On effective properties of beam-lattice structures made of flexoelectric materials

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Contents

Our Aim is

- to discuss the influence of microstructure influence on the effective properties of thin-walled structures, i.e. bars, beams, plates and shells, considering flexoelectricity[a],[b], [c].

$$\mathbf{P} \sim \nabla \mathbf{e}$$

[a] Zubko, et al., 2013. Flexoelectric effect in solids. Annual Review of Materials Research 43 (1), 387-421

[b] Yudin, P. V., Tagantsev, A. K., 2013. Fundamentals of flexoelectricity in solids. Nanotechnology 24 (43), 432001

[c] Wang, B. et al. 2019. Flexoelectricity in solids: Progress, challenges, and perspectives. Progress in Materials Science 106, 100570

Here

- we discuss an example of microstructured bar called pantographic bar.

Motivation:

- At small scales flexoelectricity may play significant and even dominant role for electromechanical coupling.

Basic relations of flexoelectricity

we introduce the following primary variables

$$\mathbf{u} = \mathbf{u}(\mathbf{x}, t), \quad \mathbf{P} = \mathbf{P}(\mathbf{x}, t), \tag{1}$$

where $\mathbf{u}$ and $\mathbf{P}$ are vectors of displacements and electric polarization, respectively, $\mathbf{x}$ is the position vector, and t is time. Here we restrict to the pure electromechanical theory, so the energy density takes the form

$$W = W(\mathbf{e}, \mathbf{P}, \nabla\nabla\mathbf{u}, \nabla\mathbf{P}), \qquad \mathbf{e} = \frac{1}{2}\left(\nabla\mathbf{u} + (\nabla\mathbf{u})^T\right), \tag{2}$$

where $\mathbf{e}$ is the strain tensor and ∇ denotes the three-dimensional nabla-operator. If we neglect the dependence on $\mathbf{P}$ and $\nabla\mathbf{P}$ in (2) we recover the Toupin–Mindlin strain gradient elasticity. On the other hand, if we omit in (2) only second deformation gradient $\nabla\nabla\mathbf{u}$ we get Mindlin's theory of dielectrics. Finally, Eq. (2) can be reduced to the piezoelectricity with constitutive equation

$$W = W(\mathbf{e}, \mathbf{P}).$$

Variational principle

For flexoelectric solids there exists the variational principle

$$\delta \int\limits_V \left(W - \frac{1}{2}\epsilon_0 \mathbf{E}\cdot\mathbf{E} - \mathbf{P}\cdot\mathbf{E}\right) dV = 0, \qquad (3)$$

where ϵ_0 is a vacuum permittivity, and $\mathbf{E}$ is the electric field, expressed through the electric potential ϕ: $\mathbf{E} = -\nabla\phi$. Last relation ensures that Maxwell's equation

$$\nabla \times \mathbf{E} = \mathbf{0}, \qquad (4)$$

is automatically satisfied. As a result, from (3) we get

$$\nabla \cdot \boldsymbol{\sigma} = \mathbf{0}, \quad \boldsymbol{\sigma} = \mathbf{T} - \nabla\cdot\mathbf{M}, \quad \mathbf{T} = \frac{\partial W}{\partial \mathbf{e}}, \quad \mathbf{M} = \frac{\partial W}{\partial \nabla\nabla\mathbf{u}}, \qquad (5)$$

$$\nabla \cdot \mathbf{D} = 0, \quad \mathbf{D} = \epsilon_0\mathbf{E} + \mathbf{P}, \quad \mathbf{E} \equiv -\nabla\phi = \frac{\partial W}{\partial \mathbf{P}} - \nabla\cdot\frac{\partial W}{\partial \nabla\mathbf{P}}. \qquad (6)$$

Here $\boldsymbol{\sigma}$ is the total stress tensor, $\mathbf{T}$ and $\mathbf{M}$ are the stress and hyper-stress tensors, respectively, and $\mathbf{D}$ is the electric displacement field. Eq. (6) is another Maxwell's equation of electrostatics.

Energy

In what follows we consider W as a quadratic form of its arguments

$$
\begin{aligned}
W =& \frac{1}{2}\mathbf{e} : \mathbf{C} : \mathbf{e} + \frac{1}{2}\mathbf{P} \cdot \mathbf{A} \cdot \mathbf{P} - \mathbf{P} \cdot \mathbf{d} : \mathbf{e} \\
&+ \frac{1}{2}\nabla\mathbf{P} : \mathbf{B} : \nabla\mathbf{P} - \nabla\mathbf{e} \,\vdots\, \mathbf{F} \cdot \mathbf{P} - \mathbf{e} : \mathbf{H} : \nabla\mathbf{P} + \frac{1}{2}\nabla\nabla\mathbf{u} \,\vdots\, \mathbf{G} \,\vdots\, \nabla\nabla\mathbf{u},
\end{aligned}
\tag{7}
$$

where $:$ and $\vdots$ stand for double and triple dot products, respectively, and several material tensors are introduced. In (7), $\mathbf{C}$ is a fourth-order tensor of elastic moduli, $\mathbf{A} = \chi^{-1}$ is a symmetric second-order reciprocal dielectric susceptibility tensor, $\mathbf{d}$ is a third–order piezoelectric tensor, $\mathbf{B}$ is a polarization gradient coupling fourth-order tensor, $\mathbf{F}$ and $\mathbf{H}$ denote fourth-order flexocoupling tensors, and $\mathbf{G}$ is a six-order tensor of elastic moduli related to strain-gradients. $C_{ijmn} = C_{mnij} = C_{jimn}$, other tensors also have symmetry properties: $d_{ijk} = d_{jik}$, $B_{ijmn} = B_{mnij}$, $F_{ijmn} = F_{jimn}$, etc. Flexocoupling tensors $\mathbf{F}$ and $\mathbf{H}$ are mutually dependent.

From (7) we get the dependence for stress tensor

$$\mathbf{T} = \mathbf{C} : \mathbf{e} - \mathbf{P} \cdot \mathbf{d} - (\mathbf{H} : \nabla \mathbf{P})^T. \qquad (8)$$

Obviously, $\mathbf{T}$ depends on polarization and its gradient. Using the relations

$$\frac{\partial W}{\partial \mathbf{P}} = \mathbf{A} \cdot \mathbf{P} - \mathbf{d} : \mathbf{e} - \nabla \mathbf{e} \,\vdots\, \mathbf{F}, \quad \frac{\partial W}{\partial \nabla \mathbf{P}} = \mathbf{B} : \nabla \mathbf{P} - \mathbf{e} : \mathbf{H}, \qquad (9)$$

Eq. (6) transforms into

$$\mathbf{E} = \mathbf{A} \cdot \mathbf{P} - \mathbf{d} : \mathbf{e} - \nabla \mathbf{e} \,\vdots\, \mathbf{F} - \nabla \cdot (\mathbf{B} : \nabla \mathbf{P}) + \nabla \cdot (\mathbf{e} : \mathbf{H}). \qquad (10)$$

Flexoelectric tensor

In the case of homogeneous materials and when the polarization gradient is constant from (10) we get the key equation of flexoelectricity

$$\mathbf{P} = \boldsymbol{\chi} \cdot \mathbf{E} + \mathbf{E} : \mathbf{e} + \boldsymbol{\mu} \vdots \nabla \mathbf{e}, \qquad (11)$$

with the fourth-order $\boldsymbol{\mu}$ defined though the relation

$$\boldsymbol{\mu} \vdots \nabla \mathbf{e} = \boldsymbol{\chi} \cdot [\nabla \mathbf{e} \vdots \mathbf{F} - \nabla \cdot (\mathbf{e} : \mathbf{H})] \quad \forall\, \mathbf{e},$$

here we also introduced another piezoelectric tensor $\mathbf{E} = \boldsymbol{\chi} \cdot \mathbf{d}$. Without electric field and for non-piezoelectric materials, that is when $\mathbf{d} = \mathbf{0}$, Eq. (11) reduces to

$$\mathbf{P} = \boldsymbol{\mu} \vdots \nabla \mathbf{e}. \qquad (12)$$

Eqs. (11) and (12) give also the possibility to introduce $\mathbf{E}$ and $\boldsymbol{\mu}$ as follows

$$\mathbf{E} = \frac{\partial \mathbf{P}}{\partial \mathbf{e}}, \quad \boldsymbol{\mu} = \frac{\partial \mathbf{P}}{\partial \nabla \mathbf{e}}. \qquad (13)$$

Cubic symmetry and isotropy

For materials with cubic symmetry there exist only three independent components of $\boldsymbol{\mu}$ that are μ_{1111}, μ_{1122}, and μ_{1212}

$$\boldsymbol{\mu} = \begin{pmatrix} \mu_{11} & \mu_{12} & \mu_{12} & 0 & 0 & 0 \\ \mu_{12} & \mu_{11} & \mu_{12} & 0 & 0 & 0 \\ \mu_{12} & \mu_{12} & \mu_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & \mu_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & \mu_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & \mu_{44} \end{pmatrix}, \qquad (14)$$

where $\mu_{11} = \mu_{1111}$, $\mu_{12} = \mu_{1122}$, and $\mu_{44} = \mu_{1212}$.
For isotropic materials $\boldsymbol{\mu}$ takes the form

$$\boldsymbol{\mu} = \mu_{ijkl}\mathbf{E}_i \otimes \mathbf{E}_j \otimes \mathbf{E}_k \otimes \mathbf{E}_l,$$

where

$$\mu_{ijkl} = \mu_1(\delta_{ik}\delta_{lj} + \delta_{il}\delta_{kj} + \delta_{ij}\delta_{kl}) + \mu_2(\delta_{ik}\delta_{lj} + \delta_{il}\delta_{kj} - 2\delta_{ij}\delta_{kl}), \qquad (15)$$

μ_1 and μ_2 are two independent flexoelectric moduli, and δ_{ij} is the Kronecker symbol.

Piezoelectric solids

Neglecting flexoelectric and strain gradient contributions we come to the constitutive equations of piezoelectric solids

$$W = W(\mathbf{e}, \mathbf{P}) = \frac{1}{2}\mathbf{e} : \mathbf{C} : \mathbf{e} + \frac{1}{2}\mathbf{P} \cdot \mathbf{A} \cdot \mathbf{P} - \mathbf{P} \cdot \mathbf{d} : \mathbf{e}, \quad (16)$$

$$\boldsymbol{\sigma} = \mathbf{T} = \mathbf{C} : \mathbf{e} - \mathbf{P} \cdot \mathbf{d}, \quad \mathbf{E} = \mathbf{A} \cdot \mathbf{P} - \mathbf{d} : \mathbf{e}. \quad (17)$$

Eq. $(17)_2$ can be written also as

$$\mathbf{P} = \boldsymbol{\chi} \cdot \mathbf{E} + \mathbf{E} : \mathbf{e}. \quad (18)$$

Pantographic bar

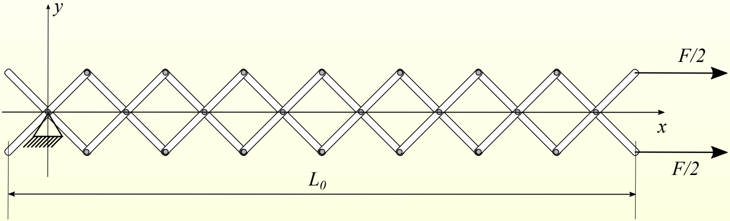

Figure: Pantographic bar loaded by a net force F. The number of cells is $n = 8$.

Deformation of a cell

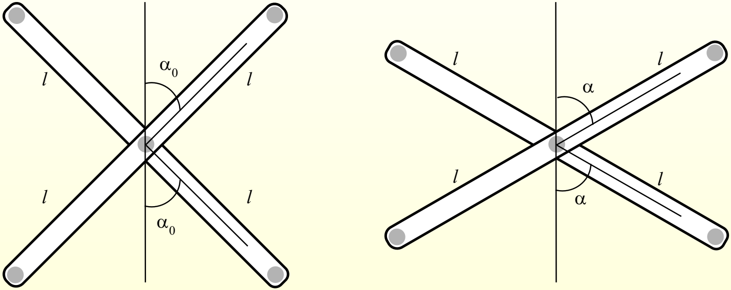

Figure: Deformation of a pantographic cell.

Kinematics and total energy

Considering pantographic bar elongation we get

$$L_0 = 2nl \sin\alpha_0, \quad L = 2nl \sin\alpha, \quad \varepsilon \equiv \frac{L - L_0}{L_0} = \frac{\sin\alpha}{\sin\alpha_0} - 1, \qquad (19)$$

For small deformations we have

$$L = L_0 + \Delta L, \quad \Delta L = 2nl\varepsilon\,\Delta\alpha, \quad \varepsilon = \cot\alpha_0\,\Delta\alpha, \quad \varepsilon_{yy} = -\tan^2\alpha_0\,\varepsilon,$$
$$M = \mathbb{K}\tau, \quad \tau = 2\Delta\alpha, \quad \mathbb{K} = \mu J_p/h. \qquad (20)$$

The total strain energy stored in all pivots is given by

$$\mathcal{E}_t = 2(3n-2)\mathbb{K}(\Delta\alpha)^2 = 2(3n-2)\frac{\mathbb{K}}{(\cot\alpha_0)^2}\varepsilon^2. \qquad (21)$$

From

$$\delta\mathcal{E}_t - \delta\mathcal{A} = 0, \quad \mathcal{A} = F(L - L_0) \quad \text{we get} \quad \varepsilon = \frac{n}{3n-2}\frac{Fl}{2\mathbb{K}}\sin\alpha_0. \qquad (22)$$

So the effective extensional stiffness is

$$\mathbb{E} = 2\frac{3n-2}{nl\sin\alpha_0}\mathbb{K}. \qquad (23)$$

Torsion: three pivots

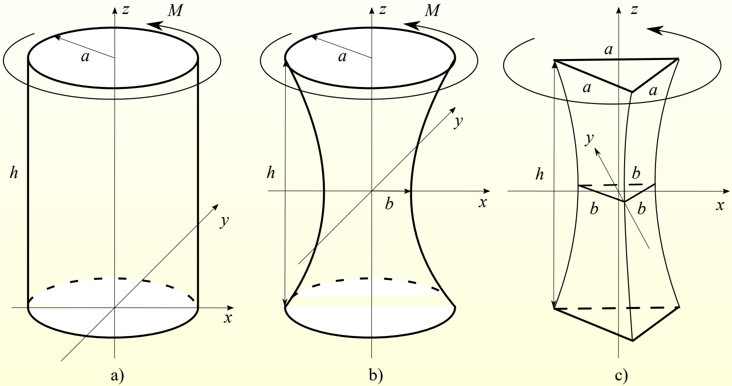

Figure: Torsion of a pivot: a) circular cylinder, $r = a$, $0 \leq z \leq h$; b) circular hyperboloid, $r = (z^2 + b^2)^{1/2}$, $-h/2 \leq z \leq h/2$, and $a^2 = h^2/4 + b^2$; c) solid with a triangular cross-section, which is an equilateral triangle of side length d, $d(0) = b$, $d(\pm h/2) = a$, $d(z) = b + 4(a - b)z^2/h^2$, $-h/2 \leq z \leq h/2$.

Circular cross-section

First, let us consider a Saint-Venant-type solution for a circular cylinder

$$\mathbf{u} = \theta(z)\mathbf{E}_z \times \mathbf{x}, \quad \theta(z) = \theta_0 z, \tag{24}$$

where r, φ, z are the polar coordinates and $\mathbf{E}_r$, $\mathbf{E}_\varphi$ and $\mathbf{E}_z$ are corresponding unit base vectors, and $\theta_0 = \tau/h$ is a twist angle per unit length. So here we have that

$$\nabla\mathbf{u} = \theta_0 \mathbf{E}_z \otimes \mathbf{E}_z \times \mathbf{x} - \theta_0 z\mathbf{I} \times \mathbf{E}_z, \quad \mathbf{e} = \gamma r(\mathbf{E}_z \otimes \mathbf{E}_\varphi + \mathbf{E}_\varphi \otimes \mathbf{E}_z), \qquad \gamma = \frac{1}{2}\theta_0$$

where $\otimes$ is the dyadic product. Obviously, here $\nabla\mathbf{e} \neq \mathbf{0}$ as $\mathbf{e}$ is a linear function of r. It is given by

$$\nabla\mathbf{e} = \gamma\left(\mathbf{E}_r \otimes \mathbf{E}_z \otimes \mathbf{E}_\varphi + \mathbf{E}_r \otimes \mathbf{E}_\varphi \otimes \mathbf{E}_z - \mathbf{E}_\varphi \otimes \mathbf{E}_z \otimes \mathbf{E}_r - \mathbf{E}_\varphi \otimes \mathbf{E}_r \otimes \mathbf{E}_z\right).$$

Nevertheless, using (12) and (14) we get that $\mathbf{P} = \mathbf{0}$. So no polarization is induced by the strain gradient term, thus flexoelectric effects do not appear for the effective homogenized pantograph. For a circular cylinder the flexoelectric effect should be expected for less symmetrical constitutive equations.

Circular cylinder with variable diameter

We assume the solution in the form with $z-$dependent twist:

$$\mathbf{u} = \theta(z)\mathbf{E}_z \times \mathbf{x}, \quad \theta(z) = \int_{-h/2}^{z} \frac{M}{\mu J_p(\xi)}\, d\xi, \tag{25}$$

and $J_p(z) = \pi r^4(z)/2$ is the polar moment of inertia and $r(z) = (z^2 + b^2)^{1/2}$ is the equation of the pivot surface. We have for cubic symmetry and for an isotropic solid

$$\mathbf{P} = (\mu_{1122} + \mu_{1212})\gamma' r\mathbf{E}_\varphi, \quad \mathbf{P} = 2(\mu_1 + \mu_2)\gamma' r\mathbf{E}_\varphi, \qquad \gamma = \frac{1}{2}\theta'. \tag{26}$$

Nevertheless, the mean polarization is zero:

$$\bar{\mathbf{P}} \equiv \langle \mathbf{P} \rangle \equiv \frac{1}{V}\int_V \mathbf{P}\, dV = \mathbf{0}. \tag{27}$$

But the flexoelectric contribution in the energy is not zero

$$W_{flexo} = \frac{1}{2}\nabla\mathbf{P} : \mathbf{B} : \nabla\mathbf{P} - \nabla\mathbf{e} \,\vdots\, \mathbf{F}\cdot\mathbf{P} - \mathbf{e} : \mathbf{H} : \nabla\mathbf{P} \neq 0. \tag{28}$$

Prismatic pivot with variable cross-section

We assume a solution in the form

$$\mathbf{u} = \theta(z)\mathbf{E}_z \times \mathbf{x} + \psi(x,y,z)\mathbf{E}_z, \quad \psi = \theta_0\eta(x,y), \tag{29}$$

where $\eta(x,y)$ is the warping (torsion) function and θ_0 is the twist per unit length given by

$$\eta(x,y) = \frac{y(3x^2 - y^2)}{6d}, \quad \mathbb{K} = \sqrt{3}\mu d^4/80h.$$

We consider the approximate solution with ψ given by

$$\psi = \theta'(z)\frac{y(3x^2 - y^2)}{6d(z)}, \tag{30}$$

where $\theta(z)$ is given as before with $J_p = \frac{\sqrt{3}d^4(z)}{48}$.
Here $\nabla\mathbf{e}$ includes the term $\psi''\mathbf{E}_z \otimes \mathbf{E}_z \otimes \mathbf{E}_z$. It produces the transverse polarization $P_3 = 3\mu_1\psi''$. Here the mean polarization does not vanish

$$\bar{\mathbf{P}} \equiv \langle \mathbf{P} \rangle = \bar{P}_3\mathbf{E}_z, \qquad \bar{P}_3 = 3\mu_1\frac{1}{V}\int_V \psi''\,dx\,dy\,dz. \tag{31}$$

Symmetry requirements

Effective piezoelectricity requires some constraints on non-centrosymmetry of flexoelectric composites

- More precisely, the microstructure should break centrosymmetry
- The first example is the most symmetric one, so for an isotropic solid we have not flexoelectricity effect
- For the second example we get polarization at the microscale but it disappears after averaging.
- For third example the mean polarization does not vanish, it presents a case which exactly corresponds to the requirement of violation of centrosymmetry and could be a good candidate for effective piezoelectric composites

Effective piezoelectric properties of the pantograph

For effective 1D piezoelectric medium we have

$$W = \frac{1}{2}\mathbf{e} : \mathbf{C} : \mathbf{e} + \frac{1}{2}\chi_0^{-1}\mathbf{P} \cdot \mathbf{P} + W_{flexo}. \qquad (32)$$

The torque is given

$$M = 2\mathbb{K} \tan \alpha_0 \, \varepsilon,$$

and

$$\theta(z) = \frac{2\mathbb{K} \tan \alpha_0}{\mu} \int_{-h/2}^{z} \frac{d\xi}{J_p(\xi)} \, \varepsilon, \quad \psi(x, y, z) = \frac{\mathbb{K} \tan \alpha_0}{3\mu J_p(z) d(z)} y(3x^2 - y^2) \, \varepsilon. \qquad (33)$$

Finally, we obtain that $\bar{P}_3 = e_{311}\varepsilon$ with the effective piezoelectric modulus e_{311} given by

$$e_{311} = \mu_1 \frac{\mathbb{K} \tan \alpha_0}{\mu V} \int_V \frac{d^2}{dz^2} \frac{y(3x^2 - y^2)}{J_p(z) d(z)} \, dx \, dy \, dz. \qquad (34)$$

References

- Eremeyev, V.A., Ganghoffer, J.F., Konopińska-Zmysłowska, V. and Uglov, N.S., 2020. Flexoelectricity and apparent piezoelectricity of a pantographic micro-bar. *International Journal of Engineering Science*, **149**, 103213.
- Mawassy, N., Reda, H., Ganghoffer, J.-F., Eremeyev, V. A., and Lakiss, H. 2021. A variational approach of homogenization of piezoelectric composites towards piezoelectric and flexoelectric effective media. *International Journal of Engineering Science* **158**, 103410
- Malikan, M. and Eremeyev, V.A., 2020. On the dynamics of a visco-piezo-flexoelectric nanobeam. *Symmetry*, **12**(4), 643.

Conclusions

1. The effective piezoelectric properties of microstructured flexoelectric structures is discussed;
2. A pantographic bar is considered as the first example;
3. The presented results shown that the effective properties strongly depend on the microstructure;
4. Other examples for bending dominant flexoelectric structures will be analyzed in more details such as laminated plates or beams.

Thank you for your attention!!!

Further questions:

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