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DISPERSION PROPERTIES IN HOMOGENIZED PIEZOELECTRIC PHONONIC MATERIALS

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Summary: We consider a composite medium made of weakly piezoelectric inclusions periodically distributed in the matrix which is made of a different piezoelectric material. The medium is subject to a periodic excitation with an incidence wave frequency independent of scale ε of the microscopic heterogeneities. Two-scale method of homogenization was applied to obtain the limit homogenized model which describes acoustic wave propagation in the piezoelectric medium when $\varepsilon \to 0$. In analogy with the purely elastic composite, the resulting model is featured by existence of the acoustic band gaps. These are identified for certain frequency ranges whenever the so-called homogenized mass becomes negative. The homogenized model can be used for band gap prediction and for dispersion analysis for low wave numbers. Modeling of these types of composite materials seems to be perspective in the context of Smart Materials design.

1. Introduction

By the *phononic materials* we understand bi-phasic elastic media with periodic structure and with large contrasts between the stiffness parameters associated with different phases, whereas their specific mass is comparable. It is well known that for certain frequency ranges, such elastic structures can suppress the elastic wave propagation, i.e. they exhibit the band gaps. Here we consider *piezoelectric* composite materials where the large contrasts are related not only to elasticity, but also to other piezoelectric parameters, namely the piezoelectric coupling coefficients and the dielectricity.

An alternative and effective way of modeling the phononic materials is the asymptotic homogenization method applied to the strongly heterogeneous elastic, or piezoelectric medium. We consider a composite made of weakly piezoelectric inclusions periodically distributed in the matrix which is made of a different piezoelectric material. The medium is subject to a periodic excitation. The homogenized model of acoustic wave propagation in the piezoelectric medium is characterized by the homogenized elastic, dielectric and piezoelectric parameters and by the homogenized mass tensor. The dispersion properties and namely the *band gap distributions* are inherited from the homogenized mass tensor which depends nonlinearly on the incident wave frequency; when this tensor is negative (in the sense of its eihenvalues) the wave equation looses its hyperbolicity. According to the number of the negative eigenvalues the wave propagation is

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restricted to a certain direction, so that the homogenized material is strongly anisotropic. We refer to interesting paper Milton and Willis (2007), where anisotropy and randomness aspect in the phononic materials are discussed.

In the context of mathematical modelling, the method of homogenization was proposed to study the heterogeneous elastic media (sometimes called *phononic crystals*) in (Auriault and Bonnet, 1985) and recently treated in (Avila et.al., 2005, 2008), where also numerical results were reported. For related photonic problem in electromagnetic wave propagation see Bouchitté and Felbacq (2004).

For elastic composites an existence of band gaps for certain wavelengths was shown in Avila et.al. (2008) as the consequence of the non positivity of the limit "homogenized mass density". In the present paper we consider acoustic wave propagation in a *piezoelectric strongly heterogeneous composite*; the problem was formulated in Rohan and Miara (2006-B). Here we summarize the esential homogenization results and propose the dispersion analysis which involves modified Christoffel acoustic tesor, due to presence of the piezoelectric coupling with the electric field. This is an extension of the recent publication (Rohan et.al., 2009) where the elastic homogeneized phononic material was discussed in detail.

2. Piezoelectric phononic material

We consider a piezoelectric medium whose material properties, being attributed to material constituents vary periodically with position; the period is denoted by ε . Throughout the text all quantities varying with this microstructural periodicity are denoted with superscript ε .

2.1. Definition of the strongly heterogeneous material

The material properties are related to the periodic geometrical decomposition which is now introduced, see Fig. 1. We consider an open bounded domain $\Omega \subset \mathbb{R}^3$ and the reference cell $Y =]0, 1[^3$ with inclusion $\overline{Y_2} \subset Y$, whereby the matrix part is $Y_1 = Y \setminus \overline{Y_2}$. Using the reference cell we generate the decomposition of Ω as follows

$$\Omega_2^{\varepsilon} = \bigcup_{k \in \mathbb{K}^{\varepsilon}} \varepsilon(Y_2 + k) , \text{ where } \mathbb{K}^{\varepsilon} = \{k \in \mathbb{Z} | \varepsilon(k + \overline{Y_2}) \subset \Omega\} ,$$
$$\Omega_1^{\varepsilon} = \Omega \setminus \Omega_2^{\varepsilon} ,$$

so that $\Omega = \Omega_1^{\varepsilon} \cup \Omega_2^{\varepsilon} \cup \Gamma^{\varepsilon}$, where Γ^{ε} is the interface $\Gamma^{\varepsilon} = \overline{\Omega_1^{\varepsilon}} \cap \overline{\Omega_2^{\varepsilon}}$.

Properties of a three dimensional body made of the piezoelectric material are described by three tensors: the elasticity tensor c_{ijkl}^{ε} , the dielectric tensor d_{ij}^{ε} and the piezoelectric coupling tensor g_{kij}^{ε} , where i, j, k = 1, 2, ..., 3. As usually we assume both major and minor symmetries of c_{ijkl}^{ε} ($c_{ijkl}^{\varepsilon} = c_{jikl}^{\varepsilon} = c_{klij}^{\varepsilon}$), symmetry of d_{ij}^{ε} , i.e. $d_{ij}^{\varepsilon} = d_{ji}^{\varepsilon}$ and the following one of g_{kij}^{ε} : $g_{kij}^{\varepsilon} = g_{kji}^{\varepsilon}$.

We assume that inclusions are occupied by a "very soft material" in such a sense that there the material coefficients are significantly smaller than those of the matrix compartment, *except the material density*, which is comparable in both the compartments; as an important feature of the modelling, the *strong heterogeneity* is related to the geometrical scale of the underlying



Figure 1: Periodic structure of the piezoelectric composite with ε^2 -scaled material in the inclusions Y_2 .

microstructure by coefficient ε^2 :

$$\rho^{\varepsilon}(x) = \begin{cases} \rho^{1} & \text{in } \Omega_{1}^{\varepsilon}, \\ \rho^{2} & \text{in } \Omega_{2}^{\varepsilon}, \end{cases} \qquad c^{\varepsilon}_{ijkl}(x) = \begin{cases} c^{1}_{ijkl} & \text{in } \Omega_{1}^{\varepsilon}, \\ \varepsilon^{2}c^{2}_{ijkl} & \text{in } \Omega_{2}^{\varepsilon}, \end{cases} \\ g^{\varepsilon}_{kij}(x) = \begin{cases} g^{1}_{kij} & \text{in } \Omega_{1}^{\varepsilon}, \\ \varepsilon^{2}g^{2}_{kij} & \text{in } \Omega_{2}^{\varepsilon}, \end{cases} \qquad d^{\varepsilon}_{ij}(x) = \begin{cases} d^{1}_{ij} & \text{in } \Omega_{1}^{\varepsilon}, \\ \varepsilon^{2}d^{2}_{ij} & \text{in } \Omega_{2}^{\varepsilon}. \end{cases} \end{cases}$$
(1)

2.2. Problem formulation

We consider stationary wave propagation in the medium introduced above. Although the problem can be treated for a general case of boundary conditions, for simplicity we restrict the model to the description of clamped structures loaded by volume forces and subject to volume distributed electric charges. Assuming a synchronous harmonic excitation of a single frequency ω

$$\tilde{\boldsymbol{f}}(x,t) = \boldsymbol{f}(x)e^{i\omega t}$$
, $\tilde{q}(x,t) = q(x)e^{i\omega t}$,

where $f = (f_i), i = 1, 2, 3$ is the magnitude field of the applied volume force and q is the magnitude of the distributed volume charge, in general, we should expect a dispersive piezoelectric field with magnitudes $(\mathbf{u}^{\varepsilon}, \varphi^{\varepsilon})$

$$\tilde{\boldsymbol{u}}^{\varepsilon}(x,\omega,t) = \boldsymbol{u}^{\varepsilon}(x,\omega)e^{i\omega t} , \quad \tilde{\varphi}^{\varepsilon}(x,\omega,t) = \varphi^{\varepsilon}(x,\omega)e^{i\omega t}$$

This allows us to study the steady periodic response of the medium, as characterized by field $(\mathbf{u}^{\varepsilon}, \varphi^{\varepsilon})$ which satisfies the following boundary value problem:

$$-\omega^{2}\rho^{\varepsilon}\boldsymbol{u}^{\varepsilon} - \operatorname{div}\boldsymbol{\sigma}^{\varepsilon} = \boldsymbol{f} \quad \text{in } \Omega,$$

$$-\operatorname{div}\boldsymbol{D}^{\varepsilon} = \boldsymbol{q} \quad \text{in } \Omega,$$

$$\boldsymbol{u}^{\varepsilon} = 0 \quad \text{on } \partial\Omega,$$

$$\varphi^{\varepsilon} = 0 \quad \text{on } \partial\Omega,$$

(2)

where the stress tensor $\sigma^{\varepsilon} = (\sigma_{ij}^{\varepsilon})$ and the electric displacement D^{ε} are defined by constitutive laws

$$\sigma_{ij}^{\varepsilon} = c_{ijkl}^{\varepsilon} e_{kl}(\boldsymbol{u}^{\varepsilon}) - g_{kij}^{\varepsilon} \partial_k \varphi^{\varepsilon},$$

$$D_k^{\varepsilon} = g_{kij}^{\varepsilon} e_{ij}(\boldsymbol{u}^{\varepsilon}) + d_{kl}^{\varepsilon} \partial_l \varphi^{\varepsilon}.$$
(3)

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The problem (2) can be weakly formulated as follows: Find $(\boldsymbol{u}^{\varepsilon}, \varphi^{\varepsilon}) \in \mathbf{H}_{0}^{1}(\Omega) \times H_{0}^{1}(\Omega)$ such that

$$-\omega^{2} \int_{\Omega} \rho^{\varepsilon} \boldsymbol{u}^{\varepsilon} \cdot \boldsymbol{v} + \int_{\Omega} c_{ijkl}^{\varepsilon} e_{kl}(\boldsymbol{u}^{\varepsilon}) e_{ij}(\boldsymbol{v}) - \int_{\Omega} g_{kij}^{\varepsilon} e_{ij}(\boldsymbol{v}) \partial_{k} \varphi^{\varepsilon} = \int_{\Omega} \boldsymbol{f} \cdot \boldsymbol{v} ,$$

$$\int_{\Omega} g_{kij}^{\varepsilon} e_{ij}(\boldsymbol{u}^{\varepsilon}) \partial_{k} \psi + \int_{\Omega} d_{kl} \partial_{l} \varphi^{\varepsilon} \partial_{k} \psi = \int_{\Omega} q \psi ,$$
(4)

for all $(\mathbf{v}, \psi) \in \mathbf{H}_0^1(\Omega) \times H_0^1(\Omega)$.

3. Homogenized model of waves in piezo-elastic composite

Problem (4) was studied in Avila et.al. (2008) using the unfolding method of homogenization to obtain a limit model when $\varepsilon \to 0$. Here the aim is to report how the numerical analysis of the band gaps based on the stationary waves corresponds with *long guided waves* and the classical form of the dispersion diagrams. Therefore we just record the theoretical results from (Rohan and Miara, 2006-B). We remark that the spirit of the homogenization was explained exhaustively in (Rohan et.al., 2009) for the case of *elastic* composites. In our present application the differences are:

- in analysis of the eigen-solutions related to the "soft" inclusion piezoelectric materials couples elastic deformations with induced electric field;
- the homogenized material piezoelectric properties involve elasticity, piezo-coupling and dielectricity tensors; these are determined by the perforated matrix exclusively, as well as in the purely elastic case;
- the macroscopic model of piezo-elastic wave propagation involves coupled system of the balance-of-forces equation and the electric field conservation.

For brevity in what follows we employ the following notations:

$$a_{Y_{2}}(\boldsymbol{u},\boldsymbol{v}) = \int_{Y_{2}} c_{ijkl}^{2} e_{kl}^{y}(\boldsymbol{u}) e_{ij}^{y}(\boldsymbol{v}),$$

$$d_{Y_{2}}(\phi,\psi) = \int_{Y_{2}} d_{kl}^{2} \partial_{l}^{y} \phi \partial_{k}^{y} \psi,$$

$$g_{Y_{2}}(\boldsymbol{u},\psi) = \int_{Y_{2}} g_{kij}^{2} e_{ij}^{y}(\boldsymbol{u}) \partial_{k}^{y} \psi,$$

$$\varrho_{Y_{2}}(\boldsymbol{u},\boldsymbol{v}) = \int_{Y_{2}} \rho^{2} \boldsymbol{u} \cdot \boldsymbol{v},$$
(5)

whereby analogical notations are used when the integrations apply over Y_1 .

3.1. Auxiliary eigenvalue problem

The auxiliary eigenvalue problem arises due to linearity – the displacement and electric potential fields waves are expanded in series based on the eigen-solution of the associated piezo-elastic problem. This represents vibrations of the piezo-material in inclusion Y_2 with clamped boundary ∂Y_2 ; the material is electrically insulated on ∂Y_2 .

Particular solution Let us define $\varphi^{2P} = q(x)\tilde{p}(y)$ where $\tilde{p} \in H_0^1(Y_2)$ is the unique solution satisfying

$$d_{Y_2}(\tilde{p}, \psi) = \int_{Y_2} \psi \qquad \forall \psi \in H_0^1(Y_2) ,$$

hence also $d_{Y_2}(\varphi^{2P}, \psi) = q(x) \int_{Y_2} \psi \qquad \forall \psi \in H_0^1(Y_2) .$ (6)

Spectral problem The spectral problem reads as: find eigenelements $[\lambda^r; (z^r, p^r)]$, where $z^r \in \mathbf{H}_0^1(Y_2)$ and $p^r \in H_0^1(Y_2)$, r = 1, 2, ..., such that

$$a_{Y_{2}}(\boldsymbol{z}^{r}, \boldsymbol{\nu}) - g_{Y_{2}}(\boldsymbol{\nu}, p^{r}) = \lambda^{r} \varrho_{Y_{2}}(\boldsymbol{z}^{r}, \boldsymbol{\nu}) \quad \forall \boldsymbol{\nu} \in \mathbf{H}_{0}^{1}(Y_{2}), g_{Y_{2}}(\boldsymbol{z}^{r}, \psi) + d_{Y_{2}}(p^{r}, \psi) = 0 \quad \forall \psi \in H_{0}^{1}(Y_{2}),$$
(7)

with the orthonormality condition imposed on eigenfunctions z^r :

$$a_{Y_2}\left(\boldsymbol{z}^r,\,\boldsymbol{z}^s\right) + d_{Y_2}\left(p^r,\,p^s\right) = \lambda^r \varrho_{Y_2}\left(\boldsymbol{z}^r,\,\boldsymbol{z}^s\right) \stackrel{!}{=} \lambda^r \delta_{rs}.$$
(8)

The orthogonality in (8) follows easily on rewriting (7) for $v = z^s$ and $\psi = p^r$,

$$a_{Y_2}(\mathbf{z}^r, \mathbf{z}^s) - g_{Y_2}(\mathbf{z}^s, p^r) = \lambda^r \varrho_{Y_2}(\mathbf{z}^r, \mathbf{z}^s), g_{Y_2}(\mathbf{z}^s, p^r) + d_{Y_2}(p^s, p^r) = 0,$$

so that on eliminating $g_{Y_2}(z^s, p^r)$ one obtains

$$\begin{aligned} a_{Y_2}\left(\boldsymbol{z}^r, \, \boldsymbol{z}^s\right) + d_{Y_2}\left(\boldsymbol{p}^s, \, \boldsymbol{p}^r\right) &= \lambda^r \varrho_{Y_2}\left(\boldsymbol{z}^r, \, \boldsymbol{z}^s\right) \\ &\stackrel{!}{=} \lambda^s \varrho_{Y_2}\left(\boldsymbol{z}^s, \, \boldsymbol{z}^r\right) \end{aligned}$$

Moreover, the ellipticity of $a_{Y_2}(\cdot, \cdot)$ and $d_{Y_2}(\cdot, \cdot)$ yields $\lambda^r > 0$ for all $r = 1, 2, \ldots$.

Perturbations in the inclusion. Using the above auxiliary problems the relative motion and electric field fluctuations in Y_2 can be described; these are described by functions $u^2(x, y)$ and $\varphi^2(x, y)$. With the eigenelements (z^r, p^r) defined in (7)-(8) and having computed φ^{2P} we have the decomposed form

$$\boldsymbol{u}^{2}(x,y) = \sum_{r\geq 1} \alpha^{r}(x)\boldsymbol{z}^{r}(y) ,$$

$$\varphi^{2}(x,y) = \varphi^{2H} + \varphi^{2P} = \sum_{r\geq 1} \alpha^{r}(x)p^{r}(y) + q(x)\tilde{p}(y) ,$$
(9)

where α^r is expressed as follows:

$$\alpha^{r} = \frac{1}{\lambda^{r} - \omega^{2}} \left[\boldsymbol{f}(x) \cdot \int_{Y_{2}} \boldsymbol{z}^{r} + \omega^{2} \boldsymbol{u}^{1}(x) \cdot \int_{Y_{2}} \rho^{2} \boldsymbol{z}^{r} + q(x) g_{Y_{2}}\left(\boldsymbol{z}^{r}, \, \tilde{p}\right) \right] \,. \tag{10}$$

3.2. Homogenized coefficients – macroscopic model

The macroscopic model of elastic waves in strongly heterogeneous piezoelectric composite involves two groups of the homogenized material coefficients:

- the homogenized coefficients depending on the incident wave frequency these are responsible for the dispersive properties of the homogenized model. This group of the coefficients pridano depends just on the material properties of the inclusion (except the material density, which is averaged over entire Y)
- the second group of coefficients is related exclusively to the matrix compartment it determines the macroscopic piezo-elastic properties.

Frequency-dependent coefficients It should be stressed out that the dispersion arises from the *inertia in* Y_2 represented by the fluctuating field u^2 , see (11) below. Due to the auxiliary eigenvalue problems and (9) it can be expressed in terms of the macroscopic quantities (u(x), q(x), f(x)) representing the *local amplitudes of displacements, electric charge and volume force*, respectively; denoting $\oint = \frac{1}{|Y|} \int$, the following holds

$$\begin{aligned}
\oint_{Y_2} \rho^2 \boldsymbol{u}^2 &= \sum_{r \ge 1} \frac{1}{\lambda^r - \omega^2} \left[\boldsymbol{f}(x) \cdot \int_{Y_2} \boldsymbol{z}^r \otimes \oint_{Y_2} \rho^2 \boldsymbol{z}^r \\
&+ \omega^2 \boldsymbol{u}(x) \cdot \int_{Y_2} \rho^2 \boldsymbol{z}^r \otimes \oint_{Y_2} \rho^2 \boldsymbol{z}^r + q(x) g_{Y_2} \left(\boldsymbol{z}^r, \, \tilde{p} \right) \oint_{Y_2} \rho^2 \boldsymbol{z}^r \right] ,
\end{aligned} \tag{11}$$

We introduce the *eigenmomentum* $\mathbf{m}^r = (m_i^r)$,

$$\boldsymbol{m}^r = \int_{Y_2} \rho^2 \boldsymbol{z}^r.$$

Due to (11) the following tensors are introduced, all depending on ω^2 :

• Mass tensor $M^* = (M^*_{ij})$

$$M_{ij}^*(\omega^2) = \int_Y \rho \delta_{ij} - \frac{1}{|Y|} \sum_{r \ge 1} \frac{\omega^2}{\omega^2 - \lambda^r} m_i^r m_j^r ; \qquad (12)$$

• Applied load tensor $\boldsymbol{B}^* = (B_{ij}^*)$

$$B_{ij}^{*}(\omega^{2}) = \delta_{ij} - \frac{1}{|Y|} \sum_{r \ge 1} \frac{\omega^{2}}{\omega^{2} - \lambda^{r}} m_{i}^{r} \int_{Y_{2}} z_{j}^{r} ; \qquad (13)$$

• Applied charge tensor $\boldsymbol{Q}^* = (Q_i^*)$

$$Q_i^*(\omega^2) = -\frac{1}{|Y|} \sum_{r \ge 1} \frac{\omega^2}{\omega^2 - \lambda^r} m_i^r g_{Y_2}\left(\mathbf{z}^r, \, \tilde{p}\right) \,. \tag{14}$$

Coefficients related to the perforated matrix domain As mentioned above, the second group of the homogenized coefficients is defined independently of the inclusions material. In other words, the elasticity C^*_{ijkl} , piezoelectricity G^*_{kij} and dielectricity D^*_{kl} homogenized coefficients can be recovered in the same form which is defined for periodically perforated piezoelectric material. Below we summarize the results which follow as consequences of the homogenization treated in Miara, Rohan et.al. (2005) for a piezoelectric bi-phasic composite.

In order to compute C^* , G^* and D^* , we must solve the local microscopic problems for the corrector functions; these are now listed.

1. Find $(\chi^{ij}, \pi^{ij}) \in \mathbf{H}^1_{\#}(Y_1) \times H^1_{\#}(Y_1), i, j = 1, \dots, 3$ such that

$$\begin{cases} a_{Y_1} \left(\boldsymbol{\chi}^{ij} + \boldsymbol{\Pi}^{ij}, \boldsymbol{\nu} \right) - g_{Y_1} \left(\boldsymbol{\nu}, \pi^{ij} \right) &= 0, \quad \forall \boldsymbol{\nu} \in \mathbf{H}^1_{\#}(Y_1), \\ g_{Y_1} \left(\boldsymbol{\chi}^{ij} + \boldsymbol{\Pi}^{ij}, \psi \right) + d_{Y_1} \left(\pi^{ij}, \psi \right) &= 0, \quad \forall \psi \in H^1_{\#}(Y_1), \end{cases}$$
(15)

where $\Pi^{ij} = (\Pi^{ij}_k) = (y_j \delta_{ik});$

2. Find $(\chi^k, \pi^k) \in \mathbf{H}^1_{\#}(Y_1) \times H^1_{\#}(Y_1), i, j = 1, \dots, 3$ such that

$$\begin{cases} a_{Y_1}(\boldsymbol{\chi}^k, \boldsymbol{\nu}) - g_{Y_1}(\boldsymbol{\nu}, \pi^k + \Pi^k) = 0, & \forall \boldsymbol{\nu} \in \mathbf{H}^1_{\#}(Y_1), \\ g_{Y_1}(\boldsymbol{\chi}^k, \psi) + d_{Y_1}(\pi^k + \Pi^k, \psi) = 0, & \forall \psi \in H^1_{\#}(Y_1), \end{cases}$$
(16)

where $\Pi^k = y_k$.

Using the corrector basis functions just defined we compute the homogenized coefficients:

$$C_{ijkl}^{*} = \frac{1}{|Y|} \left[a_{Y_{1}} \left(\boldsymbol{\chi}^{kl} + \boldsymbol{\Pi}^{kl}, \, \boldsymbol{\chi}^{ij} + \boldsymbol{\Pi}^{ij} \right) + d_{Y_{1}} \left(\pi^{kl}, \, \pi^{ij} \right) \right] ,$$

$$D_{ki}^{*} = \frac{1}{|Y|} \left[d_{Y_{1}} \left(\pi^{k} + \boldsymbol{\Pi}^{k}, \, \pi^{i} + \boldsymbol{\Pi}^{i} \right) + a_{Y_{1}} \left(\boldsymbol{\chi}^{k}, \, \boldsymbol{\chi}^{i} \right) \right] ,$$

$$G_{kij}^{*} = \frac{1}{|Y|} \left[g_{Y_{1}} \left(\boldsymbol{\chi}^{ij} + \boldsymbol{\Pi}^{ij}, \, \boldsymbol{\Pi}^{k} \right) + d_{Y_{1}} \left(\pi^{ij}, \, \boldsymbol{\Pi}^{k} \right) \right] .$$
(17)

The homogenized coefficients are involved in the macroscopic (global) equations; we find $(\boldsymbol{u}, \varphi) \in \mathbf{H}_0^1(\Omega) \times H_0^1(\Omega)$ such that

$$-\omega^{2} \int_{\Omega} (\boldsymbol{M}^{*}(\omega^{2}) \cdot \boldsymbol{u}) \cdot \boldsymbol{v}$$

+
$$\int_{\Omega} C^{*}_{ijkl} e_{kl}(\boldsymbol{u}) e_{ij}(\boldsymbol{v}) - \int_{\Omega} G^{*}_{kij} e_{ij}(\boldsymbol{v}) \partial_{k} \varphi =$$

=
$$\int_{\Omega} (\boldsymbol{B}^{*}(\omega^{2}) \cdot \boldsymbol{f}) \cdot \boldsymbol{v} + \int_{\Omega} q \boldsymbol{\mathcal{Q}}^{*}(\omega^{2}) \cdot \boldsymbol{v} \quad \forall \boldsymbol{v} \in \mathbf{H}^{1}_{0}(\Omega), \qquad (18)$$

and

$$\int_{\Omega} G_{kij}^* e_{ij}(\boldsymbol{u}) \,\partial_k \psi + D_{kl}^* \partial_l \varphi \,\partial_k \psi = \int_{\Omega} q \,\psi \quad \forall \psi \in H_0^1(\Omega) \;.$$

This variational formulation is associated with the strong formulation, which can easily be obtained from (18) on integrating there by parts. Classical solution $(\boldsymbol{u}, \varphi)$ must satisfy the following equations imposed in domain Ω :

$$\omega^2 M_{ij}^*(\omega^2) u_j^1 + \partial_j \left(C_{ijkl}^* e_{kl}(\boldsymbol{u}) - G_{kij}^* \partial_k \varphi \right) = -B_{ij}^*(\omega^2) f_j - q Q_i^*(\omega^2) ,$$

$$\partial_k \left(G_{kij}^* e_{ij}(\boldsymbol{u}) + D_{kl}^* \partial_l \varphi \right) = q ,$$
(19)

where $\boldsymbol{u} = 0$ and $\varphi = 0$ on $\partial \Omega$.

As an important feature of the limit macroscopic equations, its inertia term is defined in terms of the ω -dependent homogenized mass tensor M_{ij}^* . It was proved in Avila et.al. (2008) for the elastic media that there exist intervals of frequencies for which the limit problem admits only an evanescent solution; these intervals are called the *acoustic band gaps*. More precisely, such intervals are indicated by negative definiteness, or negative semi-definiteness of $M_{ij}^*(\omega^2)$; while the first case does not admit any oscillating solution, in the latter one the admissibility of an oscillating response depends on the assumed direction of amplitudes of propagating waves. Thus, some frequencies may result in a strongly anisotropic behaviour of the homogenized medium. Similar conclusions can be derived also in the present situation with the piezoelectric coupling.



Figure 2: Distribution of the weak band gaps (white strips) for the piezoelectric composite. The curves correspond to eigenvalues of the mass tensor $M^*(\omega)$.

3.3. Band gaps

In the context of our homogenization-based modelling of phononic materials, the band gaps are frequency intervals for which the propagation of waves in the structure is disabled or restricted in the polarization.

The band gaps can be classified w.r.t. the polarization of waves which cannot propagate. Given a frequency ω , there are three cases to be distinguished according to the signs of eigenvalues $\gamma^r(\omega)$, r = 1, 2, 3 (in 3D), which determine the "positivity, or negativity" of the mass:

- 1. **propagation zone** all eigenvalues of $M_{ij}^*(\omega)$ are positive: then homogenized model (19) admits wave propagation without any restriction of the wave polarization;
- 2. strong band gap all eigenvalues of $M_{ij}^*(\omega)$ are negative: then homogenized model (19) does *not* admit any wave propagation;
- 3. weak band gap tensor $M_{ij}^*(\omega)$ is indefinite, i.e. there is at least one negative and one positive eigenvalue: then propagation is possible only for waves polarized in a manifold determined by eigenvectors associated with positive eigenvalues. In this case the notion of wave propagation has a local character, since the "desired wave polarization" may depend on the local position in Ω .

For detailed discussion on computing the band gaps for elastic homogenized structures we refere to Avila et.al. (2008); Rohan et.al. (2009). In Fig. 2 we illustrate *weak band gap* distribution for piezoelecric composite formed by matrix *PZT5A* with embedded spherical inclusions made of *BaTiOx3*, where the scale parameter correction was by $\varepsilon = 0.01$; the procedure of rescaling the physical material parameter in the context of assumed scaleing ansatz in (1) was discussed in (Rohan et.al., 2009) for elastic composits, the principle remains valid also for piezoelectric structures.

3.4. Dispersion analysis

We consider guided waves propagating in the heterogeneous medium. For propagation of *long waves* we proposed in (Rohan et.al., 2009) to analyze the dispersion curves using the homogenized model, although this was developed for stationary waves. Such an approximate modeling is valid for a large difference in the elasticity and other piezoelectric parameters between the two compartments.

Usually the band gaps are identified from the *dispersion* diagrams. For the homogenized model the dispersion of guided plane waves is analyzed in the standard way, using the following ansatz:

$$\boldsymbol{u}(x,t) = \bar{\boldsymbol{u}} e^{-\mathrm{i}(\omega t - x_j \kappa_j)} ,$$

$$\varphi(x,t) = \bar{\varphi} e^{-\mathrm{i}(\omega t - x_j \kappa_j)} ,$$
(20)

where $\bar{\boldsymbol{u}}$ is the displacement polarization vector (the wave amplitude), $\bar{\varphi}$ is the electric potential amplitude, $\kappa_j = n_j \varkappa$, $|\boldsymbol{n}| = 1$, i.e. \boldsymbol{n} is the incidence direction, and \varkappa is the wave number. The dispersion analysis consists in computing nonlinear dependencies $\bar{\boldsymbol{u}} = \bar{\boldsymbol{u}}(\omega)$ and $\varkappa = \varkappa(\omega)$; for



Figure 3: Illustration of the dispersion analysis output for the piezoelectric composite. The dispersion curves $\varkappa^{\beta}(\omega)$ computed according to (25). In the weak band gaps (white strips) analyzed according to Figure 2 waves can propagate in one or two directions only. In the 2nd band only one polarization passes, the phase velocity determined by the blue curve, in the 1st band gap two polarization can propagate. In the "full propagation zones" (green) three curves correspond to three wave polarizations.

this one substitutes (20) into the homogenized model (19) with zero r.h.s.

$$-\omega^2 M_{ij}^*(\omega^2) u_j - C_{ijkl}^* \frac{\partial^2 u_k}{\partial x_j \partial x_l} + G_{kij}^* \frac{\partial^2 \varphi}{\partial x_j \partial x_k} = 0 ,$$

$$G_{kij}^* \frac{\partial^2 u_i}{\partial x_k \partial x_j} + D_{kl}^* \frac{\partial^2 \varphi}{\partial x_k \partial x_l} = 0 ,$$
(21)

thus on introducing

$$\Gamma_{ik} = C_{ijkl}^* n_j n_l , \quad \text{the standard Christoffel acoustic tensor,} \gamma_i = G_{kij}^* n_j n_k , \qquad (22) \zeta = D_{kl}^* n_l n_k ,$$

we obtain

$$-\omega^2 M_{ij}^*(\omega^2) \bar{u}_j + \varkappa^2 \left(\Gamma_{ik} \bar{u}_k - \gamma_i \bar{\varphi} \right) = 0 ,$$

$$\varkappa^2 \left(\gamma_k \bar{u}_k + \zeta \bar{\varphi} \right) = 0 .$$
(23)

In (23) we can eliminate $\bar{\varphi}$ (assuming $\varkappa^2 \neq 0$), thus the dispersion analysis reduces to the "elastic case" where the acoustic tensor is modified:

$$-\omega^2 M_{ij}^*(\omega^2) \bar{u}_j + \varkappa^2 H_{ik} \bar{u}_k = 0 ,$$

where $H_{ik} = \Gamma_{ik} + \gamma_i \gamma_k / \zeta .$ (24)

The dispersion is analyzed in terms of the following problem:

• for all $\omega \in [\omega^a, \omega^b]$ and $\omega \notin \{\lambda^r\}_r$ compute eigenelements $(\eta^\beta, \mathbf{w}^\beta)$:

$$\omega^2 M_{ij}^*(\omega^2) w_j^\beta = \eta^\beta H_{ik} w_k^\beta , \quad \beta = 1, 2, 3 ;$$
(25)

- if $\eta^{\beta} > 0$, then $\varkappa^{\beta} = \sqrt{\eta^{\beta}}$,
- else ω falls in an *acoustic gap*, wave number is not defined.

In heterogeneous media *in general* the polarizations of the two waves (outside the band gaps) are *not mutually orthogonal*, which follows easily from the fact that $\{w^{\beta}\}_{\beta}$ are $M^*(\omega^2)$ -orthogonal. Moreover, in the presence of the piezoelectric coupling, which introduces another source of anisotropy, the standard orthogonality is lost even for heterogeneous materials with "symmetric inclusions" (circle,hexagon, etc.), in contracst with elastic structures where these designs preserve the standard orthogonality.

4. Conclusion

The purpose of the paper was to present an extension of the homgenization-based modeling adapted from Rohan et.al. (2009) to the *piezoelectric phononic materials*.

The principal ingredient of the homogenization procedure is the scale dependence of the elastic coefficients in the mutually disconnected inclusions - this leads to acoustic band gaps due to the *negative effective mass* phenomenon appearing in the upscaled model. From the point of the mathematical model, the main difference between the elastic and the piezoelectric *homogenized phononic materials* is the eigenvalue problem – in the latter case there arises the constraint related to the induced electric field.

The main advantage of the homogenization based two-scale modeling lies in the fact, that the homogenization based prediction of the band gap distribution for stationary or long guided waves is relatively simple and effective, cf. Rohan et.al. (2009), in comparison with the "standard computational approach" based on a finite scale heterogeneous model, which requires to evaluate all the Brillouin zone for the dispersion diagram reconstruction; as the consequence, it leads to a killing complexity.

The further research in this field will face the following tasks:

- modeling validation the band gap prediction provided by the homogenized model will be compared with prediction computed on the non-homogenized medium for a given scale of heterogeneities, cf. Sigmund and Jensen (2003); similar study was reported in Rohan et.al. (2009) for the elastic situation.
- numerical study of the piezoelectric inclusion shape and polarization influence on the dispersion properties; similar studies were reported for the elastic case, showing its significant importance.

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- optimal design of the piezo-phononic material; the research related to the sensitivity analysis was published in (Rohan and Miara, 2006-B),(Rohan and Miara, 2006-C) in the context of shape sensitivity at the microscopic level (reference cell Y and the inclusion Y₂).
- modeling of more complicated microstructures w.r.t. their topology, i.e. multiple disjoint inclusions with "different orientations", or embedded inclusions, see Cimrman and Rohan (2009) for the elastic case. We expect that the topology of the "microstructural arrangement" of the composite may have remarkable influence on the dispersion properties.

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6. References

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