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APPLICATION OF FEM IN MODELLING OF THE RESONANCE CHARACTERISTICS OF PIEZOELECTRIC RESONATORS *

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Abstract. The paper describes an application of the finite element method in modelling of the resonance characteristics of piezoelectric resonators. It 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. The matrices define the generalized eigenvalue problem, from which we can obtain the frequency spectrum of the resonator. The model is tested on the problem of the longitudinally vibrating quartz resonator $XYt_{-\varphi}$ -cut (for definition see [2]), our results are compared with measured frequencies.

Key words. modelling, piezoelectric resonators, finite element method

AMS subject classifications.

1. Introduction. A piezoelectric resonator is a thin stick or wafer made of piezoelectric material. There are two or more electrodes on its surface. The voltage on the electrodes implies the deformation of the resonator. The parameters of piezoelectric resonators are closely related to properties of materials from which they are made. The most important of them are the elastic, dielectric and piezoelectric material characteristics. When we want to study the behavior of the piezoelectric resonator, the most important parameter is his resonance frequency. It depends on the origin and form of the cut, the shape and size of the electrodes, selected vibration mode, the resonator mounting and housing. The experimental testing of piezoelectric resonators is very expensive and means plenty of specimens. Thus the motivation for the using of mathematical model is to cheapen this testing. The analytic solution is able only for very simple structures. For numerical modelling, we use the finite element method (FEM). It is necessary to calibrate and verify all types of models on the simple real system. In article, described FEM model was calibrated and verified on the longitudinally vibrating quartz resonator $XYt_{-\varphi}$ -cut. This resonator has got a simple geometry, thus the resonance frequencies are very well known. In this case, we can compare the model with the real resonator.

2. Physical description. There are two differential equations governing the behavior of a piezoelectric continuum - Newton's laws of motion (2.1) and the quasistatic approximation Maxwell's equation (2.2)(see [3] - this approximation is valid, because acoustic waves are typically five orders of magnitude slower than electromagnetic waves.). Let us denote the volume of the resonator as the volume Ω and its boundary as Γ. The time range, in which we solve the problem, is $(0, \mathrm{T})$.

$$\varrho \frac{\partial^2 u_i}{\partial t^2} = \frac{\partial \mathrm{T_{ij}}}{\partial x_j} \qquad i = 1, 2, 3, \qquad x \in \Omega, \quad \mathrm{t} \in (0, \mathrm{T}) \tag{2.1}$$

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$$\nabla \cdot \mathbf{D} = \frac{\partial \mathrm{D_j}}{\partial x_j} = 0, \tag{2.2}$$

T is the stress tensor, **D** is the vector of electric flux density, ϱ is the density and **u** is the displacement vector.

The above equations are coupled by the piezoelectric equations of state:

$$\mathrm{T_{ij}} = c_{ijkl} \cdot \mathrm{S_{kl}} + d_{ijk} \cdot \mathrm{E_k} \qquad i,j = 1,2,3, \tag{2.3}$$

$$\mathrm{D}_k = d_{kij} \cdot \mathrm{S_{ij}} + \varepsilon_{kj} \cdot \mathrm{E_j} \qquad k = 1,2,3, \tag{2.4}$$

where **S** is the strain tensor, **E** is the vector of electric field, **c**, **d** and $\boldsymbol{\varepsilon}$ are the stiffness, piezoelectric and permitivity tensors of quartz (these tensors are typicall for each material). We assume the symmetry of the tensors. In generall, they are not positive definite.

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

$$\mathrm{E_k} = \frac{\partial \varphi}{\partial x_k} \qquad k = 1,2,3,$$

where φ is the electric potential. If the resonator is loaded by electric potential in the form

$$\varphi = \varphi_0(x,y,z)\cos\omega t,$$

we can expect the behavior of displacement in the form

$$\mathbf{u} = \mathbf{u}_0(x,y,z)\cos\omega t.$$

For convenience, we will write the amplitudes of vibration, $\mathbf{u_0}$ and φ_0, as **u** and φ. If we now substitute (2.3), (2.4) into (2.1), (2.2), we obtain

$$-\omega^2\varrho \cdot u_i = \frac{\partial}{\partial x_j}\left(c_{ijkl} \cdot \frac{1}{2}\left[\frac{\partial u_k}{\partial x_l} + \frac{\partial u_l}{\partial x_k}\right] + d_{ijk} \cdot \frac{\partial \varphi}{\partial x_k}\right) \qquad i = 1,2,3, \tag{2.5}$$

$$\frac{\partial}{\partial x_k}\left(d_{kij} \cdot \frac{1}{2}\left[\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right] + \varepsilon_{kj} \cdot \frac{\partial \varphi}{\partial x_j}\right) = 0. \tag{2.6}$$

Let the boundary of Ω consist of two disjoint subsets $\Gamma = \Gamma_1 \bigcup \Gamma_2$. There are stated the boundary and initial condition :

$$\begin{aligned} u_i &= u_{iD} \qquad i = 1,2,3 \qquad \text{on} \quad \Gamma_1, \\ \mathrm{T_{ij}} n_j &= t_{iN} \qquad i = 1,2,3 \qquad \text{on} \quad \Gamma_2, \end{aligned} \tag{2.7}$$

$$\begin{aligned} \varphi &= \varphi_D \qquad \text{on} \quad \Gamma_1, \\ \mathrm{D_k} n_k &= \mathrm{D_N} \qquad \text{on} \quad \Gamma_2. \end{aligned} \tag{2.8}$$

The conditions marked with subscript D are the Dirichlet boundary conditions, the subscript N marks the Neumann boundary condition (n_j is the j-th component of normal vector at the boundary Γ).

3. Weak formulation. If we want to use the FEM method to compute the the numerical solution of the problem (2.5) - (2.8), we must establish the weak formulation of the problem. We look for a weak solution, which has to be a member of the Sobolev space

$$W_2^{(1)}(\Omega) = \{\varphi \in L_2(\Omega) | \nabla\varphi \in [L_2(\Omega)]^3 \text{ in the weak sence}\}.$$

Let's define

$$V(\Omega) = \{v | v \in W_2^{(1)}(\Omega), \quad v|_{\Gamma_1} = 0 \quad \text{in the sence of traces}\}.$$

At first, for i=1,2,3 we multiply the equations (2.5) by test functions $w_i \in V$, sum them up and integrate the sum over Ω. After using the Green formula, boundary conditions and symmetry of the material tensors we obtain the integral equality

$$\text{(3.1)} \qquad \Big(c_{ijkl}\cdot \mathrm{S_{kl}}, \mathrm{R_{ij}}\Big)_\Omega - \Big(\varrho\omega^2 u_i, w_i\Big)_\Omega + \Big(d_{ijk}\cdot \frac{\partial\varphi}{\partial x_j}, \mathrm{R_{ij}}\Big)_\Omega = \Big\langle t_{iN}, w_i \Big\rangle_{\Gamma_2},$$

where

$$\mathrm{R_{ij}} = \frac{1}{2}\left[\frac{\partial w_i}{\partial x_j} + \frac{\partial w_j}{\partial x_i}\right].$$

Further, we apply the same procedure on the equation (2.6), with test function $\phi \in V$. We obtain the integral equality

$$\text{(3.2)} \qquad \Big(d_{jik}\mathbf{S}_{ik}, \frac{\partial\phi}{\partial x_j}\Big)_\Omega + \Big(\varepsilon_{ji}\frac{\partial\varphi}{\partial x_i}, \frac{\partial\phi}{\partial x_j}\Big)_\Omega = \Big\langle D_N, \phi\Big\rangle_{\Gamma_2}.$$

Let $\mathbf{u}_D \in [W_2^{(1)}(\Omega)]^3$ and $\varphi_D \in W_2^{(1)}(\Omega)$ satisfy Dirichlet boundary conditions (in the weak sence). Further, let $\mathbf{u} = (u_1, u_2, u_3) \in [V(\Omega)]^3$ and $\varphi \in V(\Omega)$ be functions, for which equalities (3.1) and (3.2) are observed for all choices of testing functions $\mathbf{w} = (w_1, w_2, w_3) \in [V(\Omega)]^3, \quad \phi \in V(\Omega)$. Than we define the weak solution of the problem (2.5) - (2.8) as

$$\mathbf{u}_D + \mathbf{u}, \quad \varphi_D + \varphi.$$

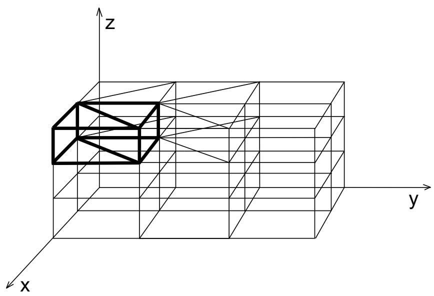

FIG. 4.1. *Division of a cubic crystal into layers and prizmatic elements*

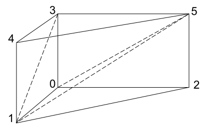

FIG. 4.2. *Division of a prizmatic element into four tetrahedrons 0125, 0153 a 1534*

4. Discretized problem. For computing an aproximation of the weak solution of our problem, we divide the area Ω (which is the volume of the resonator) in two steps to the finite set E^h of disjoint tetrahedrons covering the volume:

$$\Omega \sim \Omega^h = \bigcup_{e \in E^h} e, \quad \bigcup_{j \in J} \overline{e_j} = \overline{\Omega}.$$

For each element from the division, we define the function space and its basis

$$V^h(e) = \{\phi^h | supp(\phi^h) \subset e,\ \phi^h \in W_2^1(e),\ \phi^h|_{\partial e} = 0\}\ \Phi(e) = \{\phi_i^e(x,y,z) | i = 1,2,3,4\},$$

which satisfy

$$\phi_i^e(s^j) = \delta_{ij}, \qquad i,j = 1,2,3,4.$$

For tethrahedron the basis is made of four linear multinomials. The union

$$\Phi^h = \bigcup_{e \in E^h} \Phi^h(e) \quad \text{forms the basis of} \quad V^h(\Omega) = \{\phi \in V(\Omega), \phi|_e$$

is linear multinomial $\forall e \in E^h\}$. We look for aproximation of a weak solution from the space $V^h(\Omega)$:

$$u_i^h(x) = \sum_{\phi_j^h \in \Phi^h} u_i^j \phi_j^h(\mathbf{x}), \quad u_i^j \in \mathbf{R}, \quad \mathbf{x} \in \Omega, \quad i = 1,2,3, \tag{4.1}$$

$$\varphi^h(\mathbf{x}) = \sum_{\phi_j^h \in \Phi^h} \varphi^j \phi_j^h(\mathbf{x}), \quad \varphi^j \in \mathbf{R}, \quad \mathbf{x} \in \Omega.$$

Coefficients in the linear combination are the values of the functions $\mathbf{u}$ and φ in the nodes of division. Let the basis functions be numbered $(\phi_1^h, ..., \phi_r^h)$. Substituting (4.1) into (3.1) and (3.2), the integral equality has to be satisfied for all base function ϕ_s^h, $s \in \hat{r}$

$$\left(c_{ijkl} \cdot \mathrm{S^h_{kl}}, \mathrm{R^h_{ij}}\right)_\Omega - \left(\varrho\omega^2 u_i^h, \phi_s^h\right)_\Omega + \left(d_{ijk} \cdot \frac{\partial \varphi^h}{\partial x_j}, \mathrm{R^h_{ij}}\right)_\Omega = \left\langle t_{iN}, \phi_s^h \right\rangle_{\Gamma_2}, \tag{4.2}$$

$$\left(d_{jik} \mathbf{S}_{ik}^h, \frac{\partial \phi_s^h}{\partial x_j}\right)_\Omega + \left(\varepsilon_{ji} \frac{\partial \varphi^h}{\partial x_i}, \frac{\partial \phi_s^h}{\partial x_j}\right)_\Omega = \left\langle D_N, \phi_s^h \right\rangle_{\Gamma_2}. \tag{4.3}$$

To fulfil the above equations, the system of linear algebraic equations has to be fulfiled. The system has a block shape

$$\left(\begin{array}{c|c}\left(\begin{array}{ccc}\mathbf{K}_{11} & .. & \mathbf{K}_{1r}\\ \mathbf{K}_{21} & .. & \mathbf{K}_{2r}\\ ... & .. & ...\\ ... & .. & ...\\ \mathbf{K}_{r1} & .. & \mathbf{K}_{rr}\end{array}\right) - \omega^2 \left(\begin{array}{ccc}\mathbf{M}_{11} & .. & \mathbf{M}_{1r}\\ \mathbf{M}_{21} & .. & \mathbf{M}_{2r}\\ ... & .. & ...\\ ... & .. & ...\\ \mathbf{M}_{r1} & .. & \mathbf{M}_{rr}\end{array}\right) & \begin{array}{ccc}\mathbf{P}_{11}^{\mathrm{T}} & ... & \mathbf{P}_{r1}^{\mathrm{T}}\\ \mathbf{P}_{12}^{\mathrm{T}} & ... & \mathbf{P}_{r2}^{\mathrm{T}}\\ ... & ... & ...\\ ... & ... & ...\\ \mathbf{P}_{1r}^{\mathrm{T}} & ... & \mathbf{P}_{rr}^{\mathrm{T}}\end{array}\\ \hline \begin{array}{ccc}\mathbf{P}_{11} & ... & \mathbf{P}_{1r}\\ \mathbf{P}_{21} & ... & \mathbf{P}_{2r}\\ \vdots & \cdots & \vdots\\ \mathbf{P}_{r1} & ... & \mathbf{P}_{rr}\end{array} & \begin{array}{ccc}\mathbf{E}_{11} & ... & \mathbf{E}_{1r}\\ \mathbf{E}_{21} & ... & \mathbf{E}_{2r}\\ \vdots & \cdots & \vdots\\ \mathbf{E}_{r1} & ... & \mathbf{E}_{rr}\end{array}\end{array}\right)\left(\begin{array}{c}u_1^1\\ u_2^1\\ u_3^1\\ ...\\ u_1^r\\ u_2^r\\ u_3^r\\ \varphi^1\\ \varphi^2\\ ...\\ \varphi^r\end{array}\right)$$

$$= \left(\mathrm{R}_1^1, ..., \mathrm{R}_\mathrm{r}^1, \mathrm{R}_1^2, ..., \mathrm{R}_\mathrm{r}^2\right)^T, \tag{4.4}$$

where for $p, q \in \hat{r}$

$$\mathbf{K}_{pq} = \int_{\Omega^h} [\mathbf{B}^q]^{\mathrm{T}} \mathbf{C} \mathbf{B}^p d\Omega, \quad \mathbf{K}_{pq} \in \mathbf{R}^{3,3},$$

$$\mathbf{B}^p = \begin{pmatrix} \frac{\partial}{\partial x_1}\phi_p^h(\mathbf{x}) & 0 & 0\\ 0 & \frac{\partial}{\partial x_2}\phi_p^h(\mathbf{x}) & 0\\ 0 & 0 & \frac{\partial}{\partial x_3}\phi_p^h(\mathbf{x})\\ 0 & \frac{1}{2}\frac{\partial}{\partial x_3}\phi_p^h(\mathbf{x}) & \frac{1}{2}\frac{\partial}{\partial x_2}\phi_p^h(\mathbf{x})\\ \frac{1}{2}\frac{\partial}{\partial x_3}\phi_p^h(\mathbf{x}) & 0 & \frac{1}{2}\frac{\partial}{\partial x_1}\phi_p^h(\mathbf{x})\\ \frac{1}{2}\frac{\partial}{\partial x_2}\phi_p^h(\mathbf{x}) & \frac{1}{2}\frac{\partial}{\partial x_1}\phi_p^h(\mathbf{x}) & 0 \end{pmatrix},$$

$$(\mathbf{M}_{pq})_{ii} = \int_{\Omega^h} \phi_p^h \phi_q^h d\Omega, \quad i = 1, 2, 3, \quad \mathbf{M}_{pq} \in \mathbf{R}^{3,3},$$

$$\mathbf{P}_{pq} = \int_{\Omega^h} [\mathbf{B}^q]^{\mathrm{T}} \mathbf{D} (\nabla \phi_p^h) d\Omega, \quad \mathbf{P}_{pq} \in \mathbf{R}^{3,1},$$

$$\mathbf{E}_{pq} = \int_{\Omega^h} (\nabla \phi_q^h)^{\mathrm{T}} \mathbf{\Sigma} (\nabla \phi_p^h) d\Omega, \quad \mathbf{E}_{pq} \in \mathbf{R},$$

$$\mathrm{R}_\mathrm{p}^1 = (\langle t_{1N}, \phi_p^h \rangle_{\Gamma_2},\ \langle t_{2N}, \phi_p^h \rangle_{\Gamma_2},\ \langle t_{3N}, \phi_p^h \rangle_{\Gamma_2})^{\mathrm{T}}, \quad \mathrm{R}_\mathrm{p}^2 = \langle D_N, \phi_p^h \rangle_{\Gamma_2}.$$

4.1. Observing of the resonance frequencies. Let us write the system (4.4) as

$$\begin{pmatrix} \mathbf{K} - \omega^2 \mathbf{M} & \mathbf{P}^{\mathrm{T}} \\ \mathbf{P} & \mathbf{E} \end{pmatrix} \begin{pmatrix} \mathbf{U} \\ \Phi \end{pmatrix} = \begin{pmatrix} \mathrm{R}_1 \\ \mathrm{R}_2 \end{pmatrix}. \tag{4.5}$$

The Dirichlet boundary conditions can be introduced to the system by replacing the appropriate part of matrix with identity matrix and zeros and adding the boundary values to the vector of right side. E.g., let be prescribed the boundary condition for displacement in the j-th node of the mesh. Then we change submatrices in the j-th row and column of the matrix (other parts of the system are unchanged).

$$\left(\begin{array}{ccc|ccc} ... & 0 & ... & ... & ... & ... \\ 0 & \mathbf{I} & 0 & 0 & 0 & 0 \\ ... & 0 & ... & ... & ... & ... \\ ... & 0 & ... & ... & ... & ... \\ \hline ... & 0 & ... & ... & ... & ... \\ \vdots & ... & \vdots & \vdots & \dots & \vdots \\ ... & 0 & ... & ... & ... & ... \end{array}\right) \left(\begin{array}{c} ... \\ u^j \\ ... \\ ... \\ ... \\ \vdots \\ ... \end{array}\right) = \left(\begin{array}{c} ... \\ u_D^j \\ ... \\ ... \\ ... \\ \vdots \\ ... \end{array}\right), \tag{4.6}$$

For given parameter ω, if the matrix of the system is nonsingular, from the system with right side we can compute values of displacement and electric potential in the nodes of the mesh (it was the subject in first testing problems and shall not be presented here). The case of singularity of the matrix corresponds to the resonance. To compute the resonance frequencies involve to find out such parameters ω, for which the matrix is singular (or nearly singular). Thus we have to solve the symmetric generalized eigenvalue problem with deflated matrix of the system (we omit the parts of the matrix, which belong to the Dirichlet boundary condition):

$$\begin{pmatrix} \mathbf{K} & \mathbf{P}^{\mathrm{T}} \\ \mathbf{P} & \mathbf{E} \end{pmatrix} \begin{pmatrix} \mathbf{U} \\ \Phi \end{pmatrix} = \lambda \begin{pmatrix} \mathbf{M} & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} \mathbf{U} \\ \Phi \end{pmatrix}. \tag{4.7}$$

The solution of this problem is the eigenvalue $\lambda \in \mathbf{R}$ and the nontrivial eigenvector $(\mathbf{U}, \Phi)^{\mathrm{T}}$, which fulfil (4.7). If we have any positive eigenvalue λ from the solution of the problem (4.7), the

$$\omega = \sqrt{\lambda}$$

is the required resonance frequency. The eigenvector $(\mathbf{U}, \Phi)^{\mathrm{T}}$ contains the values of displacement and electric potential at the nodes of discretization. The resonance frequencies result from the character of the matrix, thus they are independent from the right side in (4.5). We assume the influence of the right side to the shape of the vibration, but it has not yet been studied.

5. Example problem. The designed FEM model was calibrated and verified on the longitudinally vibrating narrow quartz XYt-j -cut rods (for j $= 0^{\mathrm{o}} - 5^{\mathrm{o}}$) with parameters

$$\text{length} = (4.000 \pm 0.001)\text{cm}, \ \text{thickn.} = (0.001 \pm 0.0005)\text{cm}, \ \text{width} = (0.400 \pm 0.001)\text{cm}.$$

Both large sides of the resonator are covered by silver electrodes. Its equivalent thickness is 6.10^{-4} cm. The resonator is pinned in the center of large sides.The resonator is fixed in the center of its length, thus the problem is symmetric and we can solve it for one half of the resonator. We establish appropriate boundary conditions at the center of the resonator. The consequence of this simplification is, that we compute only symmetric vibrations of the resonator.

5.1. Boundary conditions. The values of the electric potential is established at the electrodes: $\phi = \phi_{def}$.

The boundary conditions for the displacement are established in the center of the resonator. Resonator is fixed in the center of the large sides. Through these points goes the nodal line of odd vibrations. On the nodal line we suppose zero displacements: $\mathbf{u} = 0$ at the nodal line of odd vibrations.

Zero displacements are also entered on the planes going through the nodal line of odd vibrations. These planes are supposed in two modifications.

1. $\mathbf{u} = 0$ the plane normal to the length of resonator
2. $\mathbf{u} = 0$ the nodal plane of longitudinal vibrations

The definition of the second plane depends on the cut (see [2]) and the plane is not exactly normal to the length of the resonator. This second condition represents more accurate the physical reality.

5.2. Numerical realisation. The resonator was divided into prismatic elements (fig. 5.1) and then each of the prismatic element was divided into four tetrahedrons.

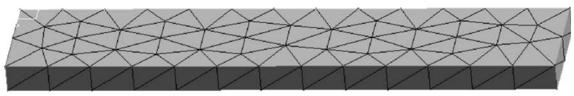

FIG. 5.1. *The mesh - prismatic elements*

The global matrix was compiled. Rows and columns, which belonged to the nodes with prescribed Dirichlet boundary conditions, were removed. The deflated matrix was an input for the computing of the resonance frequencies. The procedures for discretization with flexible discretization parameter and compilation of the matrices of the discretized problem has been implemented by us in the programming language C++. For solving the generalized eigenvalue problem we have used the procedures from LAPACK library. The LAPACK procedure input were two deflated matrices from (4.7). The programe output is the vector containing spectrum of generalized eigenvalue problem and the appropriate matrix, which columns are the standardized eigenvectors (the description of the output is in the LAPACK manual, available on the internet). The particular, eigenvector characterizes the type of vibration. The computing has been done for several meshes with various refinement. In the graph (fig. 5.2), there is shown the convergent character of the dependance of the resonance frequency on increasing number of elements in the mesh (increasing size of the global matrix).

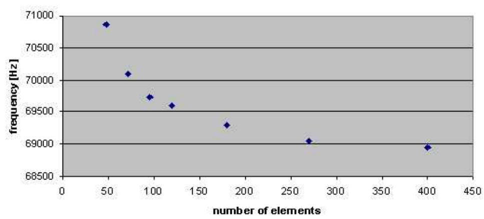

FIG. 5.2. *Frequency of the longitudinal vibration*

5.3. Some results. In next set of figures (5.3), there are shown some of first kinds of vibration of the resonator.

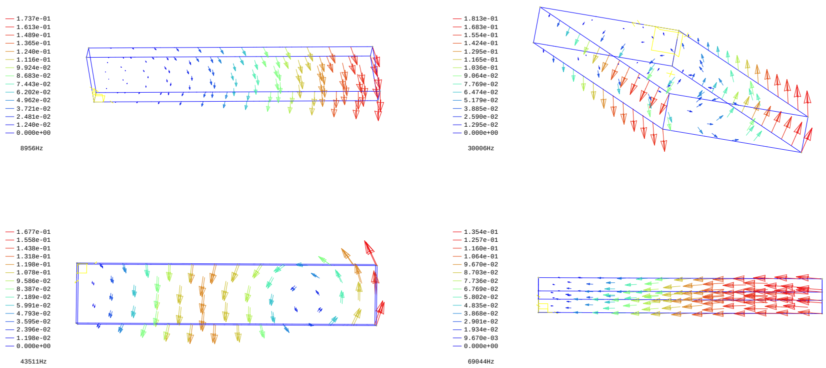

FIG. 5.3. *Some of computed modes of vibration*

Computed frequencies of longitudinall vibrations are compared with the measured frequencies (publicated in [1]) in table 5.1.

Measuring [Hz]	Model [Hz]	difference [%]	φ
67 846	68 539	1.02	0^o
68 653	68 814	0.23	2^o
70 205	69 491	1.02	5^o

TABLE 5.1
Comparation with measured frequencies

6. Conclusion. The model computing the resonance frequencies of the piezoelectric resonator has been built. The results of the described well model approximate the measured results for tested simply shaped (rod or slide) resonators. So it seems our model can have real application, e.g. in designing shape of the resonators with required frequencies. Nowadays, the program modules for computing the resonance chracteristics of planconvex and biconvex resonators and module for computing the temperature dependence of resonance frequencies are in development.

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