MODELLING OF THE RESONANCE CHARACTERISTICS OF THE PIEZOELECTRIC RESONATORS

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ABSTRACT

The paper describes an application of the FEM in modelling of the resonance characteristics of piezoelectric resonators. The paper contains derivation of the weak formulation of the problem based on the physical description of piezoelectric structures. Solving of the problem leads to the set of linear equations with large and sparse matrices, which define the generalized eigenvalue problem, from which we can obtain the frequency spectrum of the resonator. Several iterative methods for solving the generalized eigenvalue problem are used and the results are compared with measurement.

1 PROBLEM DESCRIPTION

The crystal made of piezoelectric material represents a system, where the deformation and electric field depend on each other. The deformation of the crystal induces the electric charge on the crystal's surface. As well, electric field causes the deformation of the crystal. The most important thing in studying the behavior of the piezoelectric resonator is its resonance frequency. It depends on many parameters (material properties, origin and form of the cut, etc...). The experimental testing of piezoelectric resonators is very expensive and means plenty of specimens and the analytic solution is able only for very simple structures. Thus the motivation for the mathematical modelling of piezoelectric resonators is to help to design the resonators with prescribed behavior.

1.1 PHYSICAL DESCRIPTION

Let us have the piezolectric resonator chracterized by proper material tensors. The density of the material is ρ. We denote the volume of the resonator as Ω and its boundary as Γ. There are two differential equations governing the behavior of a piezoelectric continuum

- Newton's laws of motion (1) and the quasistatic approximation to Maxwell's equation (2) (see [3])

$$\rho \frac{\partial^2 u_i}{\partial t^2} = \frac{\partial \mathrm{T_{ij}}}{\partial x_j} \qquad i = 1,2,3, \qquad x \in \Omega, \quad \mathrm{t} \in (0,\mathrm{T}) \tag{1}$$

$$\nabla \cdot \mathbf{D} = \frac{\partial \mathrm{D_j}}{\partial x_j} = 0. \tag{2}$$

We will call them *elastic* and *electric* equations. Above equations are coupled by the piezoelectric equations of state (3) and (4) (see e.g. [2])

$$\mathrm{T_{ij}} = c_{ijkl} \cdot \mathrm{S_{kl}} + d_{ijk} \cdot \mathrm{E_k}, \qquad i,j = 1,2,3. \tag{3}$$

$$\mathrm{D}_k = d_{kij} \cdot \mathrm{S_{ij}} + \varepsilon_{kj} \cdot \mathrm{E_j}, \qquad k = 1,2,3, \tag{4}$$

where

$$\mathrm{S}_{ij} = \frac{1}{2}\left[\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right], \qquad \mathrm{E_k} = \frac{\partial \varphi}{\partial x_k}, \qquad i,j,k = 1,2,3,$$

T is the stress tensor, **D** is the vector of electric flux density, **u** is the displacement vector, **S** is the strain tensor, **E** is the vector of electric field, φ is the electric potential, **c**, **d** and $\vec{\varepsilon}$ are the stiffness, piezoelectric and permitivity tensors of the crystal (these tensors are typicall for each material). We assume the symmetry of material tensors

$$c_{ijkl} = c_{jikl} = c_{ijlk} = c_{klij}, \quad d_{ijk} = d_{ikj}, \quad \varepsilon_{ij} = \varepsilon_{ji}$$

and also their positive definiteness. Assuming the harmonic electric loading of the resonator, we can expect the harmonic oscillations (ω is the frequency of voltage)

$$\varphi = \varphi_0(x,y,z)\cos\omega t, \quad \mathbf{u} = \mathbf{u}_0(x,y,z)\cos\omega t \quad \Rightarrow \quad \rho\frac{\partial^2 u_i}{\partial t^2} = -\omega^2\rho \cdot u_i. \tag{5}$$

Substituting (3), (4) and (5) into (1) and (2), we get the modified versions of elastic and electric equations, now for the unknown amplitudes $\mathbf{u}_0$ and φ_0 (we will write them without the lower index 0)

$$-\omega^2\rho \cdot u_i = \frac{\partial}{\partial x_j}\left(c_{ijkl} \cdot \frac{1}{2}\left[\frac{\partial u_k}{\partial x_l} + \frac{\partial u_l}{\partial x_k}\right] + d_{ijk} \cdot \frac{\partial \varphi}{\partial x_k}\right) \quad i = 1,2,3, \tag{6}$$

$$0 = \frac{\partial}{\partial x_k}\left(d_{kij} \cdot \frac{1}{2}\left[\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right] + \varepsilon_{kj} \cdot \frac{\partial \varphi}{\partial x_j}\right). \tag{7}$$

Boundary conditions on the part of the boundary Γ_1 are added

$$u_i = 0 \qquad i = 1,2,3, \quad \varphi = \varphi_D \qquad \text{on} \quad \Gamma_1. \tag{8}$$

1.2 POINT OF INTEREST

In (6)-(8), the problem of harmonic oscillations is defined. Our goal is to find such values of parametr ω, which set the system in resonance (= oscillations with maximal amplitudes). This means to find the case of singularity of the system (6)-(7) - it corresponds to the singularity of linear system resulting from the discretization of the problem (6)-(8).

2 NUMERICAL SOLUTION

2.1 WEAK FORMULATION

The weak formulation and discretization of the problem (6)-(8) will lead to the linear system, from which the resonance frequencies can be computed.

Comment: Let $V(\Omega) = \{v | v \in W_2^{(1)}(\Omega), \quad v|_{\Gamma_1} = 0\}$ be the set of functions from Sobolev space $W_2^{(1)}(\Omega) = \{\varphi \in C_0^{(\infty)}(\overline{\Omega}) | \varphi \in L_2(\Omega), \nabla\varphi \in [L_2(\Omega)]^3\}$, which satisfy the homogenous boundary condition on Γ_1. Further, we denote $(f,g)_\Omega = \int_\Omega fg d\Omega$ the scalar product in $L_2(\Omega)$.

We derive the weak formulation in the standard way (see e.g. [4], more precisely it is described in [5]). We multiply the equations (6) with testing functions $w_i \in V$, summarize and integrate them over Ω. As well, we multiply the equation (7) with testing function $\phi \in V$ and integrate it over Ω. Using Green formula (integrals over the border are zeros) and the symmetry of material tensors, we obtain the integral equations

$$\left(c_{ijkl} \cdot \frac{1}{2}\left[\frac{\partial u_k}{\partial x_l} + \frac{\partial u_l}{\partial x_k}\right], \frac{1}{2}\left[\frac{\partial w_i}{\partial x_j} + \frac{\partial w_j}{\partial x_i}\right]\right)_\Omega - \left(\rho\omega^2 u_i, w_i\right)_\Omega + \left(d_{ijk} \cdot \frac{\partial \varphi}{\partial x_j}, \frac{1}{2}\left[\frac{\partial w_i}{\partial x_j} + \frac{\partial w_j}{\partial x_i}\right]\right)_\Omega = 0,$$

$$\left(d_{jik}\frac{1}{2}\left[\frac{\partial u_i}{\partial x_k} + \frac{\partial u_k}{\partial x_i}\right], \frac{\partial \phi}{\partial x_j}\right)_\Omega + \left(\varepsilon_{ji}\frac{\partial \varphi}{\partial x_i}, \frac{\partial \phi}{\partial x_j}\right)_\Omega = 0. \tag{9}$$

2.2 DISCRETIZATION

For discretization of the problem (6)-(8), we use the tetrahedronal finite elements with linear base functions. The approximations of the electric potential and displacement are in (10)

$$u_i^h(x) = \sum_{\phi_j^h \in \Phi^h} u_i^j \phi_j^h(\mathbf{x}), \quad \varphi^h(\mathbf{x}) = \sum_{\phi_j^h \in \Phi^h} \varphi^j \phi_j^h(\mathbf{x}), \quad u_i^j, \varphi^j \in \mathbf{R}, \quad i = 1,2,3, \quad \mathbf{x} \in \Omega, \tag{10}$$

where Φ^h denotes the set of base functions. These approximations are piecewise linear on each element. We substitute $\mathbf{u}^h$ and φ^h into integral equalities (9). We require to them to be fulfilled for all basic functions from Φ^h:

$$\left(c_{ijkl} \cdot \frac{1}{2}\left[\frac{\partial u_k^h}{\partial x_l} + \frac{\partial u_l^h}{\partial x_k}\right], \frac{1}{2}\left[\frac{\partial \phi_i^h}{\partial x_j} + \frac{\partial \phi_j^h}{\partial x_i}\right]\right)_\Omega - \left(\rho\omega^2 u_i^h, \phi_i^h\right)_\Omega + \left(d_{ijk} \cdot \frac{\partial \varphi^h}{\partial x_j}, \frac{1}{2}\left[\frac{\partial \phi_i^h}{\partial x_j} + \frac{\partial \phi_j^h}{\partial x_i}\right]\right)_\Omega = 0,$$

$$\left(d_{jik}\frac{1}{2}\left[\frac{\partial u_i^h}{\partial x_k} + \frac{\partial u_k^h}{\partial x_i}\right], \frac{\partial \phi^h}{\partial x_j}\right)_\Omega + \left(\varepsilon_{ji}\frac{\partial \varphi^h}{\partial x_i}, \frac{\partial \phi^h}{\partial x_j}\right)_\Omega = 0. \tag{11}$$

It is equivalent to the linear system with symmetric matrix (the process of derivation of the system matrix is in detail described in [5])

$$\begin{pmatrix} \mathbf{K} - \omega^2\mathbf{M} & \mathbf{P}^{\mathrm{T}} \\ \mathbf{P} & \mathbf{E} \end{pmatrix} \begin{pmatrix} \mathbf{U} \\ \mathrm{V} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}. \tag{12}$$

U and **V** are values (of amplitudes) of displacement and electric potential in the nodes of division. Elastic matrix **K** is symmetric and positive definite, as well as mass matrix **M** and electric matrix **E**.

2.3 ALGEBRAIC PROBLEM

The system allows us, for given ω, to compute the amplitudes of vibration. But more important is to find the resonance frequencies ω_r. The resonance corresponds to the maximal amplitudes of the vibration in some characteristic direction, which equals to the singularity of the system matrix in (12). Thus we have to solve the problem

$$\begin{pmatrix} \mathbf{K} & \mathbf{P}^{\mathrm{T}} \\ \mathbf{P} & \mathbf{E} \end{pmatrix} \begin{pmatrix} \mathbf{U} \\ \mathrm{V} \end{pmatrix} = \omega_r^2 \begin{pmatrix} \mathbf{M} & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} \mathbf{U} \\ \mathrm{V} \end{pmatrix} \tag{13}$$

for unknown $\mathbf{U}$, $\mathbf{V}$, ω_r. With respect to the positive definitness of the electric matrix $\mathbf{E}$, let us denote

$$\mathbf{A} = \mathbf{C} - \mathbf{P}^{\mathrm{T}}\mathbf{E}^{-\mathbf{1}}\mathbf{P}, \quad \mathbf{B} = \mathbf{M}, \quad \lambda = \omega_r^2.$$

Then (13) is equivalent to the generalized symmetric definite eigenproblem

$$\mathbf{AX} = \lambda\mathbf{BX}. \tag{14}$$

If we have any positive eigenvalue λ, its root is the resonance frequency. The proper eigenvector $\mathbf{X}$ characterizes the mode of vibration.

For discretization and compilation of the global matrix, we use our own code. For solving the eigenvalue problem (14), we use the procedures from the Lapack++ or Arpack++ library. From Lapack++ ([3]), we use algorithms based on generalized Schur decomposition. These algorithms solve the complete eigenvalue problem. From Arpack++ ([4]), we use algorithms based on shift-invert method combined with LU factorization. These algorithms, in contrast to Lapack++ code, solve the partial eigenvalue problem and deal with the fact, that matrices are sparse.

3 SOME RESULTS

Described FEM model was calibrated and verified on the longitudinally vibrating quartz resonator XYt-α - cut (for $\alpha = 0^{o} - 5^{o}$) with equivalent thickness and both large sides covered by silver electrodes. This resonator has got a simple geometry, thus the resonance frequencies are very well known (for more precious definition of the testing problem see [5]).

Computed frequencies of longitudinally vibrations are compared with the measured frequencies (publicated in [1]) in the table below.

measured value (Hz)	deviation max.(Hz)	deviation min.(Hz)	α	computed values
67846	$+123$	-114	0°	$68,55 \cdot 10^3$
68653	$+67$	-51	2°	$68,82 \cdot 10^3$
70205	$+60$	-119	5°	$69,05 \cdot 10^3$

In the figure (1), the convergence of computed frequencies (to the value 68.82 kHz), in dependance on number of elements, is shown. The Arpack++ code was rather faster then the Lapack++ code.

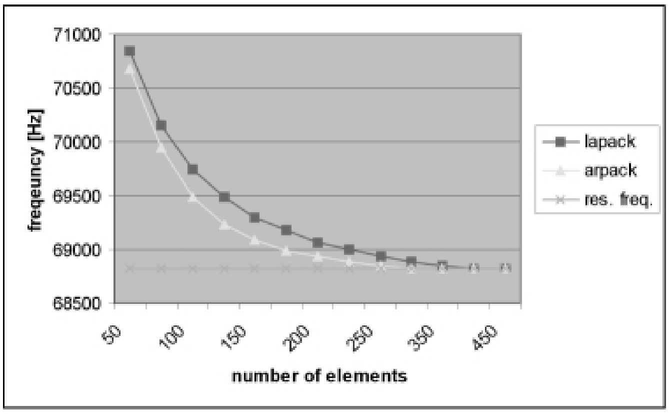

Figure 1: Convergence of the resonance frequency to the value $68,82 \cdot 10^3$ Hz

4 CONCLUSION

The mathematical model for computing the resonance frequencies of the piezoelectric resonator has been built. The results of the described model approximate well the measured results for tested simply shaped (rod or slide) resonators. It seems that our model can have real application, e.g. in desining shape of the resonators vibrating with required frekvencies. Nowadays, the more sofisticated numerical methods for solving the eigenvalue problem are in development.

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