3.3}$$

Despite their simple formulation, the properties (3.2) and (3.1) are very powerful to solve (as performed by Enakoutsa in [11, 12, 16]) BVPs involving spherical symmetries, these BVPs including geometries such as full or hollow cylinders, disks and spheres. We begin the solution of the problem by taking the first spatial derivatives of the stress and the second spatial derivatives of the ordinary Cauchy stress and hyperstress in Eq.$(2.17)_{1,2}$ to get

$$\left\{\begin{array}{lcl} \Sigma_{ij,j} & = & \lambda D_{kk,i} + 2\mu D_{ij,j} \\ M_{ijk,jk} & = & c_1\left(2D_{kp,pik} + D_{pp,jji} + D_{pp,ikk}\right) + c_2 D_{ll,kik} \\ & + & 2c_3(D_{jq,qji} + D_{iq,qjk}) + 2c_4 D_{ij,kjk} \\ & + & 2c_5(D_{ik,jjk} + D_{jk,ijk}) + (k_{12} + k_{44})\, P_{k,ik} + k_{44} P_{i,jj}. \end{array}\right. \tag{3.4}$$

Using the properties (3.2, 3.3) the expressions (3.4) and $(2.17)_3$ become

$$\left\{\begin{array}{lcl} \Sigma_{ij,j} & = & (\lambda + 2\mu)\, W_i \\ M_{ijk,jk} & = & (4c_1 + c_2 + 4c_3 + 2c_4 + 4c_5)(\Delta W)_i \\ & + & (k_{12} + k_{44})\, P_{k,ik} + k_{44}(\Delta P)_i \\ E_i & = & (k_{12} + 2k_{44})\, W_i + aP_i \end{array}\right. \tag{3.5}$$

Introducing the spatial derivatives of the stress and the hyperstress tensors $(3.5)_1, 2$ and the electric field $(3.5)_3$ in the balance equations (2.17) we obtain

$$\begin{cases} W_i - \dfrac{(4c_1 + c_2 + 4c_3 + 2c_4 + 4c_5)}{\lambda + 2\mu}(\Delta W)_i \\ \\ +\dfrac{k_{12} + k_{44}}{\lambda + 2\mu} P_{k,ik} + \dfrac{k_{44}}{\lambda + 2\mu}(\Delta P)_i + \dfrac{1}{\lambda + 2\mu} f_i = 0 \\ \\ (k_{12} + 2k_{44})\, W_i + aP_i + E_i^0 = 0 \end{cases} \tag{3.6}$$

Note that in Eq.(3.6) the displacement and polarization fields are coupled through the flexoelectricity constants K_{ijkl}. In the absence of body external forces ($f_i = E_i^0 = 0$) the system of differential equations (3.6) reduces

$$\begin{cases} W_i - k^1(\Delta W)_i + k^2 P_{k,ik} + k^3(\Delta P)_i = 0 \\ \\ k^4 W_i + aP_i = 0 \end{cases} \tag{3.7}$$

where

$$\begin{cases} k^1 &= \dfrac{(4c_1 + c_2 + 4c_3 + 2c_4 + 4c_5)}{\lambda + 2\mu} \\ \\ k^2 &= \dfrac{k_{12} + k_{44}}{\lambda + 2\mu} \\ \\ k^3 &= \dfrac{k_{44}}{\lambda + 2\mu} \\ \\ k^4 &= (k_{12} + 2k_{44}) \end{cases} \tag{3.8}$$

Using $(3.7)_2$ in $(3.7)_1$ we obtain

$$W_i - k^1(\Delta W)_i + k^2 P_{k,ik} - \frac{k^3 k^4}{a}(\Delta W_i) = 0 \tag{3.9}$$

Remembering that both the displacement and polarization vector fields only depend on the radial coordinate r, Eq.(3.9) becomes

$$W_r - \left(k^1 + \frac{\left(k^2 + k^3\right) k^4}{a}\right)(\Delta W)_r = 0 \tag{3.10}$$

or in compact form

$$\mathbf{W} - k(\Delta \mathbf{W}) = 0 \tag{3.11}$$

where $k = \left(k^1 + \frac{\left(k^2+k^3\right)k^4}{a}\right)$.

The partial derivative equation (3.11) generalizes those obtained in previous works by Enakoutsa [11, 12, 16] by accounting for flexoelectric effects through the constants K_{ijkl} in the co-factor of $(\Delta\mathbf{W})$. This equation bears some similarities with the equation of radial vibration of a sphere. The solution of this equation mainly relies on the fact that the vector $\mathbf{W}$ is assumed to be radial, deriving from a scalar field, which we shall denote here by φ. Following Enakoutsa [11, 12], Eq.(3.11) reads

$$\Delta\varphi - k^2\varphi = Cst. \tag{3.12}$$

For the sake of simplicity, we shall set the constant Cst in Eq.(3.12) to zero. Solving the resulting equation for φ we obtain

$$\varphi = \alpha e^{kr}/r + \beta e^{-kr}/r \quad \text{and} \quad \mathbf{W} \equiv W_r = \varphi' \tag{3.13}$$

where α and β represent integration constants and the symbol $'$ denotes the partial derivative $\partial/\partial r$. The radial displacement $U_r := U$ can then be obtained through the ordinary differential equation

$$W \equiv W_r = (\nabla \mathrm{tr}\, D) = (\mathrm{tr}\, D)_{,r} = (U' + 2U/r)' \tag{3.14}$$

which is solved for U as

$$U(x) = \alpha\left(1/x - 1/x^2\right)\mathrm{e}^{x} + \beta\left(1/x + 1/x^2\right)\mathrm{e}^{-x} + \gamma x + \delta/x^2. \tag{3.15}$$

In Eq.(3.15) the variable $x \equiv kr$, and α, β, γ and δ represent integration constants.

Once we have the displacement field, the polarization vector $P_r := P$ can be determined using Eqs.$(3.7)_2$ and $(3.13)_2$; we get

$$P = -\frac{k^4}{a}\varphi', \tag{3.16}$$

that is,

$$P(x) = \alpha_1\left(1/x - 1/x^2\right)\mathrm{e}^{x} + \beta_1\left(1/x + 1/x^2\right)\mathrm{e}^{-x} \tag{3.17}$$

where α_1 and β_1 are two additional constants in the solution of the problem. Overall, the displacement and polarization vector field expressions contain six unknown constants, therefore six boundary conditions (BCs) are needed to solve them. The integration constants $\alpha, \beta, \gamma, \delta$ can be determined using the following boundary conditions

$$\begin{cases} M_{rrr}(r_i) = 0, \quad U_r(r_i) = \Delta_i \\ \\ M_{rrr}(r_e) = 0, \quad U_r(r_e) = \Delta_e. \end{cases} . \tag{3.18}$$

The conditions $M_{rrr=r_{i,e}} = 0$ in Eq.(3.18) can be obtained by writing the variational formulation using the thin spherical shell as the body material. A simplified version of this formulation (not including flexoelectric effects) can be found in Enakoutsa [12] and Zhao and Pedroso [43]. The constraints $U(r_{i,e}) = \Delta_{i,e}$ are simply prescribed Dirichlet boundary conditions. Two other BCs related to the polarization vector field, Eq.(3.17), are needed; they can be obtained by fixing the values of the polarization on the inner and outer faces of the spherical shell, that is, $P(x_i) = P_i$ and $P(x_e) = P_e$ which serve to determine the constants α_1 and β_1 as

$$\left\{\begin{array}{lcl} \alpha_1 & = & \dfrac{P_e k^2\left(1/x_i + 1/x_i^2\right)e^{-x_i} - P_i k^2\left(1/x_e + 1/x_e^2\right)e^{-x_e}}{\Delta_d} \\ \\ \beta_1 & = & \dfrac{P_i k^2\left(1/x_e - 1/x_e^2\right)e^{x_e} - P_e k^2\left(1/x_i + 1/x_i^2\right)e^{x_i}}{\Delta_d} \end{array}\right. . \tag{3.19}$$

with Δ_d defined as

$$\begin{aligned} \Delta_d &= k^4\left[\left(1/x_e - 1/x_e^2\right)\left(1/x_i + 1/x_i^2\right)e^{-(x_i - x_e)}\right] \\ &- k^4\left[\left(1/x_i - 1/x_i^2\right)\left(1/x_e + 1/x_e^2\right)e^{(x_e - x_i)}\right] \end{aligned} \tag{3.20}$$

The determination of the integration constants $\alpha, \beta, \gamma, \delta$ requires the calculation of the component M_{rrr} of the hyperstress. Employing the constitutive relation $(2.17)_2$, the definition of the gradient of the strain $\nabla\mathbf{D}$ in spherical coordinates, and the polarization vector field (3.17) we obtain the component M_{rrr} as

$$M_{rrr} = \alpha \mathrm{e}^x T(x) + \beta \mathrm{e}^{-x} Q(x) + 6\delta/x^4 + (k_{12} + 2k_{44})\, P(x) \tag{3.21}$$

with

$$\left\{\begin{array}{lcl} k_1 & = & 4c_1 + c_2 + 4c_3, \quad k_2 = 2(c_4 + 2c_5) \\ \\ T(x) & = & k^2(k_1 + k_2)/x - k^2(k_1 + 3k_2)/x^2 + 6/x^3 - 6/x^4 \\ \\ Q(x) & = & k^2(k_1 + k_2)/x - k^2(k_1 + 3k_2)/x^2 + 6/x^3 + 6/x^4. \end{array}\right.$$

Assuming that $x_i = kr_i$, $x_e = kr_e$, $T_i \equiv T(x_i)$, $T_e \equiv T(x_e)$, $Q_i \equiv Q(x_i)$, and $Q_e \equiv Q(x_e)$ and using the expressions of the radial displacement and the component M_{rrr} Eqs.(3.15) and (3.21) the boundary conditions (3.18) yields the following system of equations

$$\left\{\begin{array}{l}
\alpha \mathrm{e}^{x_i} T_i + \beta \mathrm{e}^{-x_i} Q_i + 6\delta/x_i^4 = -\left(k_{12}+2k_{44}\right) P_i \\
\alpha \mathrm{e}^{x_e} T_e + \beta \mathrm{e}^{-x_e} Q_e + 6\delta/x_e^4 = -\left(k_{12}+2k_{44}\right) P_e \\
\alpha \left(1/x_i + 1/x_i^2\right) \mathrm{e}^{x_i} - \beta \left(1/x_i + 1/x_i^2\right) \mathrm{e}^{-x_i} + \gamma x_i + \delta/x_i^2 = \Delta_i \\
\alpha \left(1/x_e + 1/x_e^2\right) \mathrm{e}^{x_e} - \beta \left(1/x_e + 1/x_e^2\right) \mathrm{e}^{-x_e} + \gamma x_e + \delta/x_e^2 = \Delta_e,
\end{array}\right. .$$

which is solved for the unknown constants α, β, γ and δ as

$$\left\{\begin{array}{rcl}
\alpha & = & \left(x_e^4 Q_e \mathrm{e}^{-x_e} - x_i^4 Q_i \mathrm{e}^{-x_i}\right) \\
& \times & \left(\frac{\Delta_e}{x_e} - \frac{\Delta_i}{x_i} + \frac{x_i}{6}(k_{12}+2k_{44})P_i(1+x_i^3/x_e^3)\right)/\mathcal{D}_e \\
& - & \left(-\mathrm{e}^{-x_e}\mathcal{B}_e + \mathcal{A}_i \mathrm{e}^{-x_i}\right)(k_{12}+2k_{44})\left(x_i^4 P_i - x_e^4 P_e\right)/\mathcal{D}_e \\
\\
\beta & = & \left(x_e^4 T_e \mathrm{e}^{x_e} - x_i^4 T_i \mathrm{e}^{x_i}\right) \\
& \times & \left(\frac{\Delta_e}{x_e} - \frac{\Delta_i}{x_i} + \frac{x_i}{6}(k_{12}+2k_{44})P_i(1+x_i^3/x_e^3)\right)/\mathcal{D}_e \\
& - & \left(\mathrm{e}^{x_e}\mathcal{B}_e - \mathcal{C}_i \mathrm{e}^{x_i}\right)(k_{12}+2k_{44})\left(x_i^4 P_i - x_e^4 P_e\right)/\mathcal{D}_e \\
\\
\delta & = & -\dfrac{\alpha x_i^4 \mathrm{e}^{x_i} T_i + \beta x_i^4 \mathrm{e}^{-x_i} Qi}{6} - \dfrac{x_i^4\left(k_{12}+2k_{44}\right)}{6} P_i \\
\\
\gamma & = & \dfrac{\Delta_i}{x_i} - \left[\alpha\left(\dfrac{1}{x_i^2} - \dfrac{1}{x_i^3}\right)\mathrm{e}^{x_i} - \beta\left(\dfrac{1}{x_i^2} + \dfrac{1}{x_i^3}\right)\mathrm{e}^{-x_i} - \dfrac{\delta}{x_i^3}\right]
\end{array}\right. \tag{3.22}$$

where the values of $\mathcal{A}, \mathcal{B}, \mathcal{A}_i, \mathcal{B}_i$ and $\mathcal{D}_e$ are defined by

$$\left\{\begin{array}{rcl}
\mathcal{B}(x) & \equiv & \dfrac{1}{x^3} + \dfrac{1}{x^2} \\
\\
\mathcal{A}(x) & \equiv & \left(\dfrac{1}{x^3} + \dfrac{1}{x^2}\right) - \dfrac{xQ}{6} - \dfrac{xQ}{6x_e^3} \\
\\
\mathcal{C}(x) & \equiv & \left(\dfrac{1}{x^2} - \dfrac{1}{x^3}\right) + \dfrac{xT}{6} + \dfrac{xT}{6x_e^3} \\
\\
\mathcal{A}_i & \equiv & \mathcal{A}(x_i), \quad \mathcal{B}_i = \mathcal{B}(x_i), \quad \mathcal{C}_i = \mathcal{C}(x_i)
\end{array}\right. \tag{3.23}$$

and

$$\left\{\begin{array}{rcl}
\mathcal{D}_e & = & \left(x_e^4 T_e \mathrm{e}^{x_e} - x_i^4 T e \mathrm{e}^{x_i}\right)\left[\mathrm{e}^{-x_i}\mathcal{B}_i - \mathrm{e}^{-x_e}\mathcal{B}_e\right] \\
& - & \left(x_e^4 Q_e \mathrm{e}^{-x_e} - x_i^4 Q_i \mathrm{e}^{-x_i}\right)\left[\mathrm{e}^{x_i}\mathcal{B}_e - \mathrm{e}^{x_i}\mathcal{C}_i\right],
\end{array}\right. \tag{3.24}$$

respectively.

3.2. Discussion

The analytical solution developed raises several points of interest which are presented as follow.

- The displacement vector field (3.15) includes the combined effects of strain gradient elasticity and flexoelectricity through the parameter k. As expected, in the absence of flexoelectric effects in the model, the strain gradient elasticity displacement field of Enakoutsa [11, 12] is recovered. The relation (3.15) also shows that the magnitude of the displacement field vector is substantially reduced with respect to the classical elasticity and strain gradient elasticity solutions. This can be explained by the fact that in flexoelectric materials, some part of the external forces work is employed to polarize the material, unlike in elastic materials where all the work produced by the external forces is stored in the material as an elastic energy. Mao and Purohit ([23]) have reached the same conclusions for a closely related boundary value problem, a pressurized thick-walled cylinder.

- The polarization vector field (3.17) is also significantly affected by the flexoelectric effects. Note that the polarization in the spherical shell is determined by the combined effects of strain gradient through the constants $c_{i,1\leq i\leq 5}$ and the flexoelectric constants K_{ijkl}. When the strain gradient constants vanish (that is $c_{i,1\leq i\leq 5} = 0$), the spherical shell is still polarized (strain gradient-polarization couplings) according to the formula (3.17) through the flexoelectric constants K_{ijkl}. Eq.(3.17) also shows that the polarization vector field can be controlled by changing the mechanical loading parameters, Δ_i and Δ_e. However, it is not clear from this equation whether the polarization of the spherical shell will increase with increasing values of the mechanical loading parameters or the reverse. Similarly, the local electrical behavior can also be controlled by changing the mechanical loading parameters as demonstrated by the expression $(3.5)_3$.

4. Concluding remarks

In this paper, we presented the constitutive relations, the equilibrium equations and the boundary conditions for isotropic flexoelectric solids within the framework of small strain deformations. These governing equations are obtained using a variational formulation which includes a postulated internal energy density function that extends the one used by Toupin, Sahin and Dost, and Sharma et al. The model is used to provide the explicit analytical solution of the problem of the polarization induced by a thin-spherical shell subjected to axisymmetric loading conditions. The analytical expressions of the radial displacement and polarization vector fields are provided; these expressions involve six constitutive constants which are obtained using some suitable Dirichlet prescribed boundary conditions along with some boundary conditions given by the variational formulation. Our analytical solution could be employed to provide insights into nanoscale experiments based on flexoelectric solids. Besides, this solution could be used as a benchmark solution to assess computational tools (based on the constitutive model developed in this paper) for flexoelectric materials.

As already observed, our proposed model was intended as a first step, as our aim was to describe flexoelectric effects in the linear elastic regime of materials. The wide class of materials that experimentally show flexoelectric effects, however, will likely require at some point the need to investigate this kind of effects above the elastic regime, possibly in conjunction with dissipation phenomena. Especially considering the technological interest for both flexoelectricity and energy harvesting, this research line seems to offer plenty of prospects for the near future.

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