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MODELING OF THE PIEZOELECTRIC EFFECT USING THE FINITE-ELEMENT METHOD (FEM)

MODELIRANJE PIEZOELEKTRIČNIH POJAVOV Z METODO KONČNIH ELEMENTOV

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Some solid, crystalline materials exhibit the piezoelectric effect, which is very interesting for a variety of technological applications. Piezoelectric materials are widely used in electromechanical sensors and actuators, such as robotics' sensors, actuators, ultrasonic transducers for medical imaging and non-destructive testing. The paper presents the modeling of the piezoelectric effect in quartz, which is the most widely used material. The basic ideas of the finite-element method (FEM) for solving the problem of piezoelectric media are presented. All the results are based on linear piezoelectricity, in which the elastic, piezoelectric, and dielectric coefficients are treated as constants, independent of the magnitude and frequency of the applied mechanical stresses and electric fields. Starting with the tri-dimensional finite-element method, we have developed a numerical computational method for a determination of the electrical voltage (the direct piezoelectric effect) and the eigenmodes of vibration (the inverse piezoelectric effect).

The finite-element method is normally used for solving problems related to macrostructures. The aim of this work is to show that the finite-element method (FEM) is also a useful and convenient method for solving problems in relation to microstructures. Here we present the solution to the problem of the piezoelectric effect using the FEM, approaching the problem from the microstructural point of view.

Key-words: Finite-Element Method, Piezoelectricity, Modeling, Ansys, Quartz, Voltage, Eigenfrequencies

Nekatere kristalinične trdne snovi izkazujejo piezoelektrični pojav, kar je zelo zanimivo za številne tehnološke aplikacije. Piezoelektrični materiali se večinoma rabijo za elektromehanske senzorje in aktuatorje, na primer v robotiki, za ultrazvočne pretvornike pri raznih slikanjih v medicini in neporušnih preskušanjih. V prispevku obravnavamo modeliranje piezoelektričnega pojava v kremenu, ki se najpogosteje uporablja v piezoelektričnih napravah. Predstavljene so osnove metode končnih elementov (MKE) za numerično reševanje problemov piezoelektričnih struktur. Vsi prikazani rezultati so bili dobljeni za primer linearnega piezoelektričnega pojava, kjer smo obravnavali elastične, piezoelektrične in dielektrične koeficiente kot konstante, neodvisne od velikosti in frekvence mehanskih napetosti in električnih polj. Za obravnavo praktičnih primerov smo MKE aplicirali v treh dimenzijah in razvili numerične računske postopke za določitev električne napetosti v odvisnosti od mehanskih napetosti (neposredni piezoelektrični pojav) ter določitev lastnih nihajnih načinov in frekvenc v primeru inverznega piezoelektričnega pojava.

Ključne besede: metoda končnih elementov, piezoelektrični pojav, modeliranje, Ansys, kremen, lastne frekvence

1 INTRODUCTION

The Curie brothers, Jacques and Pierre, were two of the first people to experiment with common crystals such as quartz, topaz and sugar cane in the field of piezoelectricity in 1880 to 1882. The next 25 years (1882–1917) brought a substantial amount of information to be supported by mathematical calculations. Woldermar Voigt published a book that dealt with the physics of crystals, and research work was done in support of the book in reference to the effects of piezoelectricity such as, the changing of electrical into mechanical energy and vice versa. These French workers, along with P. Langevin, put together a submarine detector made of steel sheets and quartz.

In this paper we treat the piezoelectric effect in quartz in a theoretical way; in Section 2 we treat a mathematical formalization that describes the piezoelectric effect; and in Section 3 we present the modeling of the piezoelectric effect with the FEM.

The equations of piezoelectricity are sufficiently complex to preclude a closed form solution for all but the simplest cases. This is unfortunate since the piezoelectric effect plays an important role in the field of crystal physics and transducer technology (sensors and actuators). Previously, in the past 70 years, variational principles have been derived that serve as the basis of approximate solution techniques, such as the powerful Rayleight-Ritz method. Noteworthy contributions along these lines were made in the papers of Henno Allik and Thomas J. R. Hughes.[1,2,4,8,16]

Although these important developments have opened the way to wider class problems, they are not sufficiently general in themselves to be considered a universal method of piezoelectric analysis. For instance, a significant deficiency of the Rayleigh-Ritz technique is the necessity to select a trial function, which often becomes intractable for complex geometries.

This paper concerns the development of a general method of electrostatic analysis by incorporating the

piezoelectric effect in a finite-element method (FEM). The theory presented is, essentially, an expansion of the variational principle, which was used before by Holland and EerNisse[1], presented here in a matrix fashion. The dynamical matrix derived for linear piezoelectricity is found to be reducible, in form, to the ordinary matrix equation encountered in structural dynamics.

The electrostatic matrices for a simplex 'displacement-potential' for three-dimensional analysis are presented, thereby illustrating the method.[1,2,3,8,16]

The FEM is normally used for solving problems related to macrostructures. The aim of this work is to show that the FEM is also a useful and convenient method for solving problems in relation to micro-structures. Here we present the solution of the problem of the piezoelectric effect using the FEM, approaching the problem from the microstructural point of view.

2 FINITE ELEMENT APPROACH

The study of physical systems frequently results in partial differential equations, which either cannot be solved analytically or lack an exact analytic solution due to the complexity of the boundary condition or domain. For a realistic and detailed study, a numerical method must be used to solve the problem. The finite-element method is often found to be the most appropriate.

The FEM has successfully penetrated many areas, such as heat transfer, fluid mechanics, electromagnetism, acoustics and fracture mechanics. Basically, the finite element method consists of a piecewise application of classical variational methods to smaller and simpler sub-domains called finite elements connected to each other at a finite number of points called nodes.[6,15]

The fundamental principles of the finite-element method are:
- The continuum is divided into a finite number of elements of a geometrically simple shape.
- These elements are connected in a finite number of nodes.
- The unknowns are the displacements of these nodes.
- Polynomial interpolation functions are chosen to prescribe the unknown displacement field at each point of the element related to the corresponding field values at the nodes.
- The forces applied to the structure are replaced by an equivalent system of forces applied to the nodes.[2]

A finite-element formulation accounting for the coupling between the equations of electrostatics and elastodynamics becomes necessary when the piezo-electric material represents a non-negligible fraction of the entire structure.

Piezoelectric Finite Elements

The constitutive equations of a linear piezoelectric material[3] are:

$$\{T\}=[c^{E}]\{S\}-[e]^{T}\{E\} \tag{1}$$

$$\{D\}=[e]\{S\}-[\varepsilon^{S}]\{E\} \tag{2}$$

where $\{T\}=\left\{T_{11}\,T_{22}\,T_{33}\,T_{23}\,T_{13}\,T_{12}\right\}$ is the vector of the mechanical stress, $\{S\}=\left\{S_{11}\,S_{22}\,S_{33}\,S_{23}\,S_{13}\,2S_{12}\right\}$ is the vector of mechanical strains, $\{E\}=\left\{E_{1}\,E_{2}\,E_{3}\right\}$ is the vector of electric field, $\{D\}=\left\{D_{1}\,D_{2}\,D_{3}\right\}$ is the vector of dielectric displacement, $[c]^{E}$ is the mechanical stiffness matrix for a constant electric field E, $[\varepsilon]^{S}$ is the dielectric constant matrix for constant mechanical strain S, $[e]$ is the piezoelectric coupling coefficients matrix, $[e]^{T}$ is transposed.

The dynamic equations of a piezoelectric continuum can be derived from the Hamilton principle, in which the Lagrangian and the virtual work are properly adapted to include the electrical contribution as well as the mechanical ones. The potential energy density of a piezoelectric material includes a contribution from the strain energy and from the electrostatic energy[2].

The electric field E is related to electrical potential ϕ by

$$E = -\text{grad}\,\phi \tag{3}$$

and the mechanical strain S to the mechanical displacement u in the Cartesian coordinates by

$$S=\begin{bmatrix} \partial/\partial x & 0 & 0 & \partial/\partial y & 0 & \partial/\partial z \\ 0 & \partial/\partial y & 0 & \partial/\partial x & \partial/\partial z & 0 \\ 0 & 0 & \partial/\partial z & 0 & \partial/\partial y & \partial/\partial x \end{bmatrix}^{T}\{u\}=[B]\{u\} \tag{4}$$

The elastic behavior of piezoelectric media is governed by Newton's law:

$$\text{div}\{T\}=\rho\frac{\partial^{2}\{u\}}{\partial t^{2}} \tag{5}$$

where ρ is the density of the piezoelectric medium, whereas the electrical behavior is described by Maxwell's equation, taking into account the fact that the piezoelectric media are insulating (no free volume charge):

$$\text{div}\{D\}=0 \tag{6}$$

Equations (1) to (6) constitute a complete set of differential equations, which can be solved with the appropriate mechanical (displacement and forces) and electrical (potential and charge) boundary conditions. An equivalent description of above boundary-wave problem is Hamilton's variational principle as extended to piezoelectric media,

$$\delta\int_{t_{1}}^{t_{2}}(L+W)\mathrm{d}t=0 \tag{7}$$

where the operator δ denotes the first-order variation, t_{1} and t_{2} define the time interval (all variations must vanish at $t = t_{1}$ and $t = t_{2}$) and the Lagrangian term L is determined by the energies available in the piezoelectric

medium and W is the virtual work of the external mechanical and electrical forces[1,2,4].

In the finite-element method the body to be computed is subdivided into small, discrete elements, the so-called finite elements. The mechanical displacement u and the forces f as well as the electrical potential ϕ and the charge q are determined at the nodes of these elements. The values of these mechanical and electrical quantities at an arbitrary position on the element are given by a linear combination of the polynomial interpolation function $N(x,y,z)$ and the nodal point values of these quantities as a coefficient. For an element with n nodes (nodal coordinates: (x_i, y_i, z_i), $(i=1,2,....,n)$ the continuous displacement function $u(x, y, z)$ (vector of order three), for example, can be evaluated from its discrete nodal point vectors as follows (the quantities with "0" are the nodal point values of one element):

$$\{u(x, y, z)\} = [N_u(x, y, z)]\left\{\overset{0}{u}(x_i, y_i, z_i)\right\} \quad (8)$$

$$\phi = [N_\phi(x, y, z)]\left\{\overset{0}{u}(x_i, y_i, z_i)\right\} \quad (9)$$

where $\left\{\overset{0}{u}\right\}$ is the vector of the nodal point displacement and $[N_u]$ is the interpolation function for the displacement.

Therefore, the strain field $\{S\}$ and the electric field $\{E\}$ are related to the nodal displacement and potential by the shape-function derivatives $[B_u]$ and $[B_\phi]$ defined by,[12]

$$\{S\} = [B_u]\left\{\overset{0}{u}_i\right\} \quad (10)$$

$$\{E\} = -[B_\phi]\left\{\overset{0}{\phi}_i\right\} \quad (11)$$

The substitution of the polynomial interpolation function into (8) yields a set of linear differential equations that describe a single piezoelectric finite element.

$$\{M\}\left\{\overset{0}{\ddot{u}}\right\} + [K_{uu}]\left\{\overset{0}{u}_i\right\} + [K_{u\phi}]\left\{\overset{0}{\phi}_i\right\} = \left\{\overset{0}{f}_i\right\} \quad (12)$$

$$[K_{\phi u}]\left\{\overset{0}{u}_i\right\} + [K_{\phi\phi}]\left\{\overset{0}{\phi}_i\right\} = \left\{\overset{0}{q}_i\right\} \quad (13)$$

Each element k of the mesh is connected to its neighboring elements at the global nodes and the displacement is continuous from one element to the next. The element degrees of freedom (dof) $\left(\left\{\overset{0}{u}_i\right\}, \left\{\overset{0}{\phi}_i\right\}\right)$ are related to the global dof $(\{u\}, \{\Phi\})$ by the mean of the localization matrices $\left[\overset{0}{L}_u\right]$ and $\left[\overset{0}{L}_\phi\right]$.

Hamilton's principle (7) must be verified for the whole structure, which results in (by summation of the contribution from each finite element).[1,2,3,4,8]

$$\{M\}\{\ddot{U}\} + [K_{UU}]\{U\} + [K_{U\Phi}]\{\Phi\} = \{F\} \quad (14)$$

$$[K_{\Phi U}]\{U\} + [K_{\Phi\Phi}]\{\Phi\} = \{Q\} \quad (15)$$

where the assembled matrices are given by:

$[M] = \sum_i [L_{ui}]^T [M^{(i)}][L_{ui}]$ – kinematically consistent mass matrix

$[K_{uu}] = \sum_i [L_{ui}]^T [K_{uu}^{(i)}][L_{ui}]$ – stiffness matrix

$[K_{U\Phi}] = \sum_i [L_{ui}]^T [K_{u\phi}^{(i)}][L_{\phi i}]$ – piezoelectric "stiffness" matrix

$[K_{\Phi U}] = \sum_i [L_{\phi i}]^T [K_{\phi u}^{(i)}][L_{ui}]$ – transponse piezoelectric "stiffness" matrix

$[K_{\Phi\Phi}] = \sum_i [L_{\phi i}]^T [K_{\phi\phi}^{(i)}][L_{\phi i}]$ – dielectric "stiffness" matrix

$\{F\} = \sum_i [L_{ui}]^T [f_i]$ – external forces applied to the structure

$\{Q\} = \sum_i [L_{\phi i}]^T [q_i]$ – electrical charges brought to the electrodes

Equations (14) and (15) couple the mechanical variables $\{U\}$ and the electrical potentials $\{\Phi\}$.

Based on this formulation, a piezoelectric finite element of the type multilayered Mindlin shell and volume has been derived.[2,3]

For shell elements, it is assumed that the electric field and the displacement are uniform across the thickness and aligned on the normal to the mid-plane. The electrical degrees of freedom are the voltages ϕ_k across the piezoelectric layers; it is assumed that the voltage is constant over each element (this implies that the finite element mesh follows the shape of the electrodes). One electrical degree of freedom of the type voltage per piezoelectric layer is defined. The assembly takes into account the equipotentiality condition of the electrodes; this reduces the number of electric variables to the number of electrodes.

For volume elements, one additional degree of freedom of the type electric potential is **introduced** in each node of the piezoelectric volume element.

3 MODELING AND RESULTS

As for selecting the element types, the decision is based on the characteristics of the element type to the best model that applies to the problem, geometrically and physically. The material properties are required for most element types. Depending on the element types, the material properties may be linear or non linear; isotropic or anisotropic; and constant temperature-independent or temperature-dependent.

The starting points of the modeling of the effect of quartz are the differential equations (14) and (15). These equations are solved according to the FEM, supported by the ANSYS software, whereas the program was ADPL (ANSYS PARAMETRIC DESIGN LANGUAGE).

In this paper, ANSYS was used as a computational tool for modeling the piezoelectric effect [6,7]. For this purpose, a quartz sample is taken, with a density of 2695 kg/m^3 and these dimensions: 90 mm × 120 mm × 27 mm [5], (**Figure 2**). We know that the crystal quartz is
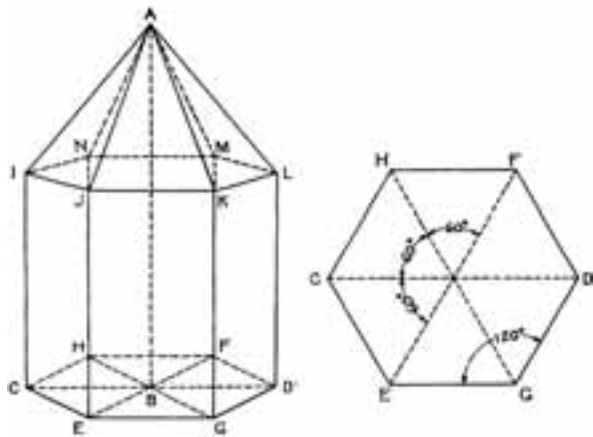
Figure1: A section of a quartz crystal showing the direction of the optical axes (AB) and the electrical axes (CD, EF, GH)[9]
Slika 1: Prerez kremenovega kristala in prikaz smeri optičnih osi (AB) in električnih osi (CD, EF, GH)
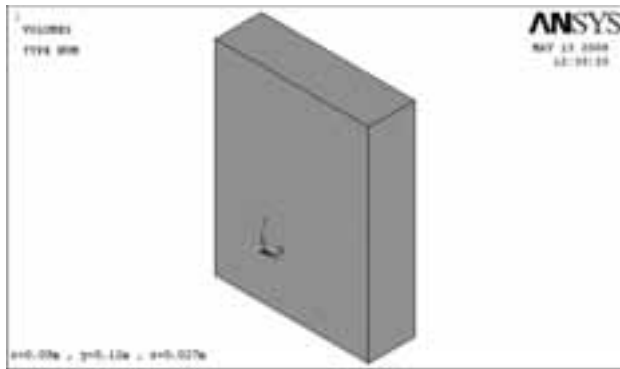
Figure 2: The quartz sample in the ANSYS window[7]
Slika 2: Kremenov vzorec v prikaznem oknu programa ANSYS

in the form of a hexagonal cylinder surmounted by a hexagonal pyramid; the faces of the crystal, which may vary in length and breadth, lie at definite angles with each other (**Figure 1**) [9,13]. Also, we know that pressure
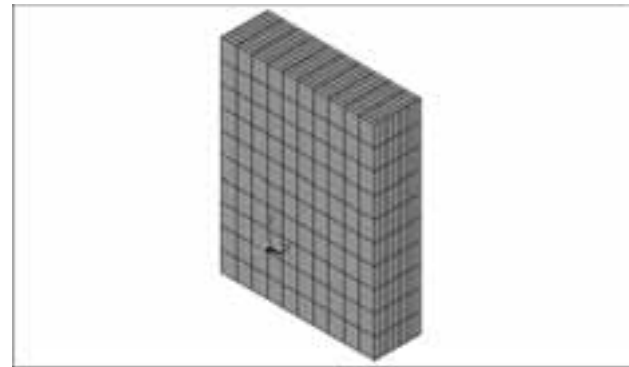
Figure 3: Meshing of the integral zone for the quartz sample[7]
Slika 3: Razdelitev integracijskega območja kremenovega vzorca v končne elemente

applied to the crystal parallel to electric axes produces a piezoelectric polarization in the same direction.

Then, according to the FEM, the meshing is carried out (the division of the domain of integration into the finite integrating elements) into 1000 elements with 1331 nodes, **Figure 3**, and **Table 1**.

As a finite element, from the library of ANSYS, the element SOLID 5 is taken, (**Figure 4**)[6,7]. The nodes of this element have degrees of freedom (dof): displacements along the axes *x, y, z*, the intensity of the electric potential, the intensity of the magnetic field and temperature, so this is a multi-field element. Since we are discussing the linear piezoelectricity, the displacements (mechanical quantities) and electric potential (electrical quantities) are of interest to us.
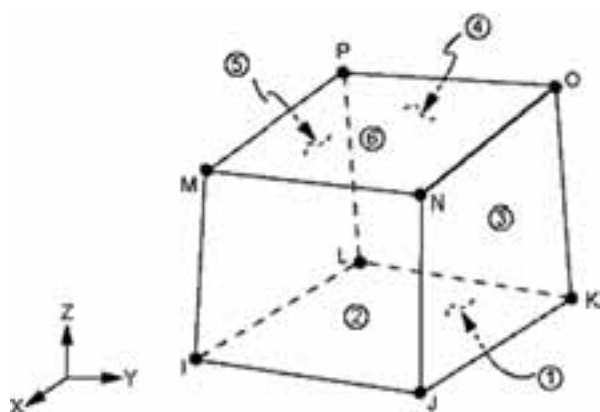
Coupled-fields in the ANSYS software can be treated on two ways to create a finite-element model: automatic meshing (also called the direct modeling in ANSYS terminology) and manual meshing (also called the direct generation in ANSY terminology). In automatic meshing the users are required to have a solid model available prior to the creation of a finite-element model. When such a solid model becomes available, the users can then

Table 1: Element and nodes of the sample[7]
Tabela 1: Matematični opis končnih elementov in vozlišč vzorca

Elements		Nodes		
LIST ALL SELECTED ELEMENTS. (LIST NODES)		LIST ALL SELECTED NODES. DSYS = 0		
		SORT TABLE ON NODE NODE NODE		
ELEM MAT TYP REL ESY SEC NODES		NODE	X	Y	Z
1 1 1 1 0 1 2 32 41 11 251 333 603 449		1 0.00000000000	0.120000000000	0.00000000000
2 1 1 1 0 1 32 33 42 41 333 334 684 603		2 0.00000000000	0.00000000000	0.00000000000
3 1 1 1 0 1 33 34 43 42 334 335 765 684		3 0.00000000000	0.108000000000	0.00000000000
4 1 1 1 0 1 34 35 44 43 335 336 846 765		4 0.00000000000	0.960000000000E-01	0.00000000000
5 1 1 1 0 1 35 36 45 44 336 337 927 846		5 0.00000000000	0.840000000000E-01	0.00000000000
6 1 1 1 0 1 36 37 46 45 337 338 1008 927		6 0.00000000000	0.720000000000E-01	0.00000000000
995 1 1 1 0 1 926 1007 396 387 197 206 148 149		1326 0.810000000000E-01	0.108000000000	0.108000000000E-01
996 1 1 1 0 1 1007 1088 405 396 206 215 147 148		1327 0.810000000000E-01	0.108000000000	0.135000000000E-01
997 1 1 1 0 1 1088 1169 414 405 215 224 146 147		1328 0.810000000000E-01	0.108000000000	0.162000000000E-01
998 1 1 1 0 1 1169 1250 423 414 224 233 145 146		1329 0.810000000000E-01	0.108000000000	0.189000000000E-01
999 1 1 1 0 1 1250 1331 432 423 233 242 144 145		1330 0.810000000000E-01	0.108000000000	0.216000000000E-01
1000 1 1 1 0 1 1331 530 350 432 242 142 133 144		1331 0.810000000000E-01	0.108000000000	0.243000000000E-01

Figure 4: Geometry of the SOLID 5 [6,7]
Slika 4: Geometrija elementa SOLID 5 v programu ANSYS

instruct ANSYS to automatically develop a finite-element model (nodes and elements). The purpose of using automatic meshing is to relieve the user of the time-consuming task of building a complicated finite-element model. In manual meshing, the users need to define the nodes and elements directly (the development of a solid model is not required). The manual meshing method offers complete control over the geometry and connectivity of every node and every element, as well as the ease of keeping track of the identities of the nodes and elements. However, this method may not be as convenient as the automatic meshing method when dealing with a complicated finite-element model. It is, however, possible to combine both methods. In this paper we used the automatic meshing method. This is provided by the element SOLID 5, because it has a degree of freedom of different physical fields. SOLID 5 is a type of element that occupies three-dimensional space. In addition, it has eight nodes. Each of these nodes has three displacements along the *x, y* and *z* axes, respectively. The SOLID 5 element is capable of modeling seven different types of disciplines. When this particular type of discipline is chosen, ANSYS will only compute the behaviors of SOLID 5 in the UX, UY, UZ and VOLT degrees of freedom. It should be noted that UX, UY and UZ are to indicate the displacements in the *X, Y* and *Z* directions (the *X, Y* and *Z* axes are based on the global coordinate system), while VOLT is to indicate the difference in the potential energy of the electrical particles between two locations [6]. More precisely, when we have the action of the mechanical field, we can automatically obtain the output quantities of the electric field from the element SOLID 5, and vice versa (the case of the inverse piezoelectric effect).

Besides the geometry of the sample, the density of the quartz and the meshing, and introducing the element SOLID 5, we also have to take into account the other physical characteristics of quartz, in order to establish the initial condition for solving the differential equation. The physical characteristics that determine the solution of the differential equation are: the stiffness matrix c^E,

the dielectric constant matrix ε^S, and the piezoelectric constant matrix e. The values for the above matrices at a temperature of 25 °C are: [8]

$$[c^E] = \begin{pmatrix} 86.74 & 6.99 & 11.91 & -17.91 & 0 & 0 \\ 6.99 & 86.74 & 11.91 & 17.91 & 0 & 0 \\ 11.91 & 11.91 & 107.2 & 0 & 0 & 0 \\ -17.91 & 17.91 & 0 & 57.94 & 0 & 0 \\ 0 & 0 & 0 & 0 & 57.94 & -17.91 \\ 0 & 0 & 0 & 0 & -17.91 & 39.88 \end{pmatrix} \cdot 10^9 \frac{N}{m^2} \quad (16)$$

$$[\varepsilon^S] = \begin{pmatrix} 39.21 & 0 & 0 \\ 0 & 39.21 & 0 \\ 0 & 0 & 41.03 \end{pmatrix} \cdot 10^{-12} \frac{C}{V \cdot m} \quad (17)$$

$$[e] = \begin{pmatrix} 0.171 & -0.171 & 0 & -0.0406 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0.0406 & -0.171 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \frac{C}{m^2} \quad (18)$$

Depending on the geometry of the sample, the physical characteristics of quartz, we have built a program to calculate the potential differences as a function of mechanical force, as well as the intensity of the deformation of the sample as a function of the electric voltage. In both cases, the calculations are carried out along the *x* axis (the electrical axis of the quartz). Below, we present the result of modeling for all cases: when the external mechanical forces compress the sample, when this force stretches the sample, and when an electric voltage is applied on the lateral faces of the sample (the inverse piezoelectric effect).

3.1.1 The direct piezoelectric effect (longitudinal)

The external mechanical forces compress sample

Assume that a mechanical force with intensity *F* is acting in the direction of the *x*-axis, i.e., in the direction of the normals of the lateral faces of the sample, in the positions *x* = 0 and *x* = 90 mm (in the opposite directions with the normal's vector)[9]. Then, as a result of the action of this force, the sample will be stressed. The intensity of this stress is the force on the unit of the surface *yz*, **Figure 5**. As a result of the action of a mechanical force, we will have the accumulation of a positive and negative
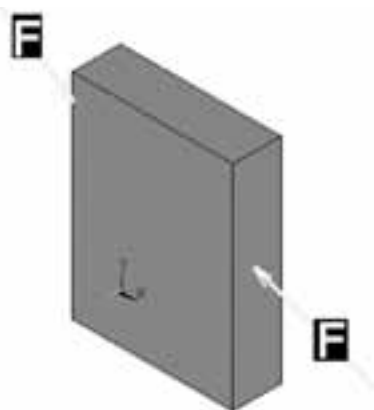
Figure 5: The force acting in the direction of the *x* axis
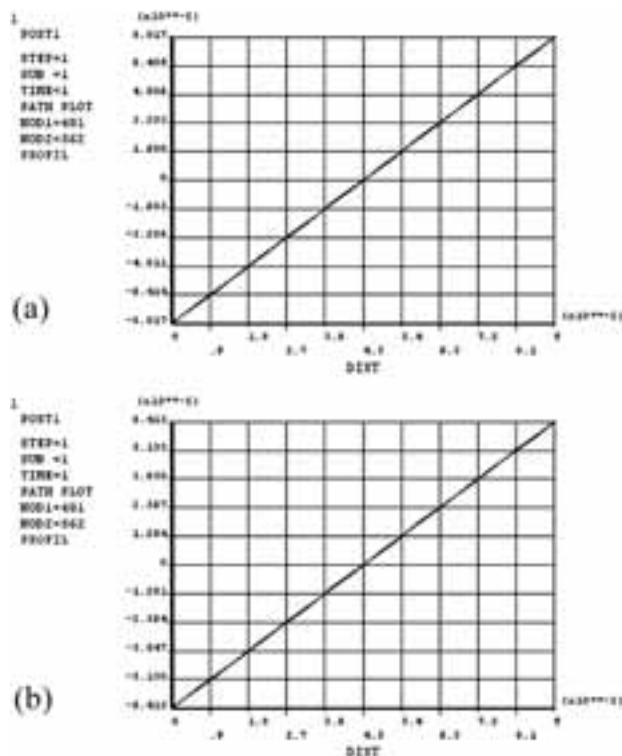**Slika 5:** Mehanska sila pri stiskanju vzorca v smeri osi *x*

electrical charge on the opposite lateral faces of the sample along the *x*-axis. In other words, we will have the transformation of mechanical energy into electric energy. This phenomenon is called the direct piezoelectric effect.

Calculations are carried out for the cases when the force has the following intensities: 0.1 N, 0.08 N, 0.06 N, 0.04 N and 0.02 N. For these values of the intensities, we have calculated the potential difference as a function of depth. But, for practical reasons, we have not taken into account the fact that the opposite sides of the electrical poles in the interior of the sample are neutralized, and as a result the electric charges appear only on the surface. We made this approximation in order to prove the dependence of the intensity of the electrical potential on the depth. In **Figure 6** we have presented the modeling result for two cases.

The main results are the potential difference as a function of depth and the mechanical force, **Figure 7**.
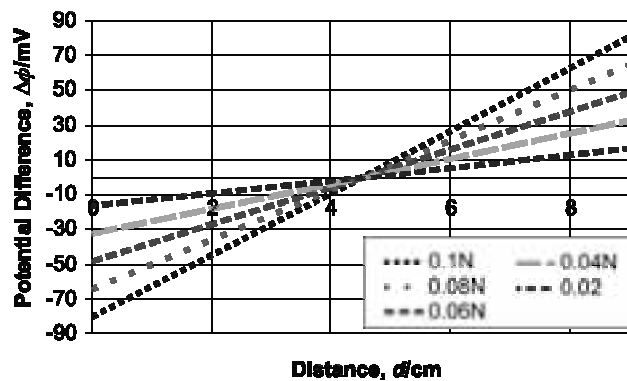
According to **Figures 6 and 7** we can conclude the following:

- The intensity of the electrical potential depends on the external mechanical force. For equal depths the intensity of the potential increases with the increase of the force. This dependence is shown in **Table 2**.

Figure 7: Potential difference [mV] as a function of depth [cm] and mechanical force F/N – compression case
Slika 7: Razlika električnega potenciala v odvisnosti od razdalje pri različnih silah stiskanja

Table 2: Potential difference [mV] as a function of depth [cm] and mechanical force F(N) – compression case
Tabela 2: Razlika električnega potenciala pri različnih silah stiskanja na robovih in v sredini vzorca

Force F/N	Depth, d/cm / Potential difference, $\Delta\phi$/mV		
	0	4.5	9
0.1	-80.17	0	80.17
0.08	-64.13	0	64.13
0.06	-48.10	0	48.10
0.04	-32.06	0	32.06
0.02	-16.03	0	16.03

- From **Table 2** and **Figures 6 and 7** we see that during the compression of the sample, in the interval from *x=0m* to *x=0.045m*, the electrical potential is negative, whereas on the other side, i.e., from *x=0.045m* to *x=0.09m* the potential is positive. It is known that the electrical potential is proportional to the intensity of the electric charge; therefore, we can conclude that on the upper part of the sample we have the accumulation of the negative charge and then, from the half-depth on, there is an accumulation of the positive charge.
- The accumulated electrical charge depends on the intensity of the external force and the depth. For a given force, the electrical charge decreases with an increase of the depth decrease of the thickness of the sample along the *x* axis, whereas for a certain depth, it increases with the increase of the force.

External mechanical forces stretches the sample

In **Figures 8 and 9** are the results of modeling for the case of stretching. From these figures we can draw the same conclusions as in the case of the stress of the sample. The only difference is that by changing the direction of the mechanical force, the sign of the electrical potential changes. More precisely, by changing the direction of the force, the side of the accumulation of the electric charges will switch. In the case of stretching, on the upper part of the sample the positive charge will be accumulated. In the other part of the sample (depth
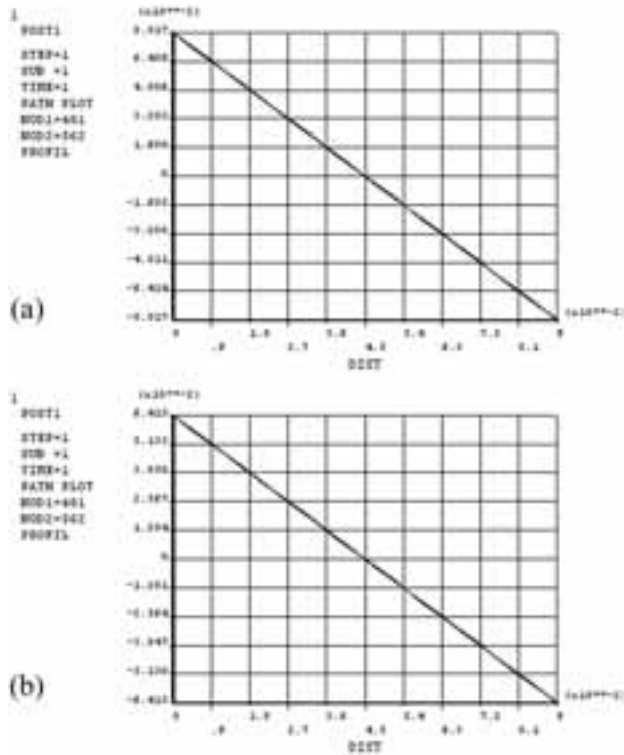

Figure 6: Potential difference as a function of depth and mechanical force – compression case: (a) F = 0.1 N, (b) F = 0.08 N
Slika 6: Prikaz izračuna razlike električnega potenciala v odvisnosti od razdalje s programom ANSYS – primer tlačne sile: (a) F = 0.1 N, (b) F = 0.08 N

Figure 8: Potential difference as a function of depth and mechanical force – stretch case: (a) F = 0.1 N, (b) F = 0.08N

Slika 8: Prikaz izračuna razlike električnega potenciala v odvisnosti od razdalje za primer raztezne sile: (a) F = 0.1 N, (b) F = 0.08N
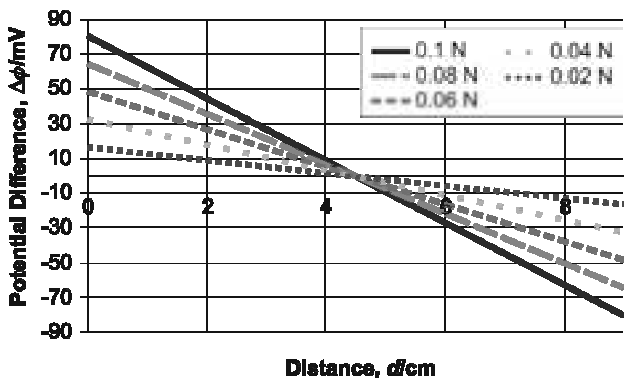

Figure 9: Potential difference [V] as a function of depth and mechanical force [F] – stretch case

Slika 9: Razlika električnega potenciala v odvisnosti od razdalje pri različnih razteznih silah

from $x=0.045m$ to $x=0.090m$) the negative charge will be accumulated. In both cases at a depth of $x=0.045m$ the electrical potential is zero, which means in the mid-depth of the sample the centers of positive electrical charges will coincide with the centers of the negative electrical charges and the net charge is zero. As a consequence, the electrical potential will also be zero.

3.1.2 The direct piezoelectric effect (transversal)

The same phenomena occur in the case when compression (stress) or stretch is applied along the *Y*-axis perpendicular to *X*. The only difference is that in the case of stress (compression) along the *Y*-axis, negative electrical charges are accumulated on the opposite side compared to the first case (when the sample was compressed or stretched in the direction of the *X*-axis. In **Figure 10**, the case for the force 0.1 N is shown, for the case when the sample is stressed or stretched along the *Y*-axis (the so-called transversal piezoelectric effect). The results presented in **Figure 10** show that the net accumulated electrical charge is not the same (for the same force in the case of transversal piezoelectricity, the net accumulated electric charge is greater). This occurs because in the case of longitudinal piezoelectricity, the net accumulated electrical charge depends only on the intensity of the applied force and the thickness of the sample, whereas in the case of the transversal piezoelectric effect, this net charge depends on the ratio between the surface area where the electrical charge is accumulated and the surface area upon which the force is exerted, $\frac{y \cdot z}{x \cdot z}$.

3.2 Converse piezoelectric effect

In this section we present the results of the inverse piezoelectric effect. The question is, what happens if an
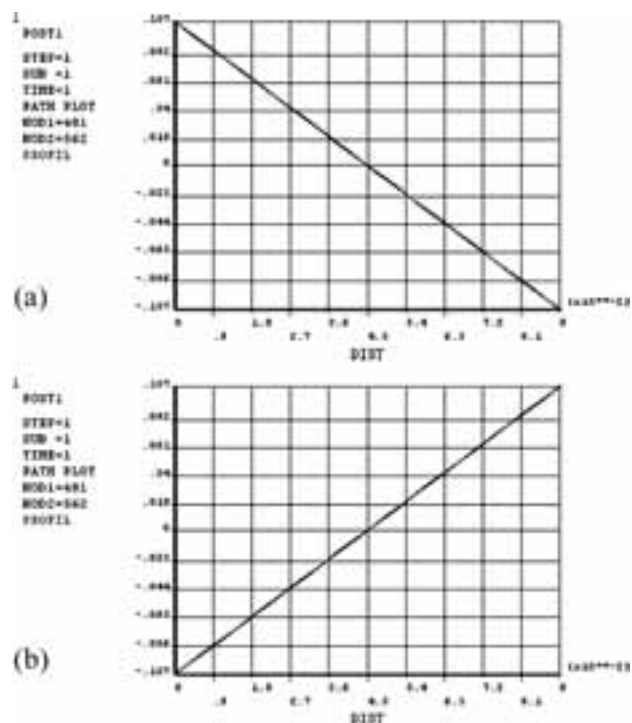

Figure 10: Transversal piezoelectric effect: (a) Case of specimen compression, (b) Case of specimen stretch

Slika 10: Transverzalni piezoelektrični pojav: (a) primer stiskanja in (b) primer raztezanja

external AC voltage is applied to the sample? From practice we know that piezoelectric materials (in our case the crystal is quartz) can change their physical dimensions with the application of an electric field. Again, we have taken a sample with the same geometry. The element for meshing is the same, whereas as the initial condition we take the voltage applied on the ends of the *x*-axis. We have analyzed what happens to a sample when an electrical voltage applied on it. This analysis belongs to the so-called modal analysis. With this analysis we can determine the process of oscillations of a system[10]. More precisely, if the system performs oscillations under the action of an external factor, then with this analysis we find the proper frequencies of these oscillations and the shape of the oscillations (deformations of the system related to the initial undeformed shape). This part of the analysis is supported by the ANSYS software, with the condition that during the solution of the equation, it must be indicated that we are dealing with the modal type. The degrees of freedom of the element SOLID 5 provide the transfer from the quantities of one physical field to another.

In our case, the applied voltage is given as $U = 220$ V. Then the element SOLID 5 provides the transfer from this electrical quantity to the mechanical quantity – the displacement of the nodes or the deformation of the sample. The software (ANSYS) automatically calculates the frequency of the deformation – the oscillations of the nodes as well as its shape. With this program we can also find the frequencies of all modes of oscillations and their shapes for any applied voltage. In **Figure 11**, the 10 first modes of oscillations and their shapes are shown. According to[11], the frequencies of the oscillations along the electric axis *x* for the quartz take values from 50 Hz to 200 kHz. From the last presentation we see that the frequency of oscillations for the 10 first modes take the values 51 815 Hz to 59 518 Hz. We have proved that the other modes, for example, the 40th mode, has a frequency of 93 000 Hz, whereas the 100th mode has the frequency 120 819 Hz. The results also prove that under the voltage applied, the geometry of the sample is deformed and that this deformation is caused by oscillations with different frequencies.

It appears that an improvement in the computational accuracy of highly ordered modes depends, above all, on the number of finite elements used, and is not limited by the use of the finite-element method.

4 CONCLUSIONS

From the results obtained, presented in **Figures 5, 6, 7, 8, 9, 10** we can conclude as follows:

- In principle, the differential equation of the coupled-field (mechanical and electrical) is solvable with the finite-element method (FEM)
- The commodity of the solution provides the application ANSYS.
- Both types of piezoelectric effect can be modeled with the aid of the FEM package, whereas simulations in ANSYS prove the corrections of the theoretical model.
- For the direct piezoelectric effect, we proved that depending on the intensity of the force and its direction (stress or stretch), we have the accumulation of the electrical charges along the electric axis *x*, which can be seen in **Figures 7 and 9**.
- Modal analyses provide an elegant presentation of the different shapes of oscillations of the sample when an
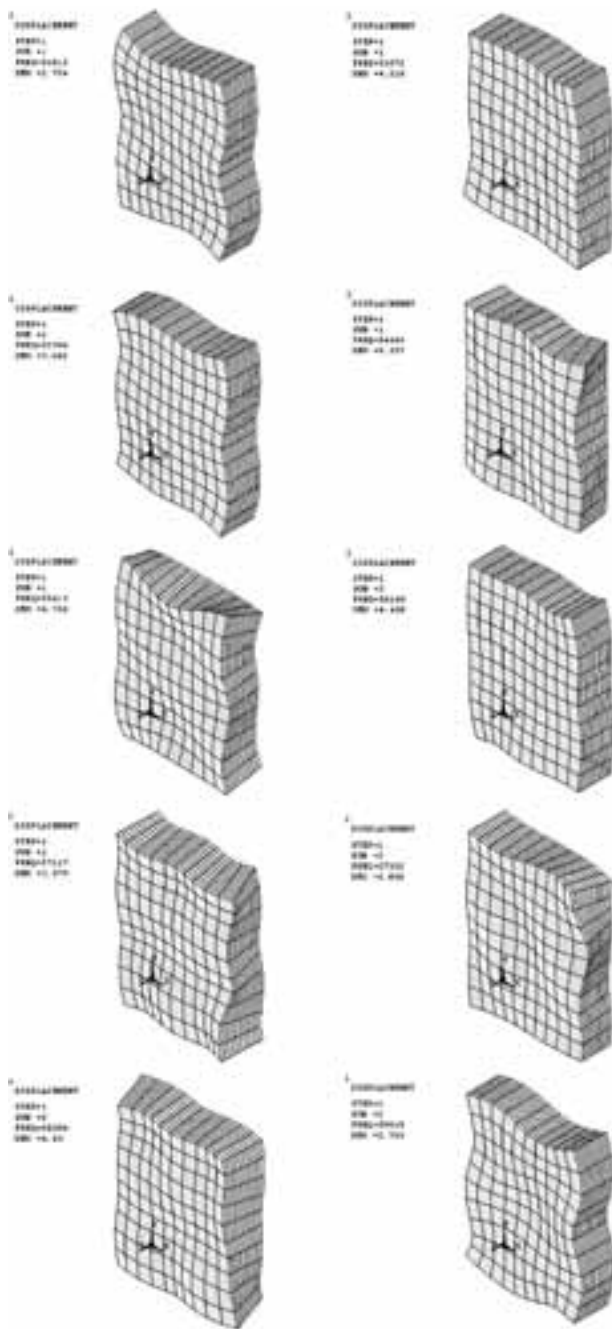
Figure 11: The first 10 modes of vibration and their shapes
Slika 11: Prvih 10 lastnih nihajnih načinov kremenovega vzorca

electric voltage is applied to it. With this analysis we have proved the inverse piezoelectric effect.

- With the same procedure the piezoelectric effect can be modeled for other materials, when only the three characteristic matrices of the material are known.

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