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On acoustic band gaps in homogenized piezoelectric phononic materials

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Abstract

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 is 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 allows 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 such composite materials seems to be perspective in the context of Smart Materials design.

Keywords: phononic material, acoustic band gap, piezoelectric material, homogenization

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 phenomenon and namely the *band gap distribution* are inherited from properties of the homogenized mass tensor which depends nonlinearly on the incident wave frequency; when this tensor is negative (in the sense of its eigenvalues) the wave equation looses its hyperbolicity. According to the number of the negative eigenvalues the

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wave propagation is restricted to a certain direction, so that the homogenized material is strongly anisotropic. We refer to interesting paper [7], where anisotropy and randomness aspects in the phononic materials are discussed.

We would like to stress out that our model is convenient for an approximate modeling of the long wave dispersion. The homogenized model involves frequency dependent homogenized mass which allows for prediction of the band gaps, i.e. for some frequencies possibly changing the hyperbolic type partial differential equation into the elliptic one.

In the context of mathematical modelling, the method of homogenization was proposed to study the heterogeneous elastic media (sometimes called *phononic crystals*) in [1] and recently treated in [2, 3], where also numerical results were reported. For related photonic problem in electromagnetic wave propagation see [4].

For elastic composites an existence of band gaps for certain wavelengths was shown in [3] 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 [9]. Here we summarize the essential homogenization results and propose the dispersion analysis which involves modified Christoffel acoustic tensor, due to presence of the piezoelectric coupling with the electric field. This is an extension of the recent publication [11] where the elastic homogenized 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 $^\varepsilon$.

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 the 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

$$
\begin{aligned}
\Omega_2^\varepsilon &= \bigcup_{k \in \mathbb{K}^\varepsilon} \varepsilon(Y_2 + k) \;, \text{ where } \mathbb{K}^\varepsilon = \{k \in \mathbb{Z}^3 |\, \varepsilon(k + \overline{Y_2}) \subset \Omega\} \;, \\
\Omega_1^\varepsilon &= \Omega \setminus \Omega_2^\varepsilon \;,
\end{aligned}
$$

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

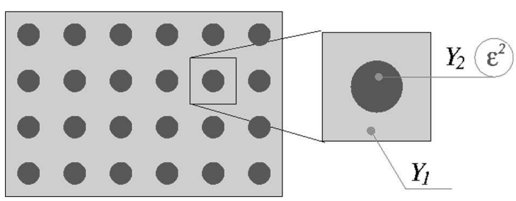

Fig. 1. Periodic structure of the piezoelectric composite with ε^2-scaled material in the inclusions Y_2

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

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 microstructure by coefficient ε^2:

$$
\begin{aligned}
\rho^\varepsilon(x) &= \begin{cases} \rho^1 & \text{in } \Omega^\varepsilon_1, \\ \rho^2 & \text{in } \Omega^\varepsilon_2, \end{cases} & c^\varepsilon_{ijkl}(x) &= \begin{cases} c^1_{ijkl} & \text{in } \Omega^\varepsilon_1, \\ \varepsilon^2 c^2_{ijkl} & \text{in } \Omega^\varepsilon_2, \end{cases} \\
g^\varepsilon_{kij}(x) &= \begin{cases} g^1_{kij} & \text{in } \Omega^\varepsilon_1, \\ \varepsilon^2 g^2_{kij} & \text{in } \Omega^\varepsilon_2, \end{cases} & d^\varepsilon_{ij}(x) &= \begin{cases} d^1_{ij} & \text{in } \Omega^\varepsilon_1, \\ \varepsilon^2 d^2_{ij} & \text{in } \Omega^\varepsilon_2. \end{cases}
\end{aligned}
\tag{1}
$$

2.2. *Problem formulation*

We consider a 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

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

where $\boldsymbol{f} = (f_i)$, $i = 1, 2, 3$ 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 $(\boldsymbol{u}^\varepsilon, \varphi^\varepsilon)$

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

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

$$
\begin{aligned}
-\omega^2 \rho^\varepsilon \boldsymbol{u}^\varepsilon - \mathrm{div}\boldsymbol{\sigma}^\varepsilon &= \boldsymbol{f} && \text{in } \Omega, \\
-\mathrm{div}\boldsymbol{D}^\varepsilon &= q && \text{in } \Omega, \\
\boldsymbol{u}^\varepsilon &= 0 && \text{on } \partial\Omega, \\
\varphi^\varepsilon &= 0 && \text{on } \partial\Omega,
\end{aligned}
\tag{2}
$$

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

$$
\begin{aligned}
\sigma^\varepsilon_{ij} &= c^\varepsilon_{ijkl} e_{kl}(\boldsymbol{u}^\varepsilon) - g^\varepsilon_{kij} \partial_k \varphi^\varepsilon, \\
D^\varepsilon_k &= g^\varepsilon_{kij} e_{ij}(\boldsymbol{u}^\varepsilon) + d^\varepsilon_{kl} \partial_l \varphi^\varepsilon.
\end{aligned}
\tag{3}
$$

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

$$
\begin{aligned}
-\omega^2 \int_\Omega \rho^\varepsilon \boldsymbol{u}^\varepsilon \cdot \boldsymbol{v} + \int_\Omega c_{ijkl}^\varepsilon e_{kl}(\boldsymbol{u}^\varepsilon) e_{ij}(\boldsymbol{v}) - \int_\Omega g_{kij}^\varepsilon e_{ij}(\boldsymbol{v}) \partial_k \varphi^\varepsilon &= \int_\Omega \boldsymbol{f} \cdot \boldsymbol{v} \;, \\
\int_\Omega g_{kij}^\varepsilon e_{ij}(\boldsymbol{u}^\varepsilon) \partial_k \psi + \int_\Omega d_{kl} \partial_l \varphi^\varepsilon \partial_k \psi &= \int_\Omega q \psi \;,
\end{aligned}
\tag{4}
$$

for all $(\boldsymbol{v}, \psi) \in \mathbf{H}_0^1(\Omega) \times H_0^1(\Omega)$, where $\boldsymbol{f} \in \mathbf{L}^2(\Omega)$, $q \in L^2(\Omega)$.

3. Homogenized model of waves in piezo-elastic composite

Problem (4) was studied in [3] using the unfolding method of homogenization to obtain a limit model when $\varepsilon \to 0$. Here the aim is to compare the band gaps predicted by analyzing the stationary waves in the homogenized continuum with the dispersion diagrams obtained for *long waves* propagating in this continuum. For this, we record the theoretical results from [9]. We remark that the spirit of the homogenization was explained exhaustively in [11] 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 couple elastic deformations with an induced electric field;
- piezoelectric properties of the homogenized material involve elasticity, piezo-coupling and dielectricity tensors; these are determined by the perforated matrix exclusively, analogously to 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 notation:

$$
\begin{aligned}
a_{Y_2}(\boldsymbol{u}, \boldsymbol{v}) &= \int_{Y_2} c_{ijkl}^2 e_{kl}^y(\boldsymbol{u})\, e_{ij}^y(\boldsymbol{v}), \\
d_{Y_2}(\phi, \psi) &= \int_{Y_2} d_{kl}^2 \partial_l^y \phi \, \partial_k^y \psi, \\
g_{Y_2}(\boldsymbol{u}, \psi) &= \int_{Y_2} g_{kij}^2 e_{ij}^y(\boldsymbol{u})\, \partial_k^y \psi, \\
\varrho_{Y_2}(\boldsymbol{u}, \boldsymbol{v}) &= \int_{Y_2} \rho^2 \boldsymbol{u} \cdot \boldsymbol{v},
\end{aligned}
\tag{5}
$$

whereby analogical notation is used when integrating over Y_1.

3.1. Auxiliary eigenvalue problem

The auxiliary eigenvalue problem arises due to linearity of the limit model. The displacement and electric potential fields waves are expanded in series based on the eigen-solution of the associated piezo-elastic problem representing 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

$$\begin{aligned} d_{Y_2}(\tilde{p},\, \psi) &= \int_{Y_2} \psi \qquad \forall \psi \in H_0^1(Y_2)\;, \\ \text{hence also } d_{Y_2}\left(\varphi^{2P},\, \psi\right) &= q(x) \int_{Y_2} \psi \qquad \forall \psi \in H_0^1(Y_2)\;. \end{aligned} \tag{6}$$

Spectral problem Find eigenelements $[\lambda^r; (\boldsymbol{z}^r, p^r)]$, where $\boldsymbol{z}^r \in \mathbf{H}_0^1(Y_2)$ and $p^r \in H_0^1(Y_2)$, $r = 1, 2, \dots$, such that

$$\begin{aligned} a_{Y_2}(\boldsymbol{z}^r,\, \boldsymbol{v}) - g_{Y_2}(\boldsymbol{v},\, p^r) &= \lambda^r \varrho_{Y_2}(\boldsymbol{z}^r,\, \boldsymbol{v}) \quad \forall \boldsymbol{v} \in \mathbf{H}_0^1(Y_2), \\ g_{Y_2}(\boldsymbol{z}^r,\, \psi) + d_{Y_2}(p^r,\, \psi) &= 0 \quad \forall \psi \in H_0^1(Y_2), \end{aligned} \tag{7}$$

with the orthonormality condition imposed on eigenfunctions $\boldsymbol{z}^r$:

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

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

$$\begin{aligned} a_{Y_2}(\boldsymbol{z}^r,\, \boldsymbol{z}^s) - g_{Y_2}(\boldsymbol{z}^s,\, p^r) &= \lambda^r \varrho_{Y_2}(\boldsymbol{z}^r,\, \boldsymbol{z}^s)\,, \\ g_{Y_2}(\boldsymbol{z}^s,\, p^r) + d_{Y_2}(p^s,\, p^r) &= 0, \end{aligned}$$

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

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

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

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

$$\begin{aligned} \boldsymbol{u}^2(x, y) &= \sum_{r \geq 1} \alpha^r(x) \boldsymbol{z}^r(y)\;, \\ \varphi^2(x, y) &= \varphi^{2H} + \varphi^{2P} = \sum_{r \geq 1} \alpha^r(x) p^r(y) + q(x)\tilde{p}(y)\;, \end{aligned} \tag{9}$$

where α^r is expressed as follows:

$$\alpha^r = \frac{1}{\lambda^r - \omega^2} \left[\boldsymbol{f}(x) \cdot \int_{Y_2} \boldsymbol{z}^r + \omega^2 \boldsymbol{u}(x) \cdot \int_{Y_2} \rho^2 \boldsymbol{z}^r + q(x) g_{Y_2}(\boldsymbol{z}^r,\, \tilde{p}) \right]\;, \tag{10}$$

where $\boldsymbol{u}(x)$ is the homogenized displacement (amplitude) field satisfying the macroscopic equations (18), see below.

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 depends just on the material properties of the inclusion (except the material density, which is averaged over whole 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 $\boldsymbol{u}^2$, see (11) below. Due to the auxiliary eigenvalue problems and (9) it can be expressed in terms of the macroscopic quantities $(\boldsymbol{u}(x), q(x), \boldsymbol{f}(x))$ representing the *local amplitudes of displacements, electric charge and volume force*, respectively; denoting $\fint = \frac{1}{|Y|}\int$, the following holds

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

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

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

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

- Mass tensor $\boldsymbol{M}^* = (M_{ij}^*)$

$$M_{ij}^*(\omega^2) = \fint_Y \rho \delta_{ij} - \frac{1}{|Y|} \sum_{r\geq 1} \frac{\omega^2}{\omega^2 - \lambda^r} m_i^r m_j^r \,; \tag{12}$$

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

$$B_{ij}^*(\omega^2) = \delta_{ij} - \frac{1}{|Y|} \sum_{r\geq 1} \frac{\omega^2}{\omega^2 - \lambda^r} m_i^r \int_{Y_2} z_j^r \,; \tag{13}$$

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

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

Coefficients related to the perforated matrix domain As mentioned above, the second group of the homogenized coefficients is defined independently of the material in the inclusions. In other words, the homogenized tensors of elasticity C^*_{ijkl}, piezoelectricity G^*_{kij} and dielectricity D^*_{kl} 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 [6] 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 $(\boldsymbol{\chi}^{ij}, \pi^{ij}) \in \mathbf{H}^1_\#(Y_1) \times H^1_\#(Y_1)$, $i, j = 1, \ldots, 3$ such that

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

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

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

$$\left\{ \begin{array}{ll} a_{Y_1}\left(\boldsymbol{\chi}^{k},\, \boldsymbol{v}\right) - g_{Y_1}\left(\boldsymbol{v},\, \pi^{k} + \Pi^k\right) = 0\,, & \forall \boldsymbol{v} \in \mathbf{H}^1_\#(Y_1)\,, \\ g_{Y_1}\left(\boldsymbol{\chi}^{k},\, \psi\right) + d_{Y_1}\left(\pi^{k} + \Pi^k,\, \psi\right) = 0\,, & \forall \psi \in H^1_\#(Y_1)\,, \end{array} \right. \tag{16}$$

where $\Pi^k = y_k$.

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

$$\begin{aligned} C^*_{ijkl} &= \frac{1}{|Y|}\left[a_{Y_1}\left(\boldsymbol{\chi}^{kl} + \boldsymbol{\Pi}^{kl},\, \boldsymbol{\chi}^{ij} + \boldsymbol{\Pi}^{ij}\right) + d_{Y_1}\left(\pi^{kl},\, \pi^{ij}\right)\right]\,, \\ D^*_{ki} &= \frac{1}{|Y|}\left[d_{Y_1}\left(\pi^{k} + \Pi^{k},\, \pi^{i} + \Pi^{i}\right) + a_{Y_1}\left(\boldsymbol{\chi}^{k},\, \boldsymbol{\chi}^{i}\right)\right]\,, \\ G^*_{kij} &= \frac{1}{|Y|}\left[g_{Y_1}\left(\boldsymbol{\chi}^{ij} + \boldsymbol{\Pi}^{ij},\, \Pi^{k}\right) + d_{Y_1}\left(\pi^{ij},\, \Pi^{k}\right)\right]\,. \end{aligned} \tag{17}$$

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

$$\begin{aligned} & - \omega^2 \int_\Omega (\boldsymbol{M}^*(\omega^2) \cdot \boldsymbol{u}) \cdot \boldsymbol{v} \\ & + \int_\Omega C^*_{ijkl} e_{kl}(\boldsymbol{u})\, e_{ij}(\boldsymbol{v}) - \int_\Omega G^*_{kij} e_{ij}(\boldsymbol{v})\, \partial_k \varphi = \\ = & \int_\Omega (\boldsymbol{B}^*(\omega^2) \cdot \boldsymbol{f}) \cdot \boldsymbol{v} + \int_\Omega q \boldsymbol{Q}^*(\omega^2) \cdot \boldsymbol{v} \quad \forall \boldsymbol{v} \in \mathbf{H}^1_0(\Omega)\,, \end{aligned} \tag{18}$$

and

$$\int_\Omega G^*_{kij} e_{ij}(\boldsymbol{u})\, \partial_k \psi + D^*_{kl} \partial_l \varphi\, \partial_k \psi = \int_\Omega q\, \psi \quad \forall \psi \in H^1_0(\Omega)\,.$$

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:

$$\begin{aligned} \omega^2 M^*_{ij}(\omega^2)\, u_j + \partial_j\left(C^*_{ijkl} e_{kl}(\boldsymbol{u}) - G^*_{kij} \partial_k \varphi\right) &= -B^*_{ij}(\omega^2) f_j - q Q^*_i(\omega^2)\,, \\ \partial_k\left(G^*_{kij} e_{ij}(\boldsymbol{u}) + D^*_{kl} \partial_l \varphi\right) &= q\,, \end{aligned} \tag{19}$$

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 [3] 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 polarization 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.

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 completely, or restricted just for some polarizations.

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 refer to [3, 11]. In Fig. 2 we illustrate *weak band gap* distribution for piezoelectric composite formed by matrix *PZT5A* with embedded spherical inclusions made of *BaTiOx3*, where the scale parameter correction was $\varepsilon = 0.01$. The procedure of rescaling the physical material parameters in the context of assumed scaling ansatz in (1) was discussed in [11] for elastic composites, 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 [11] 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:

$$
\begin{aligned}
\boldsymbol{u}(x,t) &= \bar{\boldsymbol{u}}\, e^{-\mathrm{i}(\omega t - x_j \kappa_j)}\,, \\
\varphi(x,t) &= \bar{\varphi}\, e^{-\mathrm{i}(\omega t - x_j \kappa_j)}\,,
\end{aligned}
\tag{20}
$$

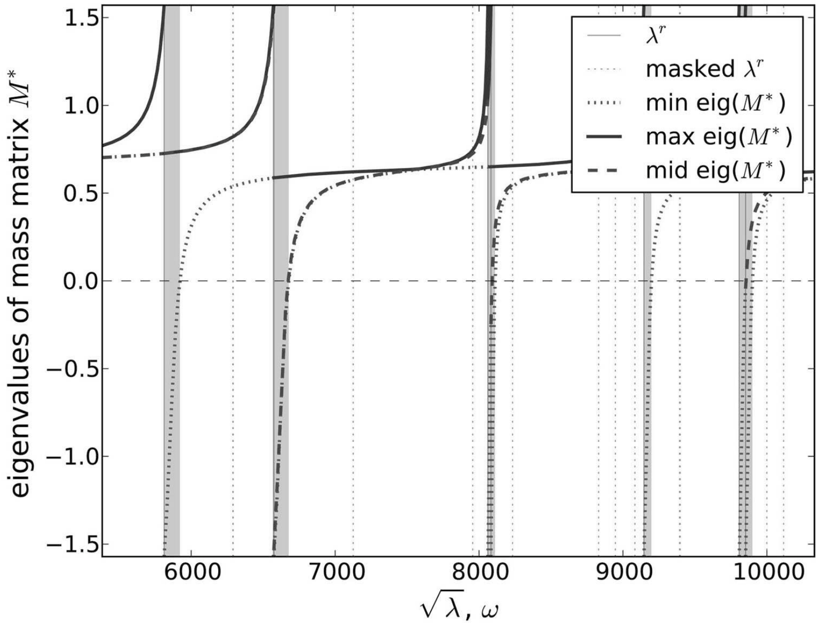

Fig. 2. Distribution of the weak band gaps (white strips) for the piezoelectric composite. The curves correspond to eigenvalues of the mass tensor $\boldsymbol{M}^*(\omega)$

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

$$
\begin{aligned}
-\omega^2 M^*_{ij}(\omega^2) u_j - C^*_{ijkl} \frac{\partial^2 u_k}{\partial x_j \partial x_l} + G^*_{kij} \frac{\partial^2 \varphi}{\partial x_j \partial x_k} &= 0 \;, \\
G^*_{kij} \frac{\partial^2 u_i}{\partial x_k \partial x_j} + D^*_{kl} \frac{\partial^2 \varphi}{\partial x_k \partial x_l} &= 0 \;.
\end{aligned}
\tag{21}
$$

Thus on introducing

$$
\begin{aligned}
\Gamma_{ik} &= C^*_{ijkl} n_j n_l \;, \qquad \text{the standard Christoffel acoustic tensor,} \\
\gamma_i &= G^*_{kij} n_j n_k \;, \\
\zeta &= D^*_{kl} n_l n_k \;,
\end{aligned}
\tag{22}
$$

we obtain

$$
\begin{aligned}
-\omega^2 M^*_{ij}(\omega^2) \bar{u}_j + \varkappa^2 \left(\Gamma_{ik} \bar{u}_k - \gamma_i \bar{\varphi} \right) &= 0 \;, \\
\varkappa^2 \left(\gamma_k \bar{u}_k + \zeta \bar{\varphi} \right) &= 0 \;.
\end{aligned}
\tag{23}
$$

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:

$$
\begin{aligned}
-\omega^2 M^*_{ij}(\omega^2) \bar{u}_j + \varkappa^2 H_{ik} \bar{u}_k &= 0 \;, \\
\text{where} \quad H_{ik} &= \Gamma_{ik} + \gamma_i \gamma_k / \zeta \;.
\end{aligned}
\tag{24}
$$

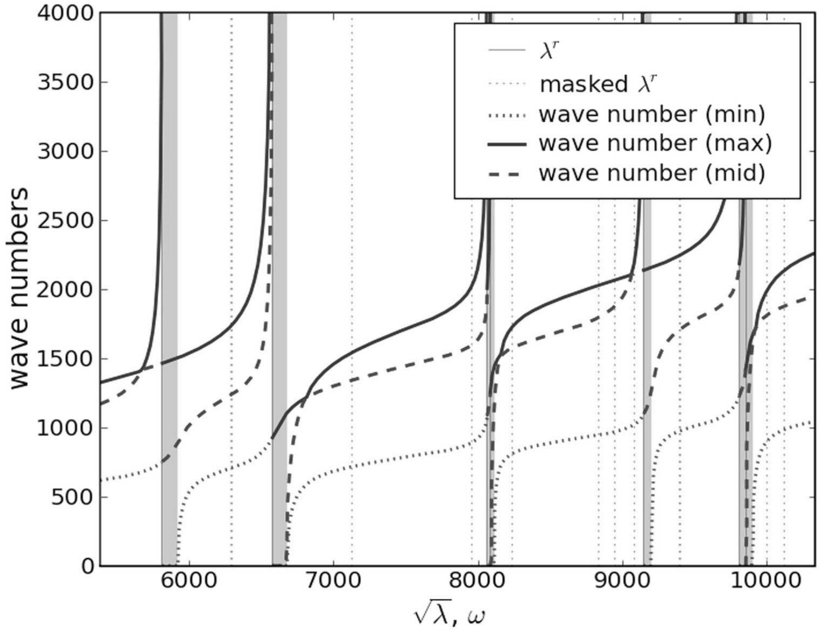

Fig. 3. Illustration of the dispersion analysis output for the piezoelectric composite, angle of incidence is 45deg. The dispersion curves $\varkappa^\beta(\omega)$ computed according to (25). In the weak band gaps (grey/green strips) analyzed according to Fig. 2 waves can propagate in one or two directions only. In the second band gap only one polarization exists, with the phase velocity determined by the blue (solid) curve, in the first band gap two polarizations can propagate. In the "full propagation zones" (white) the three curves correspond to the three wave polarizations

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 $(\eta^\beta, \boldsymbol{w}^\beta)$:

$$\omega^2 M^*_{ij}(\omega^2) w^\beta_j = \eta^\beta H_{ik} w^\beta_k \;, \quad \beta = 1, 2, 3 \;; \tag{25}$$

- 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 three (or two in 2D) waves (outside the band gaps) are *not mutually orthogonal*, which follows easily from the fact that $\{\boldsymbol{w}^\beta\}_\beta$ are $\boldsymbol{M}^*(\omega^2)$-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 contrast with elastic structures where these designs preserve the standard orthogonality.

4. Conclusion

The purpose of the paper was to present an extension of the homogenization-based modeling adapted from [11] 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 solved in the inclusions – 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. [11], in comparison with the "standard computational approach" based on a finite scale heterogeneous model, requiring to evaluate the whole Brillouin zone for the dispersion diagram reconstruction which, as the consequence, leads to a killing complexity. Here we treated the stationary waves in a finite domain. An infinite domain could be considered when guided waves were in our focus, however, here we do not treat guided "short" waves such that the wave length interfere with the microstructure scale. If it were the case, the short wave dispersion should rather be studied in the framework of the Bloch wave theory.

Usually in realistic media a small damping exists. Adding a small viscosity to our model changes completely the theoretical homogenization result. In contrast with the purely non-dissipative material where existence of a small band gap is guaranteed by virtue of the homogenized mass tensor (a band gap is distributed in the vicinity of any eigenfrequency of the inclusion problem (7)), in the viscous case we are not able to prove a similar result. However the band gaps in our sense, i.e. identified by the negative (semi)definiteness of the homogenized mass, still may exist depending on the proportion of the viscose damping. This was obsereved in our numerical tests and will be subject of a forthcoming paper.

The further research in this field will address 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. [12]; similar study was reported in [11] 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.

- optimal design of the piezo-phononic material; the research related to the sensitivity analysis was published in [9], [10] in the context of shape sensitivity at the microscopic level (reference cell Y and the inclusion Y_2).

- modeling of more complicated microstructures w.r.t. their topology, i.e. multiple disjoint inclusions with "different orientations", or embedded inclusions, see [5] 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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