phononic Documentation

Release 0.1

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April 09, 2010

CONTENTS

This documentation describes a software for prediction of band gaps in phononic materials.

CHAPTER

ONE

ABSTRACT

The phononic materials are 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. For certain frequency ranges, such elastic structures can suppress the elastic wave propagation, i.e. they exhibit the band gaps. 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. The software can predict distribution of the band gaps in such media for stationary or long guided waves very effectively, due to the use of the homogenization based two-scale modeling.

Keywords: phononic materials; band gaps; elasticity; piezo-elasticity

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1.1 User's Guide

The purpose of this software is to predict distribution of acoustic band gaps in phononic materials in 2D and 3D.

1.1.1 Introduction

We will briefly recall the notions of a *phononic material* and *acoustic band gaps* using the piezoelastic material. The purely elastic case is its special simplified version.

For a more complete description involving details of application of the theory of homogenization, see e.g. [rohan-miara-seifrt-2009].

Strongly heterogeneous material

The material properties are related to the periodic geometrical decomposition like in Fig. *Periodic structure of the piezoelectric composite with -scaled material in the inclusions* ..

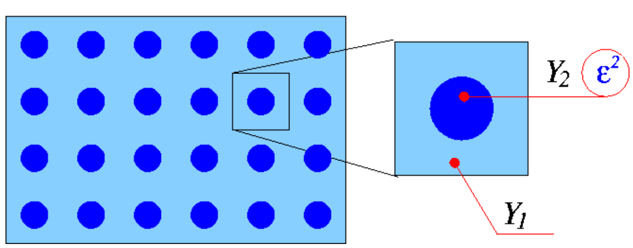

Figure 1.1: Periodic structure of the piezoelectric composite with ε^2 -scaled material in the inclusions Y_2.

Properties of a 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 $i, j, k = 1, 2, \ldots, 3$.

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:

$$\rho^\varepsilon(x) = \begin{cases} \rho^1 & \text{in } \Omega_1^\varepsilon, \\ \rho^2 & \text{in } \Omega_2^\varepsilon, \end{cases} \qquad c^\varepsilon_{ijkl}(x) = \begin{cases} c^1_{ijkl} & \text{in } \Omega_1^\varepsilon, \\ \varepsilon^2 c^2_{ijkl} & \text{in } \Omega_2^\varepsilon, \end{cases}$$
$$g^\varepsilon_{kij}(x) = \begin{cases} g^1_{kij} & \text{in } \Omega_1^\varepsilon, \\ \varepsilon^2 g^2_{kij} & \text{in } \Omega_2^\varepsilon, \end{cases} \qquad d^\varepsilon_{ij}(x) = \begin{cases} d^1_{ij} & \text{in } \Omega_1^\varepsilon, \\ \varepsilon^2 d^2_{ij} & \text{in } \Omega_2^\varepsilon. \end{cases}$$

Problem formulation

We consider a stationary wave propagation in the medium introduced above. For simplicity we restrict the model to the description of clamped structures loaded by volume forces and subject to volume distributed electric charges. For 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, we have in general 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:

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

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

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

The problem eq{eq-11} can be weakly formulated as follows: Find $(\boldsymbol{u}^\varepsilon, \varphi^\varepsilon) \in \mathbf{H}^1_0(\Omega) \times H^1_0(\Omega)$ such that

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

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

Spectral problem

Let us denote

$$
\begin{aligned}
a_{Y_2}\left(\boldsymbol{u},\,\boldsymbol{v}\right) &= \int_{Y_2} c^2_{ijkl} e^y_{kl}(\boldsymbol{u})\, e^y_{ij}(\boldsymbol{v}),\\
d_{Y_2}\left(\phi,\,\psi\right) &= \int_{Y_2} d^2_{kl} \partial^y_l \phi\, \partial^y_k \psi,\\
g_{Y_2}\left(\boldsymbol{u},\,\psi\right) &= \int_{Y_2} g^2_{kij} e^y_{ij}(\boldsymbol{u})\, \partial^y_k \psi,\\
\varrho_{Y_2}\left(\boldsymbol{u},\,\boldsymbol{v}\right) &= \int_{Y_2} \rho^2 \boldsymbol{u}\cdot\boldsymbol{v},
\end{aligned}
$$

whereby analogical notation is used when integrating over Y_1.

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

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

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

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

Homogenized coefficients

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 entire Y)
- the second group of coefficients is related exclusively to the matrix compartment – it determines the macroscopic piezo-elastic properties.

Let us summarize just the first group of coefficients, as those are connected with the appearance of the band gaps.

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

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

Then the following tensors are introduced, all depending on ω^2: - Mass tensor $\boldsymbol{M}^* = (M^*_{ij})$

$$
M^*_{ij}(\omega^2) = \fint_Y \rho\delta_{ij} - \frac{1}{|Y|}\sum_{r\geq 1} \frac{\omega^2}{\omega^2 - \lambda^r} m^r_i m^r_j \ ;
$$

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

$$
B^*_{ij}(\omega^2) = \delta_{ij} - \frac{1}{|Y|}\sum_{r\geq 1} \frac{\omega^2}{\omega^2 - \lambda^r} m^r_i \int_{Y_2} z^r_j \ ;
$$

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

$$
Q^*_i(\omega^2) = -\frac{1}{|Y|}\sum_{r\geq 1} \frac{\omega^2}{\omega^2 - \lambda^r} m^r_i g_{Y_2}\left(\boldsymbol{z}^r,\,\tilde{p}\right) \ .
$$

Band gaps

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:

- {bf propagation zone} – all eigenvalues of $M^*_{ij}(\omega)$ are positive: then homogenized model eq{eq-45s} admits wave propagation without any restriction of the wave polarization;
- {bf strong band gap} – all eigenvalues of $M^*_{ij}(\omega)$ are negative: then homogenized model eq{eq-45s} does {it not} admit any wave propagation;
- {bf 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.

In Fig. *Distribution of the band gaps.* we illustrate *weak band gap* distribution for piezoelectric composite formed by matrix PZT5A with embedded spherical inclusions made of BaTiOx3.

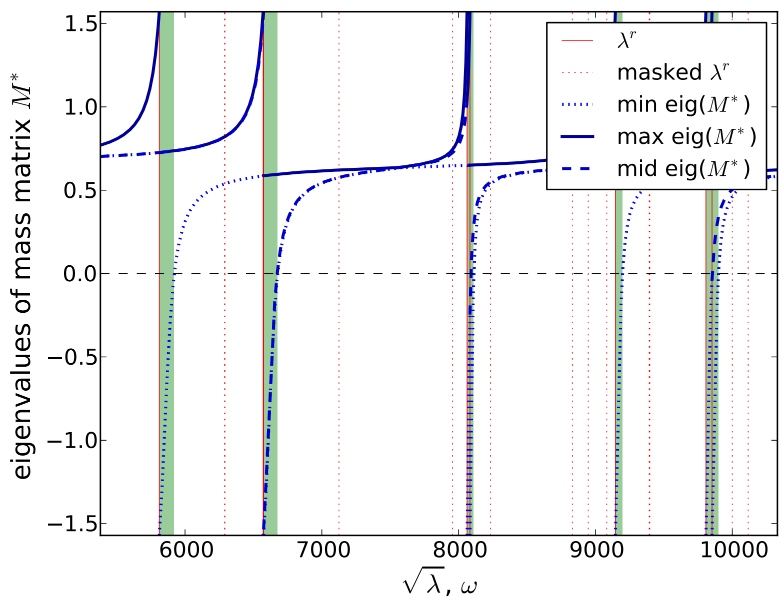

Figure 1.2: Distribution of the band gaps.

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

The software can also perform dispersion analysis of *long guided waves*, a example result is shown in Fig. *The dispersion analysis.*.

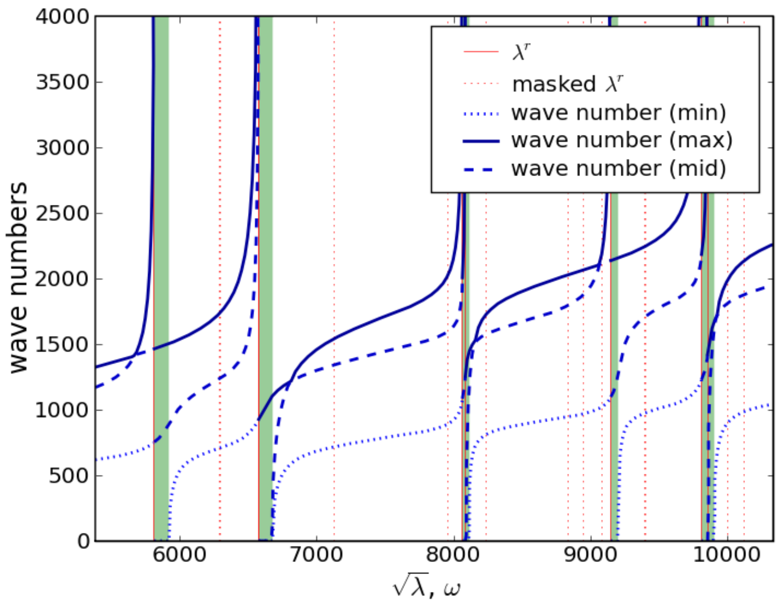

Figure 1.3: The dispersion analysis.

Illustration of the dispersion analysis output for the piezoelectric composite, angle of incidence is 45 $\deg$. In the weak band gaps (grey/green strips) analyzed according to Fig. *Distribution of the band gaps.* 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.}

References

1.1.2 Running a simulation

The band gap related problems can be solved by running the *eigen.py* script:

```
Usage: eigen.py [options] filename_in

Options:
  --version          show program's version number and exit
  -h, --help         show this help message and exit
  -o filename        basename of output file(s) [default: <basename of input
                     file>]
  -b, --band-gaps    detect frequency band gaps
  -d, --dispersion   analyze dispersion properties (low frequency domain)
  -p, --plot         plot frequency band gaps, assumes -b
  --phase-velocity   compute phase velocity (frequency-independet mass only)
```

Above *filename_in* stands for one of the problem definition files listed below. Each of the files contains all the necessary information to compute acoustic band gaps (ABG) and/or dispersion properties (DP) , namely:

- *band_gaps.py* (ABG + DP in elastic material)
- *band_gaps_liquid.py* (ABG in elastic material with fluid-like inclusion)
- *band_gaps_piezo.py* (ABG + DP in piezoelastic material)
- *band_gaps_rigid.py* (ABG in elastic material with rigid inclusion)

Each of the above files includes further options, that can be set to influence both the computation and subsequent postprocessing of results (accuracy settings, names and format of result files etc.).

1.1.3 Postprocessing

Results of a simulation are:

- graphical representation of ABG and eventually DP; the figure are saved to the directory specified in options of each problem definition file,
- text file of ABG, DP logs for custom postprocessing using *plot_gaps.py* script,
- eigenfunctions of the related elasticity or piezoelasticity eigenvalue problems in the standard VTK format or a custom HDF5-based format, eigenvalues in text files.

1.2 Developer Guide

This section purports to document the *phononic* internals.

1.2.1 band_gaps module

clip (*data, plot_range*)

clip_sqrt (*data, plot_range*)

incwd (*filename*)

normalize (*data, plot_range*)

select_in_plane (*vec, shape, normal_direction, eps*)

1.2.2 band_gaps_liquid module

get_pars (*lam, mu, dim, full=False*)

incwd (**filename*)

select_y3_circ (*x, y, z, diameter*)

vary_eta (*problem*)
Vary viscosity.

1.2.3 band_gaps_piezo module

get_inclusion_pars (*ts, coor, region, ig, mode='inclusion'*)

get_iw_dir (*dim*)

get_pars_BaTiOx3 ()
Material Ba Ti O_3, Tetragonal, type 4mm.

get_pars_PZT5A ()
Material PZT5A.

piezo_transfrom_3to2 (*C3=None, D3=None, B3=None, iplane=None*)
Transforms all coefficients of the piezoelectric constitutive law from 3D to plane stress problem in 2D: strain/stress ordering/ 11 22 33 12 13 23 –> if no arguments passed, demo example returns 2D restriction of a piezoelectric material obtained by get_pars_BaTiOx3().

Example: C2, D2, B2 = piezo_transfrom_3to2(C3, D3, B3, iplane)

1.2.4 band_gaps_rigid module

define_elastic_problem (*filename_mesh, dim, y3_diameter=None*)

extend_cell_data (*data, pb, rname, val=None*)

incwd (*filename*)

post_process (*out, problem, mtx_phi*)

prepare_shift (*problem, y3_diameter=None*)

save_log (*filename, bg, log_item*)
Saves band gaps, valid flags, eigenfrequencies.

select_rigid (*x, y, z*)

select_y3_circ (*x, y, z, diameter*)

shift_y3 (*problem*)

solve_shift (*epb, ebcs, shift*)

vary_teps (*problem*)
Vary eigenmomentum threshold.

vary_y3_size (*problem*)
Vary size of Y3 inclusion.

1.2.5 coef_conf_elastic module

define_input (*filename, region, dim, geom, define_regions=True*)
Uses materials, fe of master file, merges regions.

expand_regions (*eqs, expand*)

1.2.6 coef_conf_piezo module

define_input (*filename, region, bbox, dim, geom*)
Uses materials, fe of master file, merges regions.

expand_regions (*eqs, expand*)

1.2.7 gen_mesh module

gen_concentric (*filename, a, el_size_out, el_size_in, r0, r1, n_circ*)

1.2.8 macro_piezo module

1.2.9 parametric module

Various parametric hooks.

save_log (*filename, bg, log_item, save_eigs=False, save_angles=False*)
Saves band gaps, valid flags, eigenfrequencies, and polarization angles, if present.

vary_iw_dir_dispersion (*problem*)
Vary incident wave direction for dispersion computation. The x-y plane is used in 3D.

Assumes –dispersion option!

vary_iw_dir_phase_velocity (*problem*)
Vary incident wave direction for phase velocity computation. The x-y plane is used in 3D.

Assumes –phase-velocity option!

1.2.10 phase_velocity module

1.2.11 plot_gaps script

main ()

Log file format: par_name: par squared: <bool> header header f0 f1 flag_min f_min v_min flag_max f_max v_max kind desc

1.2.12 postproc_evp script

add_glyphs (*obj, position, color=(0, 0, 0)*)

add_scalar_cut_plane (*obj, position, normal, opacity=0.5*)

add_surf (*obj, position, opacity=0.5*)

add_text (*obj, position, text, color=(0, 0, 0)*)

cycle(*bounds*)

Cycles through all combinations of bounds, returns a generator.

More specifically, let bounds=[a, b, c, ...], so cycle returns all combinations of lists [0<=i<a, 0<=j<b, 0<=k<c, ...] for all i,j,k,...

Examples: In [9]: list(cycle([3, 2])) Out[9]: [[0, 0], [0, 1], [1, 0], [1, 1], [2, 0], [2, 1]]

In [14]: list(cycle([3, 4])) [[0, 0], [0, 1], [0, 2], [0, 3], [1, 0], [1, 1], [1, 2], [1, 3], [2, 0], [2, 1], [2, 2], [2, 3]]

main()

1.2.13 utils module

clip(*data, plot_range*)

clip_sqrt(*data, plot_range*)

get_pars(*lam, mu, dim, full=False*)

normalize(*data, plot_range*)

select_in_plane(*vec, shape, normal_direction, eps*)

to_degrees(*data*)

CHAPTER

TWO

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BIBLIOGRAPHY

[rohan-miara-seifrt-2009] Rohan, E., Miara, B. and Seifrt, F., 2009. Numerical simulation of acoustic band gaps in homogenized elastic compo sites. International Journal of Engineering Science. 4(47):573-594. doi://10.1016/j.ijengsci.2008.12.003.

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