MODELLING OF THE RESONANCE CHARACTERISTICS OF THE PIEZOELECTRIC RESONATORS*

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1. ABSTRACT

The contribution describes the application of the finite element method in modelling of the resonance characteristics of the piezoelectric resonators. It deals with derivation of the variation formulation of the problem, which is product of the physical description of the piezoelectric structures behaviors and testing of the model on the the longitudinally vibrating quartz resonator $XYt_{-\varphi}$ **-cut**, where the correspondence between computed frequency spectrum and measured frequency spectrum of this resonator is studied.

Keywords: modelling, piezoelectric resonators, finite element method

2. INTRODUCTION

The parameters of piezoelectric resonators are closely related to the properties of the materials from which they are made. Elastic, dielectric and piezoelectric properties are most important material characteristics. The most important parameter of the piezoelectric resonators is the resonance frequency. It depends on the origin and form of the cut, the shape and size of the electrodes, the vibration mode selected, the resonator mounting and housing.

Because the experimental testing of piezoelectric resonators is very expensive, useful is the mathematical model. For simple structures is able analytic solution, but for complicated structures we have to use numerical solution. 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. Described FEM model was calibrated and verifyied on the longitudinally vibrating quartz resonator $XYt_{-\varphi}$ -cut. This resonator has got simple geometry, thus the resonance frequencies are very well known. In this case we can compare model with real resonator.

3. PHYSICAL DESCRIPTION

The differential equations governing the behaviors of a piezoelectric continuum are Newton's laws of motion and the quasistatic approximation to Maxwell's equation [Ref. 2] (This later approximation is valid, because acoustic waves are typically five orders of magnitude slower than electromagnetic waves.). The volume of the resonator is area Ω and it's boundary is Γ. Time range, which we solve the problem are $\langle 0, T \rangle$. Thus,

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

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$$\frac{\partial D_i}{\partial x_i} = 0 \tag{2}$$

where $\boldsymbol{T}$, ρ, $\boldsymbol{u}$ and $\boldsymbol{D}$ are stress, density, particle displacement and electric flux density. These equations are coupled by the piezoelectric equations of state,

$$T_{ij} = c_{ijkl} S_{kl} + d_{kij} E_k \tag{3}$$

$$D_k = d_{kij} S_{ij} + \varepsilon_{kj} E_j \tag{4}$$

where $\boldsymbol{S}$, $\boldsymbol{E}$, $\boldsymbol{c}$, e and $\boldsymbol{\varepsilon}$ are strain, electric field and the stiffness, piezoelectric and permitivity tensors of the crystal. In addition,

$$S_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \tag{5}$$

$$E_i = -\frac{\partial \varphi}{\partial x_i} \tag{6}$$

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

$$\varphi = \varphi_0 \cdot \sin \omega t,$$

where t is time, then we can expect the behavior of the displacement in this shape:

$$u_i = u_{0i} \cdot \sin \omega t, \quad i = 1,2,3.$$

We will write the amplitudes of the vibration, u_{i0} and φ_0, as u_i and φ. We can now rewrite the problem (1) as

$$-\rho \omega^2 u_i = \frac{\partial T_{ij}}{\partial x_j}, \ i = 1,2,3, x \in \Omega, \tag{7}$$

Two types of boundary conditions are added. Dirichlet's boundary conditions on boundaries Γ_{1s}, Γ_{1e} and Neumann's boundary conditions on boundaries Γ_{2s}, Γ_{2e}. boundary Γ_{2s} without places where is Γ_{1s} . The situation is on the picture. The boundary conditions are:

$$u_i = u_{iD} \quad \text{on} \quad \Gamma_{1s} \tag{8}$$

$$T_{ij} \cdot n_j = t_{iN} \quad \text{on} \quad \Gamma_{2s} \tag{9}$$

$$\varphi = \varphi_D \quad \text{on} \quad \Gamma_{1e} \qquad (10)$$

$$D_k \cdot n_k = D_N \quad \text{on} \quad \Gamma_{2e} \qquad (11)$$

Boundary condition (8) can represent e.g. places of fixation of resonator, boundary condition (10) represents the position of electrodes.

4. FINITE ELEMENT FORMULATION

This method is based on the theory of weak solution. When we substitute equations (3) and (4) into (7) and (2), we obtain a set of equations with unknown functions **u** and φ:

$$-\rho\omega^2 u_i = \frac{\partial}{\partial x_j}\left[c_{ijkl}\frac{1}{2}\left(\frac{\partial u_k}{\partial x_l} + \frac{\partial u_l}{\partial x_k}\right) - d_{ijk}\frac{\partial \varphi}{\partial x_k}\right] \quad (12)$$

$$0 = \frac{\partial}{\partial x_k}\left[d_{kij}\frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) - \varepsilon_{kj}\frac{\partial \varphi}{\partial x_j}\right] \quad (13)$$

We look for weak solution of these equation, which has to be contained in the Sobolev space $W_{2,1}(\Omega)$.

Let`s for i=1,2,3 multiply the equations (12) with testing functions $w_i \in V(\Omega)=\{v \mid v \in W_{2,1}(\Omega), \mathrm{Trace}(v) = 0 \text{ on } \Gamma_1\}$, count them up and integrate over Ω. Using Green formula, boundary conditions and symmetricity of material tensors we obtain the integral equality

$$\int_\Omega c_{ijkl} S_{kl} R_{ij} - \rho\omega^2 \int_\Omega u_i w_i - \int_\Omega d_{ijk}\frac{\partial \varphi}{\partial x_k} R_{ij} = \int_{\Gamma_{2s}} t_{iN} w_i$$

(14)

Further, let`s multiply the equation (13) with testing function $\phi \in V(\Omega)$. With the same procedure we obtain the integral equality

$$-\int_\Omega d_{ijk} S_{jk}\frac{\partial \phi}{\partial x_i} + \int_\Omega \varepsilon_{ij}\frac{\partial \varphi}{\partial x_j}\frac{\partial \phi}{\partial x_i} = \int_{\Gamma_{2e}} D_N \phi$$

(15)

We say, that functions **u** and φ are the weak solution of the problem (1) and (2), if equalities (13) and (14) are observed for all choices of testing functions ψ_i and Φ.

For computing an aproximation of weak solution of our problem, we divide the area Ω (which is the volume of the resonator) into the finite set of disjoint tetrahedrons covering the area:

$$E^h = \{e_j \mid j \in J\}, \bigcup_{j\in J} \overline{e_j} = \overline{\Omega}$$

Area Ω is aproximated by the union

$$\bigcup_{j\in J} e_j = \Omega^h \approx \Omega.$$

For each element e from division we set up the basis $\Phi(e)$ of the space $V(e)=\{v \mid supp\ v \subset e, v \in W_{2,1}(e), v|_{\partial e} = 0\}$ made of four linear multinominals. Union

$$\bigcup_{e\in E^h} \Phi(e) = \Phi^h$$

form the basis of the space $V(\Omega^h)$.Now, we look for the aproximations $\mathbf{u}^h$ and φ^h of functions **u** and φ as linear combinations of the basic functions:

$$u_i^h(x) = \sum_{\phi_j \in \Phi^h} u_i^j \phi_j(x),$$

$$u_i^j \in \mathbf{R}, x \in \Omega, i = 1,2,3.$$

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

(16)

Coefficients in the linear combination are the values of the functions **u** and φ in the nodes of division.

Weak formulation (substituting (16) into (14) and (15), with basic functions as testing functions) leads to the system of linear algebraic equations with right side. It has this block shape

$$\begin{bmatrix} \mathbf{K} - \omega^2\mathbf{M} & \mathbf{D} \\ \mathbf{D}^T & \mathbf{E} \end{bmatrix} \cdot \begin{bmatrix} \mathbf{u} \\ \varphi \end{bmatrix} = \begin{bmatrix} \mathbf{R}_1 \\ \mathbf{R}_2 \end{bmatrix},$$

where **K** is elastic block, **M** is mass block, **D** is piezoelectric block and **E** is electric block. The vector of unknowns is made of coefficients from (16). The vector of right side contains boundary conditions.

From this system we can either compute the function values of displacement and electric potential (we just solve the system) or compute resonance frequencies by solving the generalized eigenvalue problem

$$\begin{bmatrix} \mathbf{K} & \mathbf{D} \\ \mathbf{D}^T & \mathbf{E} \end{bmatrix} \mathbf{X} = \lambda \begin{bmatrix} \mathbf{M} & 0 \\ 0 & 0 \end{bmatrix} \mathbf{X}.$$

The positive eigenvalues λ are the squares of the resonance frequencies. Appropriate eigenvectors characterize the sort of vibration.

5. TESTING OF THE MODEL

Designed FEM model was calibrated and verifyied on the the longitudinally vibrating narrow $XYt_{-\varphi}$ -cut rods (for $\varphi = 0^o$ to 5^o) with parameters

length $l = (4.000 \pm 0.001)cm$

thickness $t = (0.100 \pm 0.0005)cm$

beam $b = (0.400 \pm 0.001)cm$

On both large sides of resonator are electrodes. Electrodes are made from silver. Its equivalent thickness is $6 \cdot 10^{-4}$ cm. Resonator is pinned in the center of large sides.

We need bring under effect of error, which is due to irregularity of mesh, and have an area which easy to meshing. This type of resonators is advantageous for previous reasons. Measured resonance frequencies, how they are presented in [Ref.1] are in the Table 1.

av. val. [Hz]	max. dif. [Hz]	min. dif. [Hz]	φ
67 846	+88	-108	0^o
68 653	+17	-13	2^o
70 205	+81	-81	5^o

Table 1: Measured resonance frequencies

Some types of vibrations calculated for this resonator didn't have to excited. This is due to coupling between some elements of tenzors of piezoelectric or elastic modulus. Study of existention of vibrations is not aim of this work and won't be discussed.

Resonator is fixed in the center of its length and then we can suppose symmetry in regard to center of the resonator. Then we can say, that it is symmetry problem and we can solve it only on one half of resonator and the second part we can substitute with competent boundary conditions. Consequence of this simplification is computation only symmetric vibrations of resonator.

5.1 Boundary conditions

On the large sides are electrodes. In mesh nodes, which belong to these areas are entered values of electric potential. That is very simply. More interesting is assigning of elastic boundary conditions. Resonator is fixed in the center of large sides. Through these points going the nodal line of odd vibrations. On the nodal line we suppose zero displacements. Zero dispalcements are also entered on the planes going through the nodal line of odd vibrations. These planes are supposed in two modifications:

- plane normal to the length of resonator
- nodal plane of longitudinal vibrations

The first version is used by model calibration and the second for accuracy computation of longitudinal vibrations on selected mesh.

5.2 Selecting of efficient mesh

Computes were achieved for several meshes, which differed to number of elements. The type of used meshes is on the Figure 1.

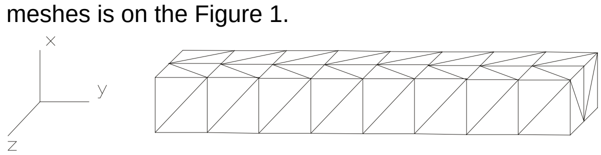

Fig 1 : Type of used meshes

Meshes had 48, 72, 96 and 120 elements. Criterium of mesh quality is vibration frequencies convergence. Between results for longitudinal vibrations computed on the meshes with 96 and 120 elements is very small difference, so we can say that refinement of mesh is not effective. Graph of convergence of results is shown on the Figure 2. Consequence of mesh refinement is enlargement of global matrix. Enlargement of matrix pose claim to computational capacity and can be cause of large numerical error, which depreciates result. Development of numerical methods, which solve described algebraic problem is very important for practicability of FEM in design of piezoelectric resonators. In this case was made computation only for angle $\varphi = 0^o$. Computed results for selected types of vibrations are in Table 2.

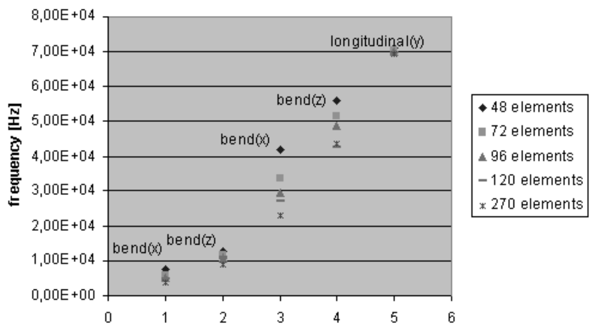

Fig. 2 : Convergence of computed results

Type of vibrations	Resonance freq. [Hz] for mesh with number of elements				
	48	**72**	**96**	**120**	**270**
bend – ***x*** ax	7 803	6 027	5 236	4 759	3 980
bend – ***z*** ax	12 480	11 383	10 925	10 702	8 956
bend – ***x*** ax	41 780	33 474	29407	27 193	23 166
shear – ***xz*** plane	86 261	69 949	60274	48 500	30 006
bend – ***z*** ax	55 952	51 269	48 640	42 640	43 511
bend – ***x*** ax	104070	83 749	73 649	68 163	59 902
longitudinal – ***y*** ax	70 873	70 091	69 730	69 600	69 044
bend – ***z*** ax	131921	117045	110751	107739	-
bend – ***x*** ax	174667	148107	129470	119323	-
shear – ***xz*** plane	207280	176270	144716	126342	89 988

Table 2 : Computed res. freq. for different meshes

We made verification, that the model is relative independent on the choice of the mesh. For computation was used different type of the mesh with different number of elements. This mesh is on the Fig. 3.

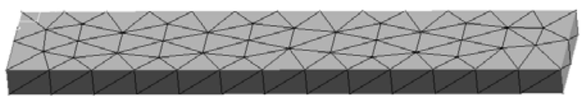

Fig. 3 : Verification mesh

This mesh has 270 elements. Results are in the Table 2. Visualization of some types of vibrations is on Fig. 4. From listed above resulting, that on figures is only one half of the resonator. On the left side is the centre of the resonator.

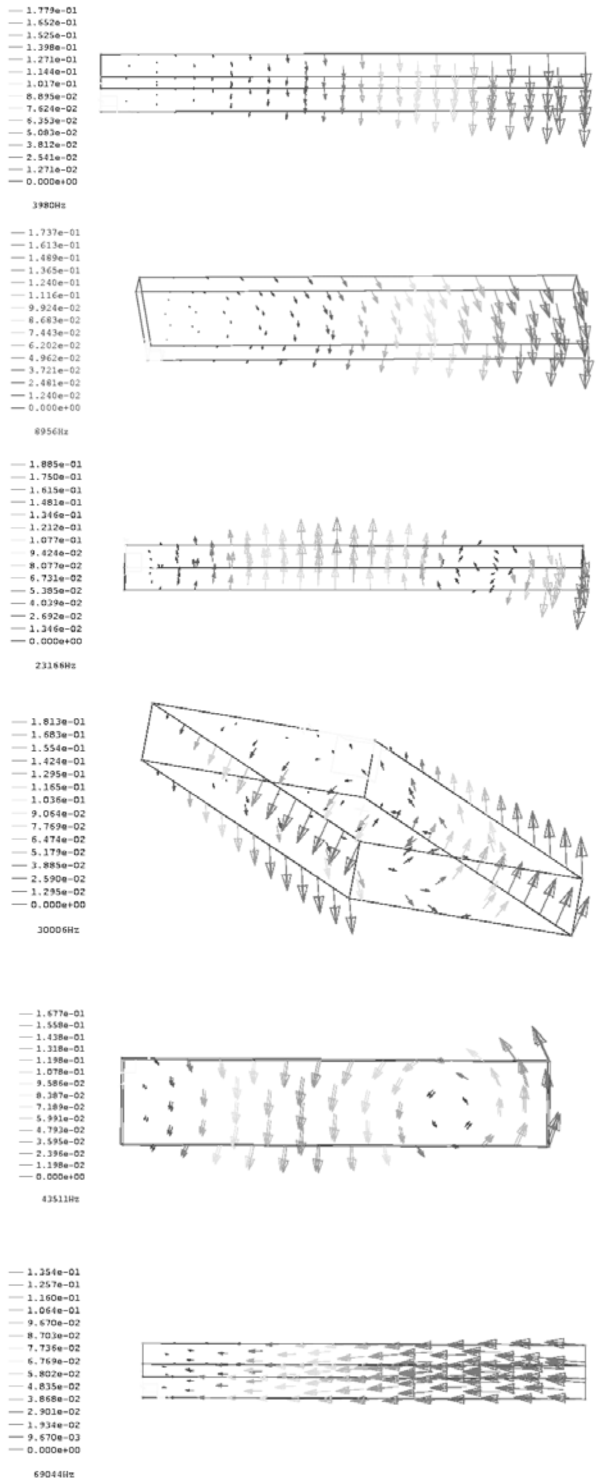

Fig. 4 : Visualization of vibrations - bend *x* ax, bend *z* ax, bend *x* ax, shear *xz* plane, longitudinal *y* ax.

5.3. Accuracy computation of longitudinal vibrations

The elastic behaviors of isotropic materials are characterised by Young's modulus ***E*** and Poisson's ratio ***ν***. These quantities are for isotropic materials constants. Also elastic behaviors of anisotropic piezoelectric materials we can express by means of expressions listed above, but ***E*** and ***ν*** are not constants, they have in various directions various values. If we plot values of ***E*** in corresponding directions, we get the area of elasticity [Ref. 3]. Similar area we get for Poisson's ratio.

From listed above resulting, that the nodal plane of longitudinal vibrations of resonators $XYt_{-\varphi}$-cut is not generally identical with the plane normal to the length of resonator. The nodal plane of longitudinal vibrations contains with the plane normal to the length angle ϑ - vide Fig. 5. This angle correspond with minimum of Young's modulus in the plane ***xy***. We can explain this effect on the base of the principle of the minimal potential energy [Ref. 4.] Angle ϑ we can get from the plane of elasticity. For $XYt_{-\varphi}$-cut is $\vartheta = 20^{o}$.

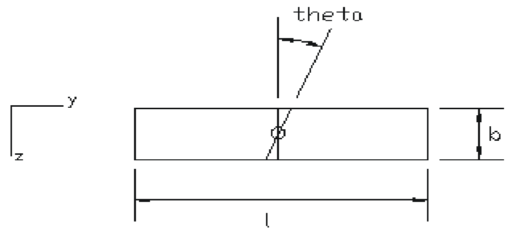

Fig. 5 : Angle ϑ.

Elastic boundary conditions – zero displacements were applied on the nodal plane of longitudinal vibrations. For this computation was used mesh with 270 elements – Fig. 3. Computed values of longitudinally vibrations and difference between measured and computed are shown in Table 3.

measured [Hz]	computed [Hz]	difference [%]	φ
67 846	68 139	0.43	*0^{o}*
68 653	68 714	0.09	*2^{o}*
70 205	69 991	0.30	*5^{o}*

Table 1 : Comparation between measured and computed frequencies.

6. CONCLUSION

Described model should be the support for development of the system for computer aided design of piezoelectric resonators. At present is in development modul for computing resonance chracteristics of planconvex and biconvex resonators and modul for computing of temperature dependence of resonance frequencies.

REFERENCES

[1] Tichý J., Zelenka J.: Podélně a plošně střižně kmitající piezoelektrické rezonátory ze synthetického křemene, Čs. Čas. Fys. 10 (1960), pp. 328 – 332.

[2] Milsom R. F., Elliot D. T., Terry Wood S., Redwood M.: Analysis and Design of Couple Mode Miniature Bar Resonator and Monolothic Filters. *IEEE Trans Son. Ultrason.*, , Vol. 30 (1983), pp. 140-155.

[3] Petržílka V.: Piezoelektřina I., Přírodovědecké vydavatelství, Praha 1951.

[4] Hlaváček I., Nečas J.: Úvod do matematické teorie pružných a pružně plastických těles, Praha, SNTL 1983.

[5] Zelenka J.: Piezoelektrické rezonátory a jejich použití v praxi, Academia, Praha 1981.

[6] Maryška J., Novák J., Rálek P.: Modelling of Piezoelectric materials, Proceesings of Simona 2000, ISBN 80-7083-451-X, Liberec 2000.