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Electrostatic Potential Induced by Flexoelectric Effects in Nanowires. Part I: Analytical Study

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1. Introduction

With the rapid developement of nanoscale technologies, there is a resurgence of interest in the study of the flexoelectric effect in solid materials. The flexoelectric effect describes the generation of an electric polarization under mechanical strain or stress gradient or the reverse, that is, the mechanical field response to an electric field gradient. The flexoelectric effect was first theoretically predicted for crystalline dielectrics by Maskevich and Tolpygo [34], and later observed and described from a phenomenological standpoint by Kogan [27].

The theory of flexoelectricity is analogous to the polarization-gradient approach suggested by Mindlin [38] which links the polarization gradient to the strain field, see Askar and co-workers [1], Bursian and Trunov [2] and Catalan and co-workers [3] to name few. More generally, most of the works on the theoretical modeling of the flexoelectric effect result from generalized continuum approaches. The later comes 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 and co-workers [47], Sedov [45], Madeo and co-workers [32, 31], Rosi and co-workers [43], Pideri and Seppecher [40], Placidi and co-workers [41], dell'Isola and co-workers [7] among others. Generalized continuum theories such as micropolar and micromorphic approaches of Eringen [19] and Eringen and Suburi [20, 21] were applied to model flexoelectric effect in materials, see for instance Chen [4] and Romeo [42].

Other fundamental models of flexoelectric effect based on generalized continuum approaches result from the application of Toupin [50]-like variational principle. Among them we can mention the works of Mao and Purohit [33] and of Sharma and co-workers [49]. The governing equations of the flexoelectric effect in the works of Mao and Purohit are analagous to those of Mindlin [35, 36] strain gradient elasticity theory. The constitutive relations of the flexoelectricity model presented by Sharma and co-workers are inspired from a previous work by Sahin and Dost [44] and include both the polarization and the second gradient of the displacement field; the contributions of the higher order terms (fifth and higher order tensors) in the internal energy were not account for. These approximations were necessary to reduce the number of parameters involved in Sharma and co-workers model so that practical numerical nanoscale electromechanical coupling applications based on this model are amenable.

Recent works by Enakoutsa and co-workers [16, 17] went beyond these approximations. Namely, these authors proposed a model for flexoelectric effect in materials resulting from Toupin [50] and Gao and Park [22]-like variational approaches. This model is based on an internal energy density function which generalizes the one suggested by Mao and Purohit [33] by accounting for a fifth-order tensor which represents the coupling between first and second order gradient effects (as a general rule these effects exist in all non-centrosymmetric materials) following an earlier suggestion by dell'Isola et al. [8, 10, 9, 11]. Enakoutsa and co-workers [16, 17]'s proposal was recently studied by Enakoutsa [15, 18]. In the latter works, a benchmark analytical solution of the problem of a thin-walled cylinder deformed in plane strain based on the proposed model for flexoelectric effect was developed as an application of this model. The outcome of the solution developed has clearly evidenced the correlation between the strain gradient and the electrical polarization generated, establishing thus some analytical foundations of flexoelectric based nanodevices, especially nanogenerators and nanopiezotronics devices. Also, Enakoutsa and co-workers [16, 17]'s works are the same vein of the previous ones of Wang and co-workers [51, 52] who developed a nanogenerator system which has the potential to convert the mechanical energy produced by the mechanical bending of a zinc oxide nanowire into an electricical energy, see [5].

Similar studies aimed at designing nanoscale piezoelectric based devices exit. Among them, we can mention the works of Gao and Wang [24] where a perturbation theory was used to derive an analytical solution for the piezoelectric potential repartition in the cross section of a bending nanowire; also, Shao and co-workers [48] presented a simplified but efficient constitutive model to calculate the piezoelectric potential in a bending nanowire. Furthermore, Moemeni and co-workers [39] fabricated a nano-composite generator which consits of an array of zinc oxide nanowires based on some analytical solution. The contributions of the flexoelectric effect, which is known to be tremendous at the material lower level length scales, were neglected in the studies mentioned above, perhaps as a first step.

The objective of this paper is to rectify this drawback and/or to complete the very few exsiting studies that account for the flexoelectric effect in their proposed flexoelectric based nanodevice prototypes. To do so we shall use the new flexoelectric effect model developed by Enakoutsa and co-workers [16, 17]. The advantage of this model over its few competitors is that it accounts for more detailed physics description, which is by now required by both theoretical and applicative reasons. This model will be used to predict the repartition of the electric potential a thin wire structures made of zinc oxide. The plan of this paper is the following.

- In Section 2, we review the governing equations of the flexolectric effect model as presented by Enakoutsa and co-workers [16, 17]. This model is derived from Toupin [50]-like variational formulation for electromechanical problems. Enakoutsa and co-workers's constitutive relations mainly consist of three independent constitutive relations, each of them defining some electromechanical "stress" which result from a postulated internal energy density function. A simplified version of Enakoutsa and co-workers [16, 17]'s model for the flexoelectric effect in material, which differs from the simplifications introduced by Sharma and co-workers [49], is also presented.

- Next, in Section 3 the simplified version of Enakoutsa and co-workers [16, 17]'s model presented in Section 2 is used to predict analytically the distribution of the electrostatic potential in a thin-walled nanowire made of zinc oxide, subjected to some external pressure load conditions. The procedure of the solution of this problem is analogous to those developed in Gao [23], Gao and Park [22], Collins and co-workers [6], and Enakoutsa [14] and reduces to find the solution of a modified Bessel-type differential equation. The analytical expression of the distribution of the electrostatic potential is provided and depends on modified Bessel functions.

- Finally, Section 4 discusses the implications of the solutions obtained in the course of this work. This Section also establishes the relevance of the model proposed by Enakoutsa and co-workers [16, 17] to describe the flexoelectric effect in materials and to simulate nanoscale flexoelectric based devices at the early stage of the fabrication of these devices.

2. Continuum model of flexoelectric effect in materials

This section presents the governing equations of Enakoutsa and co-workers [16, 17]'s model for the flexoelectric effect in materials as well as its simplified version.

2.1. Generalities

The constitutive relations of Enakoutsa and co-workers [16, 17]'s model are derived from a postulated internal energy density function $\mathcal{W}$ wich depends on the strain and its gradient as well as the polarization and its gradient, that is, $\mathcal{W} \equiv \mathcal{W}(D_{ij}, D_{ij,k}, P_i, P_{i,j})$ in the context of small displacement and deformation assumptions. The proposed internal energy density function generalizes the one suggested by Sahin and Dost [44] and adopted by Sharma and co-workers [49]; this function is defined as

$$\boldsymbol{\mathcal{W}} \equiv \left\{ \begin{array}{cl} & \frac{1}{2}C_{ijkl}D_{ij}D_{kl} + \frac{1}{2}H_{ijklmn}D_{ij,k}D_{lm,n} + \frac{1}{2}\chi_{ij}P_iP_j \\ + & e_{ijk}P_iD_{jk} + G_{ijklm}D_{ij}D_{kl,m} + K_{ijkl}P_iD_{jk,l} + a_{ij}P_{i,j} \\ + & \frac{1}{2}b_{ijkl}P_{i,j}P_{k,l} + d_{ijkl}P_{i,j}D_{kl} + g_{ijk}P_iP_{k,j} \end{array} \right. \quad (1)$$

with

- $\boldsymbol{\mathcal{C}} \equiv C_{ijkl,1\leq i,j,k,l\leq 3}$ is the usual fourth-rank "simple" elastic (stiffness) constants tensor;

- $\boldsymbol{e} \equiv e_{ijk,1\leq i,j,k\leq 3}$ represents the third-rank piezoelectric constants tensor;

- $\boldsymbol{\mathcal{H}} \equiv H_{ijklmn,1\leq i,j,k,l,m,n\leq 3}$ and $\boldsymbol{\mathcal{G}} \equiv G_{ijklm,1\leq i,j,k,l,m\leq 3}$ denote the sixth-rank and fifth-rank SGE elastic constants as suggested by dell'Isola and co-workers [8, 10, 9, 11];
- $\boldsymbol{\mathcal{K}} \equiv K_{ijkl,1\leq i,j,k,l\leq 3}$ is the fourth-rank flexoelectric constants tensor;
- $\boldsymbol{\chi} \equiv \chi_{ij,1\leq i,j\leq 3}$ is the familiar second order reciprocal dielectric susceptibility tensor;
- $\boldsymbol{d} \equiv d_{ijkl,1\leq i,j,k,l\leq 3}$ is a Mindlin [37]'s fourth-order tensor which connects the gradient of polarization to the strain;
- $\boldsymbol{b} \equiv b_{ijkl,1\leq i,j,k,l\leq 3}$ is the polarization gradient-polarization gradient coupling fourth order tensor;
- the material constant tensor $\boldsymbol{g} \equiv g_{ijk,1\leq i,j,k\leq 3}$, which was introduced by Mindlin [37], links the polarization with the gradient of the polarization;
- the material constant tensor $\boldsymbol{a} \equiv a_{ij,1\leq i,j\leq 3}$, which was also introduced by Mindlin [37], is linked to the gradient of the polarization and is introduced to avoid strain and polarization localization at the surface of the body, see Mindlin [37];
- the vector $\boldsymbol{\mathcal{P}} \equiv P_{i,1\leq i\leq 3}$ is the polarization vector field while $P_{i,j 1\leq i,j\leq 3}$ is a second order tensor representing the gradient of the polarization vector;
- the comma denotes the differentiation with respect to spatial variables;
- $\boldsymbol{\mathcal{D}} \equiv D_{ij,1\leq i,j\leq 3}$ is the second-rank symmetric strain tensor which is defined as

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

with $\boldsymbol{u} \equiv u_{i,1\leq i\leq 3}$ denoting the displacement vector field.

The elastic constants tensor $\boldsymbol{\mathcal{C}}$, and the SGE constants tensors $\boldsymbol{\mathcal{H}}$ and $\boldsymbol{\mathcal{G}}$ in Eq.(1) obey the following symmetry properties

$$\left\{\begin{array}{lcl} C_{ijkl} & = & C_{klij} \\ H_{ijklp} & = & H_{lpijkl} \\ G_{ijklpq} & = & G_{lpqijk}. \end{array}\right. \tag{3}$$

Using the symmetry properties of the strain tensor $\boldsymbol{\mathcal{D}}$ we obtained some additional symmetry properties upon the tensors $\boldsymbol{\mathcal{C}}$, $\boldsymbol{\mathcal{H}}$, and $\boldsymbol{\mathcal{G}}$ defined as

$$\left\{\begin{array}{lcl} C_{ijkl} & = & C_{ijlk} = C_{jikl} \\ H_{ijklp} & = & H_{jiklp} = H_{ijkpl} \\ G_{ijklpq} & = & G_{jiklpq} = G_{ijkplq}. \end{array}\right. \tag{4}$$

Details on the symmetry properties of the material constant tensors $\boldsymbol{b}$ and $\boldsymbol{d}$ are provided, for instance, in Mindlin [38], while Kogan [26, 27] can be consulted for the flexoelectric effect constants tensor $\boldsymbol{\mathcal{K}}$. Details studies of the mathematical properties of the flexoelectric effect constants tensor can be found in Le Quang and He [28]. The piezoelectric constants tensor $\boldsymbol{e}$ obeys the usual symmetry properties given by

$$e_{ijk} = e_{jik}. \tag{5}$$

2.2. Governing equations

The internal energy density function (1) is used to define an internal energy $\boldsymbol{\mathcal{E}}^i$ as

$$\boldsymbol{\mathcal{E}}^i = \int_\Omega \boldsymbol{\mathcal{W}} dv = \frac{1}{2}\int_\Omega \left(\Sigma_{ij} D_{ij} + M_{ijk} D_{ij,k} - E_i P_i + E_{ij} P_{i,j}\right) dv \tag{6}$$

with the components of the Cauchy stress, Σ_{ij}, the hyperstress, M_{ijk}, the local electric force, E_i, the higher order local electric force, E_{ij}, and the gradient of the strain, $D_{ij,k}$, given by

$$\left\{\begin{array}{lcl} \Sigma_{ij} & = & \dfrac{\partial \mathcal{W}}{\partial D_{ij}} = C_{ijkl} D_{jk} + G_{ijklm} D_{kl,m} + e_{ijk} P_l \\ M_{ijk} & = & \dfrac{\partial \mathcal{W}}{\partial D_{ij,k}} = G_{ijklp} D_{lp} + H_{ijklpq} D_{lp,q} + K_{ijkl} P_l \\ E_i & = & -\dfrac{\partial \mathcal{W}}{\partial P_i} = e_{ijk} D_{jk} + K_{ijkl} D_{jk,l} + \chi_{ij} P_j \\ E_{ij} & = & \dfrac{\partial \mathcal{W}}{\partial P_{i,j}} = b_{ijkl} P_{k,l} + d_{ijkl} D_{kl} + g_{ijk} P_{k,j} + a_{ij} \end{array}\right. \tag{7}$$

and

$$D_{ij,k} = \frac{1}{2}\left(u_{i,jk} + u_{j,ik}\right), \tag{8}$$

$u_{i,1\leq i\leq 3}$ being the displacement vector field.

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

$$\boldsymbol{\mathcal{E}}^e = \int_\Omega \left(f_i u_i + E_i^0 P_i\right) dv + \int_{\partial\Omega} \left(t_i u_i + q_i D u_i\right) da \tag{9}$$

where

- f_i is the external body force;
- E_i^0 denotes the external electric body force;
- 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

$$Du_i = n_l u_{i,l} \tag{10}$$

with n_l being the outward unit normal vector to the surface $\partial\Omega$. Let us mention that the integrand $(t_i u_i + q_i Du_i)$ in the right-hand of Eq.(9) was also adopted by Gao and Park [22].

We shall now apply Toupin and Mindlin [50, 37]-like variational approaches to obtain both the balance equations and the boundary conditions. To do so, an additional term is needed in the integrand (the energy density function) of the energy density (1) to be consistent with Toupin [50] and Mindlin [37] variational approaches; thus the new energy density function is given by

$$\mathcal{W} = \left\{ \begin{array}{cl} & \frac{1}{2}\left(\Sigma_{ij}D_{ij} + M_{ijk}D_{ij,k} - E_iP_i + E_{ij}P_{i,j}\right) \\ - & \frac{1}{2}\epsilon_0\left(\nabla\Phi\right)_i\left(\nabla\Phi\right)_i + \left(\nabla\Phi\right)_i P_i \end{array} \right. \tag{11}$$

with Φ being an electric potential which is related to the local electric force E_i as

$$E_i = \left(\nabla\Phi\right)_i \tag{12}$$

With this new expression of the density function, the variational approaches of Toupin and Mindlin [50, 37] as well as Gao and Park [22] can be applied to the internal energy (11) and the external energy (9) in a body occupying a volume Ω bounded by a surface $\partial\Omega$, separating Ω from the external environement $\Omega^\star$ to obtain, in the context of quasi-static analyses, the following balance equations

$$\left\{ \begin{array}{l} \Sigma_{ij,j} - M_{ijk,jk} + f_i = 0 \\ \\ E_i + E_{ij,j} - \left(\nabla\Phi\right)_i + E_i^0 = 0 \\ \\ -\epsilon_0\left(\nabla\Phi\right)_{ii} + P_{i,i} = 0 \quad in \quad \Omega \\ \\ \left(\nabla\Phi\right)_{ii} = 0 \quad in \quad \Omega^\star \end{array} \right. \tag{13}$$

and the boundary conditions

$$
\begin{cases}
\Sigma_{ij} n_j - (M_{ijk} n_k)_{,j} + (M_{ijk} n_k n_j)_{,l} n_j & = \quad t_i \\
M_{ijk} n_j n_k = q_i \\
n_i \left(-\epsilon_0 \left[\left[(\nabla\Phi)_i\right]\right] + P_i\right) = 0 \\
n_i E_{ij} = 0
\end{cases}
\tag{14}
$$

where $\left[\left[(\nabla\Phi)_i\right]\right]$ is the jump in $(\nabla\Phi)_i$ across the bounding surface of the body Ω.

Eqs.(8) and (7) along with the boundary conditions (14) constitute the governing equations for the model proposed by Enakoutsa [16, 17] for elastic flexoelectric materials under small deformation assumptions.

2.3. Simplified version

This section presents a version of Enakoutsa and co-workers [16, 17]'s model when the material is centrosymetric where the classical piezoelectric effect is absent. In this case, according to Mindlin [37], the piezoelectric coefficients tensor $e_{ijk,1\leq i,j,k\leq 3}$, the "Mindlin constants" tensor $g_{ijkl,1\leq i,j,k,l\leq 3}$ which links polarization with the gradient of the polarization as well as the fifth rank strain gradient elastic tensor $G_{ijklmn,1\leq i,j,k,l,m,m\leq 3}$ vanish. Therefore, the electromechanical forces (7) reduce to

$$
\begin{cases}
\Sigma_{ij} & = & C_{ijkl} D_{jk} \\
M_{ijk} & = & H_{ijklpq} D_{lp,q} + K_{ijkl} P_l \\
E_i & = & K_{ijkl} D_{jk,l} + \chi_{ij} P_j \\
E_{ij} & = & b_{ijkl} P_{k,l} + d_{ijkl} D_{kl} + a_{ij}
\end{cases}
\tag{15}
$$

For the particular case of linear isotropic materials, the strain gradient elastic constants in the reduced electromechanical forces relations Eq.(15) are reduced to those of dell'Isola and co-workers [8] which result from some material symmetry arguments previously proposed by Suicker and Chang [46]. Also, the electromechanical coupling coefficients tensors $\chi_{ij,1\leq i,j\leq 3}$, $K_{ijkl,1\leq i,j,k,l\leq 3}$, $d_{ijkl,1\leq i,j,k,l\leq 3}$ and $b_{ijkl,1\leq i,j,k,l\leq 3}$ simplified to those obtained by Masson [29] and Mindlin [37] and used in Maranganti and coworkers [30] so that the electromechanical stress relations (15) become:

$$
\begin{cases}
\Sigma_{ij} & = \lambda D_{kk}\delta_{ij} + 2\mu D_{ij} \\
M_{ijk} & = 2c_1 D_{kp,p}\delta_{ij} + c_1 D_{pp,j}\delta_{ik} + c_1 D_{pp,i}\delta_{jk} + c_2 D_{ll,k}\delta_{ij} \\
 & + 2c_3(D_{jq,q}\delta_{ik} + D_{iq,q}\delta_{jk}) + 2c_4 D_{ij,k} + 2c_5(D_{ik,j} + D_{jk,i}) \\
 & + \delta_{ij}k_{12}P_k + k_{44}\left(\delta_{ik}P_j + \delta_{jk}P_i\right) \\
E_i & = k_{12}D_{ik,k} + k_{44}\left(D_{ji,j} + D_{jj,i}\right) + \chi P_i \\
E_{ij} & = b_{12}\delta_{ij}P_{k,k} + b_{44}(P_{j,i} + P_{i,j}) + b_{77}(P_{j,i} - P_{i,j}) \\
 & + d_{12}\delta_{ij}D_{kk} + 2d_{44}D_{ij} + a\delta_{ij}
\end{cases}
\tag{16}
$$

where

- the symbol δ_{ij} denote the Kronecker delta tensor;
- the coefficients $c_{i,1\leq i\leq 5}$ are the strain gradient elastic material constants of dell'Isola and co-workers [8];
- the constants k_{ij} represent the non-zero flexoelectric coupling effect moduli;
- the constants b_{ij} and d_{ij} are the Masson [29] and Mindlin [37] non-zero electromechanical coupling effect moduli;
- λ and μ denote the usual Lame elastic stiffness tensor

The relations (16) include sixteen constitutive constants; along with the balance equations and boundary conditions Eqs.(13, 14), these relations define a simplified version of Enakoutsa and co-workers [16, 17]'s model for the flexoelectric effect in linear elastic solids. The practical used of this version of the model is demonstrated in the two following sections. The first application consists of an analytical study of the distribution of the electrostatic potential in a thin-walled nanowire made of zinc oxyde and subjected to an external pressure while the second application deals with the numerical solution of the same model problem using *COMSOL Multiphysics* finite element software.

3. Thin-walled nanowire under external pressure, analytical study

3.1. The thin-walled nanowire problem

In this section, we developed a closed form analytical solution for the problem of a thin-walled cylindrical nanowire made of zinc oxide subjected to some external pressure. The nanowire is of inner and outer radii r_i and r_e, respectively and obeys the constitutive relations (16) where the strain gradient elastic coefficients $c_{i,1\leq i\leq 5}$ are given as functions of the Lame elastic coefficients λ and μ, following a suggestion made by Gologanu and co-workers [25] and studied by Enakoutsa [12] and Enakoutsa and Leblond [13] some years ago. In Gologanu and co-workers [25]'s proposal, the strain gradient elastic constants are related to the Lame elastic coefficients as

$$\left\{\begin{array}{lcl} c_1/(b^2/5) & = & -\frac{\lambda}{4} \\ c_2/(b^2/5) & = & \lambda \\ c_3/(b^2/5) & = & \left(\frac{\lambda}{16}-\frac{\mu}{4}\right) \\ c_4/(b^2/5) & = & \mu \\ c_5 & = & 0 \end{array}\right. \tag{17}$$

with the parameter b representing some material charateristic length scale. The problem is assumed to be a plane strain problem and for this reason the component of the displacement in the z-direction is assumed to be equals to zero. Use will be made of the classical cylindrical coordinates r, θ and z and the corresponding orthogonal basis e_r, e_θ, e_z and the following property on a radial vector $\mathbf{W} \equiv \Delta\mathrm{U}$:

$$(\nabla \mathrm{D})_{hhi} = \mathrm{U}_{h,hi} = W_i \quad \text{and} \quad (\nabla \mathrm{D})_{ihh} = U_{i,hh} = \Delta U_i, \tag{18}$$

that is,

$$(\nabla \mathrm{D})_{hhi} = (\nabla \mathrm{D})_{ihh} = W_i. \tag{19}$$

The canonic decomposition Eq.(19) was invented by Enakoutsa [12] and later used in the solution of several boundary problems involving curvilinear coordinates, see Enakoutsa [14, 15] to name few. Figures (1; 2) illustrate this model problem.

3.2. Derivation of the analytical solution

We want to find axi-symmetric solutions where the displacement vector field $\mathbf{U}$, the polarization vector field $\mathbf{P}$ and the electric potential field Φ are assumed to be radial, which means that $\mathbf{U} \equiv U(r)e_r$, $\mathbf{P} \equiv P(r)e_r$ and $\Phi \equiv \Phi(r)$. The procedure of solution of the thin-walled cylindrical problem consists of finding the radial displacement field and deduces the polarization vector field using the balance equations Eqs.$(13)_{1,2}$ and then calculate the electric potential Φ. We start by taking the spatial derivatives of the stress and the higher order electric force as well as the second spatial derivatives of the hyperstress in Eq.$(16)_{1,2}$. Using the properties (19) and the constitutive constants (17) we get, after derivation and application of the Kronecker delta symbol:

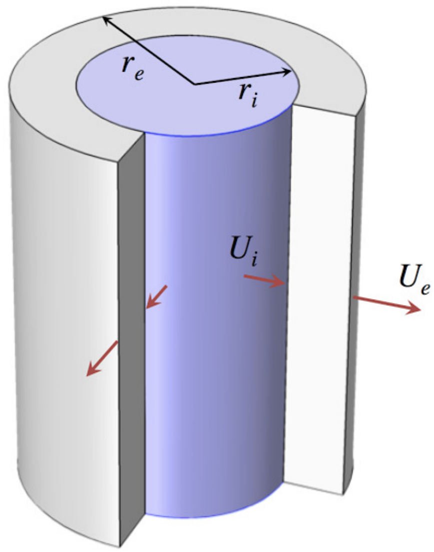

Figure 1: Illustration of the polarization of a thick walled cylindrical tube undergoing axisymmetric loading model problem. The thick walled cylindrical tube is of inner and outer radii r_i and r_e, respectively and use is made of the curvilinear cylindrical coordinates system e_r, e_θ, e_z.

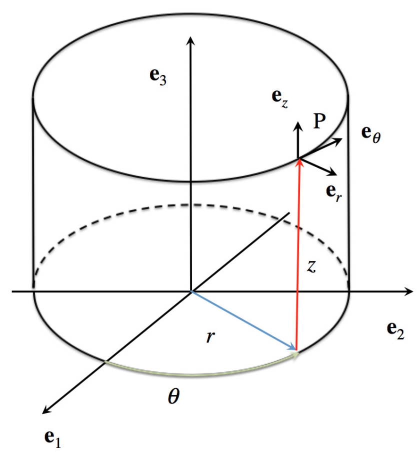

Figure 2: Illustration of the classical cylindrical coordinates r, θ and z and the corresponding orthogonal basis e_r, e_θ, e_z used to solve the problem model considered.

$$\left\{ \begin{array}{lcl} \Sigma_{ij,j} & = & (\lambda + 2\mu)\, W_i \\ M_{ijk,jk} & = & 2\dfrac{\mu b^2}{5}\dfrac{\lambda + 2\mu}{\lambda + 4\mu}(\Delta W)_i + (k_{12} + k_{44})\, P_{k,ik} + k_{44}(\Delta P)_i \\ E_i & = & (k_{12} + 2k_{44})\, W_i + aP_i \\ E_{ij,j} & = & (d_{12} + 2d_{44} + b_{12} + 2b_{44})\, W_i. \end{array} \right. \tag{20}$$

Using the relations (20) in the balance equations (13) we get the following reduced system of equations:

$$\left\{ \begin{array}{l} W_i - \dfrac{2\mu}{\lambda + 4\mu}\dfrac{b^2}{5}(\Delta W)_i + \dfrac{k_{12} + k_{44}}{\lambda + 2\mu} P_{k,ik} + \dfrac{k_{44}}{\lambda + 2\mu}(\Delta P)_i = 0 \\ \\ \left(k_{12} + 2k_{44} + d_{12} + 2d_{44} + b_{12} + 2b_{44}\right) W_i + aP_i - \left(\nabla\Phi\right)_i = 0 \end{array} \right. \tag{21}$$

in the absence of body external mechanical and electrical forces, that is $f_i = E_i^0 = 0$. The system of equations (21) then reduces

$$\left\{ \begin{array}{l} W_i - \dfrac{2\mu}{\lambda + 4\mu}\dfrac{b^2}{5}(\Delta W)_i + k^2 P_{k,ik} + k^3(\Delta P)_i = 0 \\ \\ k^4 W_i - \left(\nabla\Phi\right)_i + \chi P_i = 0 \end{array} \right. \tag{22}$$

where

$$\left\{ \begin{array}{lcl} k^2 & = & \dfrac{k_{12} + k_{44}}{\lambda + 2\mu} \\ \\ k^3 & = & \dfrac{k_{44}}{\lambda + 2\mu} \\ \\ k^4 & = & k_{12} + d_{12} + b_{12} + 2\left(k_{44} + d_{44} + b_{44}\right). \end{array} \right. \tag{23}$$

Using the component $(13)_3$ of the balance equations (13), Eqs.(24, 23) reduce to

$$\left\{ \begin{array}{l} W_i - 2\dfrac{\mu b^2}{5}\dfrac{\lambda + 2\mu}{\lambda + 4\mu}(\Delta W)_i + k^2 P_{k,ik} + k^3(\Delta P)_i = 0 \\ \\ k^4 W_i - \chi' P_i = 0 \end{array} \right. \tag{24}$$

Upon substituting of $(24)_2$ into Eq.$(24)_1$, we find

$$W_i - 2\frac{\mu b^2}{5}\frac{\lambda + 2\mu}{\lambda + 4\mu}(\Delta W)_i + k^2 P_{k,ik} - \frac{k^3 k^4}{\chi'}(\Delta W_i) = 0. \tag{25}$$

Remembering that both the displacement and polarization vector fields only depend on the radial coordinate r, Eq.(25) becomes

$$W_r - \left(2\frac{\mu b^2}{5}\frac{\lambda + 2\mu}{\lambda + 4\mu} + \frac{\left(k^2 + k^3\right) k^4}{\chi'}\right)(\Delta W)_r = 0 \tag{26}$$

or in compact form

$$\mathbf{W} - k(\Delta \mathbf{W}) = 0; \quad k = 2\frac{\mu b^2}{5}\frac{\lambda + 2\mu}{\lambda + 4\mu} + \frac{\left(k^2 + k^3\right) k^4}{\chi'} \tag{27}$$

The solution of the differential equation is well-known and yields

$$U(\rho) = D_1 I_1(\rho) + D_2 K_1(\rho) + D_3 \rho + \frac{D_4}{\rho}. \tag{28}$$

In Eq.(28)

- $\rho = \sqrt{k} r$ and the definitions of the constants $D_{i,1\leq i\leq 4}$ (the values of these constants will be fixed by the boundary conditions of this problem) have been changed
- I_1 and K_1 are the modified Bessel functions of the first and second kinds of order one, respectively.

Once we have the displacement field, the polarization vector $P \equiv P_r$ is computed as:

$$P = -\frac{k^4}{\chi'}\Phi', \tag{29}$$

that is,

$$P \equiv P(\rho) = A_1 I_1(\rho) - A_2 J_1(\rho), \tag{30}$$

with $A_{1,2}$ being two integration constants.

The solution of the electrical potential can easily be worked out through the use of Eq.13_3 whose solution is given by

$$\phi(\rho) = B_1 I_0(\rho) - B_2 J_0(\rho) + B_3, \tag{31}$$

where $B_{1,2,3}$ defines three integration constants.

To summarize, the analytic expressions for the displacement, polarization and electric potential fields for the problem considered are given by

$$\begin{cases} U(\rho) &=& D_1 I_1(\rho) + D_2 K_1(\rho) + D_3 \rho + \dfrac{D_4}{\rho} \\ P(\rho) &=& A_1 I_1(\rho) - A_2 J_1(\rho) \\ \Phi(\rho) &=& B_1 I_0(\rho) - B_2 J_0(\rho) + B_3, \end{cases} \tag{32}$$

where $A_{i,1\leq i\leq 2}$, $B_{i,1\leq i\leq 3}$ and $D_{i,1\leq i\leq 4}$ represent some integration constants that can be fixed by an appropriate choice of the boundary conditions. The integration constants $D_{i,1\leq i\leq 4}$ can be found by prescribing $U(r_i)$, $U(r_e)$, $\partial_r U(r_i)$ and

$\partial_r U(r_e)$. The integration constants $A_{i,1\leq i\leq 2}$ in the expression of the polarization field vector can also be obtained by prescribing the values of $P(r_i)$ and $P(r_e)$ on the inner and outer surface of the cylindrical tube, respectively. Calculations are straightforward. The same conditions on the displacement and polarization fields were recently applied by the authors and several other authors to analytically solve a closely related boundary value problem, see [6].

The integration constants $B_{i,1\leq i\leq 3}$ can be obtained by assuming a potential at both the inner and the outer surfaces of the cylinder, that is, $\Phi(r_i) = 0$ and $\Phi(r_e) = V$. This will provide two out of three integration constants; the remaining constant, B_3, can of course be adjusted to zero.

4. Discussion of the analytic results

An interesting point of interest of the analytical solution developped is that the displacement field, the polarization and the electric potential are significantly perturbed by the presence of flexoelectric effects. Also, in the absence of flexoelectric effects strain gradient elasticity (SGE) solution for the same model problem is recovered. Also, the presence of flexoelectric effects in the model reduces the magnitude of the displacement vector with respect to the classical and SGE solutions. The explanation is that a part of the energy induced by the external forces on the flexoelectric material has served to polarize the cylindrical tube. This is in contrast with purely elasticity where all the work done by the external loads is stored as elastic energy in the body. As a result, the circumfacial normal (orthonormal) strain in the presence of flexoelectric effects is also significantly reduced with respect to its values in the case of elastic and strain gradient elastic solutions.

5. Conclusion

We derive a close-form solution to the problem of a thick walled cylindrical tube subjected to axisymmetric loading in terms of modified Bessel functions. The solution of this problem demonstrates how the mechanical behavior of a flexoelectric material can be influenced (at the nanoscale) by the use of electric fields. This solution, besides allowing a comparision with simple elastic and SGE solutions, could be used as a benchmark solution to assess future computational design tools for flexoelectric nano-structure materials.

Future work will present a numerical solution for the same benchmark problem described in Section 3 using *COMSOL Multiphysics*, a finite element analyses software package for various multiphysics and engineering applications, expecially coupled phenomena, or multiphysics. Comparisons between the analytical and numerical predictions for the mechanical and electriccal field variables distribution in the nanostructure will also provided. We anticipate the numerical simulations of the benchmark problem will show an increasing of the electrostatic potential for decreasing values of the thickness of the cylinder (size effects).

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