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# Surface and Bulk Acoustic Waves in Multilayer Structures

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## 1. Introduction

The application of various layers on a piezoelectric substrate is a way of improving the parameters of propagating electroacoustic waves. For example, a metal film of certain thickness may provide the thermal stability of the wave for substrate cuts, corresponding to a high electromechanical coupling coefficient. The overlayer can vary the wave propagation velocity and, hence, the operating frequency of a device. The effect of the environment (gas or liquid) on the properties of the wave in the layered structure is used in sensors. The layer may protect the piezoelectric substrate against undesired external impacts. Multilayer compositions allow to reduce a velocity dispersion, which is observed in single-layer structures. In multilayer film bulk acoustic wave resonators (FBAR) many layers are necessary for proper work of such devices. Therefore, analysis and optimization of the wave propagation characteristics in multilayer structures seems to be topical. General methods of numerical calculations of the surface and bulk acoustic wave parameters in arbitrary multilayer structures are described in this chapter.

## 2. Surface acoustic waves in multilayer structures

In the linear theory of piezoelectricity and in the quasistatic electric approximation the system of differential equations, describing the mechanical displacements  $u_i$  along the three spatial coordinates  $x_i$  ( $i = 1, 2, 3$ ) and the electric potential  $\varphi$  in the solid piezoelectric medium, may be written in such view (Campbell and Jones, 1968):

$$c_{ijkl} \frac{\partial^2 u_k}{\partial x_i \partial x_l} + e_{kij} \frac{\partial^2 \varphi}{\partial x_k \partial x_i} = \rho \frac{\partial^2 u_j}{\partial t^2} \quad (1)$$

$$e_{ikl} \frac{\partial^2 u_k}{\partial x_i \partial x_l} - \varepsilon_{ik} \frac{\partial^2 \varphi}{\partial x_i \partial x_k} = 0 \quad i, j, k, l = 1, 2, 3 \quad (2)$$

In these equations  $c_{ijkl}$  is the forth rank tensor of the elastic stiffness constants,  $e_{ijk}$  is the third rank tensor of the piezoelectric constants,  $\varepsilon_{ij}$  is the second rank tensor of the dielectric constants,  $\rho$  - the mass density,  $t$  - time, and the summation convention for repeated indices is used. The expression (1) contains three equations and (2) gives one more equation, totally

four equations. These equations must be solved for each medium of all the multilayer system, which is shown in Fig. 1.

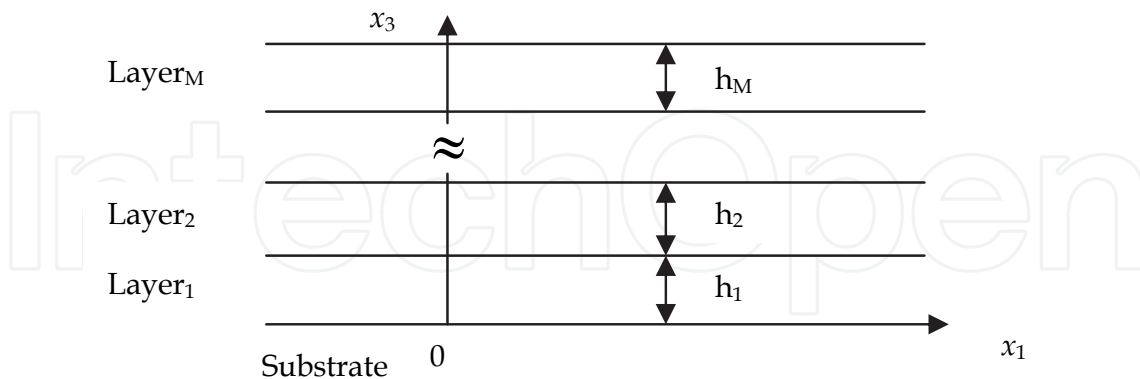


Fig. 1. Multilayer structure - substrate and M layers.

The coordinate axis  $x_1$  direction coincides with the wave phase velocity  $v$ , the coordinate axis  $x_3$  is normal to the substrate surface and the axis origin is set on this surface, as shown in Fig 1. A solution of equations (1) and (2) we will seek in the following form:

$$u_j = \alpha_j \exp[ik(b_i x_i - vt)] \quad i, j = 1, 2, 3 \quad (3)$$

$$\varphi = \alpha_4 \exp[ik(b_i x_i - vt)]$$

Here  $\alpha_j$  - amplitudes of the mechanical displacements,  $\alpha_4$  - the amplitude of the electric potential,  $b_i$  - directional cosines of the wave velocity vector along the corresponding axes,  $k = \omega/v = 2\pi/\lambda$  - the wave number,  $\omega$  - a circular frequency,  $\lambda$  - a wavelength. Substitution of (3) into (1) and (2) gives the system of four linear algebraic equations for wave amplitudes:

$$c_{ijkl} b_i b_l \alpha_k + e_{kij} b_k b_i \alpha_4 = \rho v^2 \alpha_j \quad (4)$$

$$e_{ikl} b_i b_l \alpha_k - \varepsilon_{ik} b_i b_k \alpha_4 = 0 \quad (5)$$

The detailed form of these equations is following:

$$\begin{aligned} (\Gamma_{11} - \rho v^2) \alpha_1 + \Gamma_{12} \alpha_2 + \Gamma_{13} \alpha_3 + \Gamma_{14} \alpha_4 &= 0 \\ \Gamma_{21} \alpha_1 + (\Gamma_{22} - \rho v^2) \alpha_2 + \Gamma_{23} \alpha_3 + \Gamma_{24} \alpha_4 &= 0 \\ \Gamma_{31} \alpha_1 + \Gamma_{32} \alpha_2 + (\Gamma_{33} - \rho v^2) \alpha_3 + \Gamma_{34} \alpha_4 &= 0 \\ \Gamma_{41} \alpha_1 + \Gamma_{42} \alpha_2 + \Gamma_{43} \alpha_3 + \Gamma_{44} \alpha_4 &= 0 \end{aligned} \quad (6)$$

Here:

$$\Gamma_{jk} = \Gamma_{kj} = c_{ijkl} b_i b_l, \quad \Gamma_{j4} = \Gamma_{4j} = e_{ikj} b_i b_k, \quad \Gamma_{44} = -\varepsilon_{ik} b_i b_k \quad i, j, k, l = 1, 2, 3 \quad (7)$$

For the existence of a nontrivial solution of the system (6) a determinant of this system must be equal to zero:

$$\begin{vmatrix} \Gamma_{11} - \rho v^2 & \Gamma_{12} & \Gamma_{13} & \Gamma_{14} \\ \Gamma_{21} & \Gamma_{22} - \rho v^2 & \Gamma_{23} & \Gamma_{24} \\ \Gamma_{31} & \Gamma_{32} & \Gamma_{33} - \rho v^2 & \Gamma_{34} \\ \Gamma_{41} & \Gamma_{42} & \Gamma_{43} & \Gamma_{44} \end{vmatrix} = 0 \quad (8)$$

This equation allows to determine the unknown directional cosine  $b_3$ , if the values  $v$ ,  $b_1$ , and  $b_2$  are set. For flat pseudo-surface acoustic wave the values of the directional cosines are following:

$$b_1 = 1 + i\delta, \quad b_2 = 0, \quad b_3 = b, \quad (9)$$

where  $\delta$  is the wave attenuation coefficient along the propagation direction. For surface acoustic wave the attenuation is absent and  $\delta = 0$ . The equation (8) with taking into account (9) gives the following eighth power polynomial equation with respect to the  $b$  value:

$$a_8 b^8 + a_7 b^7 + a_6 b^6 + a_5 b^5 + a_4 b^4 + a_3 b^3 + a_2 b^2 + a_1 b + a_0 = 0 \quad (10)$$

Coefficients  $a_i$  of this equation are represented by very complicated expressions, depending on material constants of the medium, a phase velocity  $v$ , and the attenuation coefficient  $\delta$ . For pseudo-surface acoustic waves  $\delta \neq 0$  and therefore coefficients  $a_i$  are complex values. For surface acoustic waves  $\delta = 0$  and coefficients  $a_i$  are pure real values. In this case roots of the equation (10) are either real or complex conjugated pairs. If  $\delta \neq 0$ , roots of the equation (10) are complex but not conjugated. So, solving (numerically certainly) the equation (10), we get eight roots  $b^{(n)}$  ( $n = 1, 2, \dots, 8$ ), which are complex values in general case. These values are the eigenvalues of the problem. Substituting each of these values into (7) and then into equation system (6), we can define all four complex amplitudes  $\alpha_j^{(n)}$  for each root  $b^{(n)}$ . Values  $\alpha_j^{(n)}$  represent the eigenvectors of the problem. This procedure must be performed for the substrate and for each layer. Found solutions are the partial solutions of the problem or partial modes.

The general solution for each medium is formed as a linear combination of partial solutions (partial modes). Quantity partial modes in the general solution for each medium must be equal to quantity of boundary conditions on its surfaces. Four boundary conditions on each surface are used, namely three mechanical and one electrical one. The substrate is semi-infinite, i.e. it has only one surface. Hence only four partial solutions are required for forming the general solution for the substrate. It means that some procedure of roots selection is required for substrate. For surface acoustic wave four roots with negative imaginary parts are selected from four complex conjugated pairs. This condition of roots selection corresponds to decreasing of the wave amplitude along the  $-x_3$  direction (into the depth of the substrate), i.e. to condition of the localization of the wave near the surface. Practically the procedure of roots sorting with increasing imaginary parts order is performed and then four first roots are used for forming of the general solution.

For pseudo-surface wave roots are not complex conjugated, but they also contain four roots with negative imaginary part and also these four roots are first in the sorted roots sequence. In this case the roots selection rule is some different. Three first roots in the sorted sequence are selected, but the fourth root of this sequence is replaced with the fifth one (with the positive imaginary part of minimal value). This condition corresponds to increasing of the

wave amplitude into the depth of the substrate and provide the energy conservation law satisfaction (wave attenuates along the propagation direction  $x_1$  due to nonzero value of  $\delta$  in the direction cosine  $b_1$ , see (9)). For high velocity pseudo-surface wave (the second order pseudo-surface wave or quasi-longitudinal pseudo-surface wave) only two first roots of the sorted sequence are selected, the third and the fourth roots are replaced with the fifth and the sixth ones.

All these rules of roots selection are applied for substrate only. For each layer of the structure shown in Fig. 1 there is no problem of roots selection, because each layer has two surfaces and all eight roots (all eight partial modes) are used for forming of the general solution for each layer.

One must to note, that in some special cases the quantity of partial modes may be less, than four for substrate and less, than eight for layers. This must be taken into account at forming of the general solution for corresponding case.

So, the general solution for each medium is formed as a linear combination of corresponding partial modes:

$$(u_j)_m = \sum_{n=N_{m-1}+1}^{N_m} C_n (\alpha_j^{(n-N_{m-1})})_m \exp \left\{ ik \left[ (b_i^{(n-N_{m-1})} x_i)_m - vt \right] \right\} \quad (11)$$

$$(\varphi)_m = \sum_{n=N_{m-1}+1}^{N_m} C_n (\alpha_4^{(n-N_{m-1})})_m \exp \left\{ ik \left[ (b_i^{(n-N_{m-1})} x_i)_m - vt \right] \right\} \quad (12)$$

Here  $m$  is the medium number,  $N_m = n_0 + n_1 + \dots + n_m$ ,  $n_m$  – the quantity of partial modes in the medium number  $m$  ( $m = 0$  corresponds to a substrate,  $m = 1$  corresponds to the 1<sup>st</sup> layer etc.,  $N_{0-1} = n_{0-1} = 0$ ),  $C_n$  – unknown coefficients and a continuous numeration is used for them (strange upper indices support this continuous numeration here and further).

The substrate is assumed the piezoelectric medium in all the cases and  $n_0 = 4$  in general case (or less in some special cases). There are eight partial modes for each layer in the general case if it is piezoelectric or six modes in the general case, if the layer is anisotropic nonpiezoelectric or isotropic medium (dielectric or metal). For isotropic medium the second component of the mechanical displacement  $u_2$  is decoupled with  $u_1$  and  $u_3$  and may be arbitrary, for example one can set  $u_2 = 1$ .

Unknown coefficient  $C_n$  in (11) and (12) can be determined using the boundary conditions on all the internal boundaries and on the external surface of the upper layer. Unfortunately it is impossible to formulate boundary conditions in the universal form, applicable to all the combinations of the substrate and layers materials. Therefore we must investigate different variants of material combinations separately.

For piezoelectric layers conditions of continuity of the mechanical displacements, electric potential, normal components of the stress tensor and the electric displacement must be satisfied for all the internal boundaries. On the external surface of the top layer normal components of the stress tensor must be equal to zero. If this surface is open (free), the continuity of the normal component of the electric displacement must be satisfied, if this surface is short circuited, then electric potential must be equal to zero. The stress tensor and electric displacement in piezoelectric medium can be calculated by means of following expressions:

$$T_{ij} = c_{ijkl} \frac{\partial u_k}{\partial x_l} + e_{kij} \frac{\partial \varphi}{\partial x_k}, \quad i, j, k, l = 1, 2, 3 \quad (13)$$

$$D_i = -\varepsilon_{ij} \frac{\partial \varphi}{\partial x_j} + e_{ijk} \frac{\partial u_j}{\partial x_k}, \quad i, j, k = 1, 2, 3 \quad (14)$$

Substituting (11) and (12) into (13) and (14) we can get following boundary conditions equations:

$$\sum_{n=N_{m-1}+1}^{N_m} C_n \left( \alpha_j^{(n-N_{m-1})} \right)_m \exp[ik(b_3^{(n-N_{m-1})})_m x_3^{(m)}] = \sum_{n=N_m+1}^{N_{m+1}} C_n \left( \alpha_j^{(n-N_m)} \right)_{m+1} \exp[ik(b_3^{(n-N_m)})_{m+1} x_3^{(m)}] \quad (15a)$$

$$\begin{aligned} & \sum_{n=N_{m-1}+1}^{N_m} C_n \left( c_{3jkl} \alpha_k^{(n-N_{m-1})} b_l^{(n-N_{m-1})} + e_{k3j} \alpha_4^{(n-N_{m-1})} b_k^{(n-N_{m-1})} \right)_m \exp[ik(b_3^{(n-N_{m-1})})_m x_3^{(m)}] = \\ & = \sum_{n=N_m+1}^{N_{m+1}} C_n \left( c_{3jkl} \alpha_k^{(n-N_m)} b_l^{(n-N_m)} + e_{k3j} \alpha_4^{(n-N_m)} b_k^{(n-N_m)} \right)_{m+1} \exp[ik(b_3^{(n-N_m)})_{m+1} x_3^{(m)}] \end{aligned} \quad (15b)$$

$$\sum_{n=N_{m-1}+1}^{N_m} C_n \left( \alpha_4^{(n-N_{m-1})} \right)_m \exp[ik(b_3^{(n-N_{m-1})})_m x_3^{(m)}] = \sum_{n=N_m+1}^{N_{m+1}} C_n \left( \alpha_4^{(n-N_m)} \right)_{m+1} \exp[ik(b_3^{(n-N_m)})_{m+1} x_3^{(m)}] \quad (15c)$$

$$\begin{aligned} & \sum_{n=N_{m-1}+1}^{N_m} C_n \left( e_{3jk} \alpha_j^{(n-N_{m-1})} b_k^{(n-N_{m-1})} - \varepsilon_{3j} \alpha_4^{(n-N_{m-1})} b_j^{(n-N_{m-1})} \right)_m \exp[ik(b_3^{(n-N_{m-1})})_m x_3^{(m)}] = \\ & = \sum_{n=N_m+1}^{N_{m+1}} C_n \left( e_{3jk} \alpha_j^{(n-N_m)} b_k^{(n-N_m)} - \varepsilon_{3j} \alpha_4^{(n-N_m)} b_j^{(n-N_m)} \right)_{m+1} \exp[ik(b_3^{(n-N_m)})_{m+1} x_3^{(m)}] \end{aligned} \quad (15d)$$

In these equations  $j, k, l = 1, 2, 3, m = 0, 1, 2, \dots, M-1$  (not up to  $M$ !), where  $M$  is the quantity of layers,  $x_3^{(m)} = h_1 + h_2 + \dots + h_m$ ,  $x_3^{(0)} = 0$ . Equations (15a) represent the continuity of mechanical displacements, (15b) – the continuity of the stress normal components, (15c) – the continuity of the electrical potential, (15d) – the continuity of the electric displacement normal component. If surface  $x_3 = x_3^{(m)}$  is short circuited by metal layer of zero thickness, equations (15c) and (15d) must be changed. The right part of the (15c) must be replaced with zero, the left part of (15d) also must be replaced with zero and the right part of (15d) must be replaced with the right part of (15c).

The boundary conditions equations for stress on the external surface of the top layer ( $m = M$ ) can be obtained from equations (15b) by replacing the right part of this equation with zero. Analogously by replacing the right part with zero the equation (15c) gives electric boundary condition for the short circuited external surface. In order to formulate the boundary condition on the free external surface, the potential in the free space must be written in the following form:

$$\varphi^{(f)} = \varphi^{(M)} e^{-kb_1(x_3 - x_3^{(M)})}, \quad x_3 \geq x_3^{(M)} \quad (16)$$

Here  $\varphi^{(M)}$  is the potential of the external surface ( $x_3 = x_3^{(M)}$ ). The potential (16) satisfies Laplace equation (that can be checked by direct substitution of (16) into this equation) and vanishes at  $x_3 \rightarrow \infty$ .

The normal component of the electric displacement in the free space:

$$D_3^{(f)} = -\varepsilon_0 \frac{\partial \varphi^{(f)}}{\partial x_3} = kb_1 \varepsilon_0 \varphi^{(M)} e^{-kb_1(x_3 - x_3^{(M)})} \quad (17)$$

Here  $\varepsilon_0$  is the dielectric permittivity of the free space. Using the expression (17) we can get the condition of the continuity of the normal component of the electric displacement on the free (open) external surface:

$$\begin{aligned} i \sum_{n=N_{M-1}+1}^{N_M} C_n \left( e_{3jk} \alpha_j^{(n-N_{M-1})} b_k^{(n-N_{M-1})} - \varepsilon_{3j} \alpha_4^{(n-N_{M-1})} b_j^{(n-N_{M-1})} \right)_M \exp[ik(b_3^{(n-N_{M-1})})_M x_3^{(M)}] = \\ = b_1 \varepsilon_0 \sum_{n=N_{M-1}+1}^{N_M} C_n (\alpha_4^{(n-N_{M-1})})_M \exp[ik(b_3^{(n-N_{M-1})})_M x_3^{(M)}] \end{aligned} \quad (18)$$

The system of the boundary conditions equations contains  $n_0 + n_1 + n_2 + \dots + n_M$  equations with the same number of unknown coefficients  $C_n$ . In general case  $n_0 = 4$ ,  $n_1 = n_2 = \dots = n_M = 8$ . For metal layers mechanical boundary conditions are the same as for the previous case (only one must take into account, that piezoelectric constants of layers are zero) and the electric boundary condition is formulated only for the substrate surface:

$$\sum_{n=1}^{n_0} C_n (\alpha_4^{(n)})_0 = 0 \quad (19)$$

This variant of boundary conditions is also valid, if the first layer is metal and all other layers are non-piezoelectric dielectrics and metals in an arbitrary combination. For this variant in the general case  $n_0 = 4$ ,  $n_1 = n_2 = \dots = n_M = 6$ .

For isotropic dielectric layers the mechanical boundary conditions are the same as for the previous case. Electric boundary conditions became complicated and multi-variant because any boundary may be either free or short circuited. Only the single variant is simple – the first boundary is short circuited. For this variant the electric boundary condition is presented by the single equation (19), such as for previous case.

In general case the dependence of the potential in the free space is defined by equation (16) and inside the  $m$ -th dielectric isotropic layer it must be written as:

$$\varphi^{(m)}(x_3) = A_m e^{-kb_1(x_3 - x_3^{(m-1)})} + B_m e^{kb_1(x_3 - x_3^{(m-1)})}, \quad x_3^{(m-1)} \leq x_3 \leq x_3^{(m)} \quad (20)$$

Coefficients  $A_m$  and  $B_m$  can be expressed by potentials on the layer boundaries, which depend on the electric conditions on this boundaries (free or short). Using conditions of the continuity of the potential and the normal component of the electric displacement one can exclude all the boundary potentials and express the potential  $\varphi^{(1)}$  in the first layer as function of  $x_3$ . This function will content only  $\varphi^{(0)}(x_3 = 0)$  – potential on the substrate surface. From the potential  $\varphi^{(1)}$  one can express the normal component of the electric displacement on the substrate surface and use the condition of the continuity of this value for formulation of the electric boundary condition equation. This is the single equation, but its view significantly depends on the electric conditions on other boundaries.

If all the boundaries are electrically free and there is only the single layer, the equation, which describes the electric boundary conditions, can be written so:



$$i \sum_{n=1}^{n_0} C_n \left( e_{3jk} \alpha_j^{(n)} b_k^{(n)} - \varepsilon_{3j} \alpha_4^{(n)} b_j^{(n)} \right)_0 = \frac{b_1 \varepsilon_1 \varepsilon_0}{sh(kb_1 h_1)} S_1 \sum_{n=1}^{n_0} C_n (\alpha_4^{(n)})_0 \quad (21a)$$

where

$$S_1 = ch(kb_1 h_1) - \frac{\varepsilon_1}{\varepsilon_1 ch(kb_1 h_1) + R_2 sh(kb_1 h_1)} \quad (21b)$$

Here and hereinafter  $\varepsilon_m$  ( $m = 1, 2, \dots, M$ ) is the relative permittivity of the  $m$ -th layer.  $R_2$  in (21b) is the recurrent coefficient, which allows to obtain the equation for two layers from equations (21) for one layer. For the single layer  $R_2 = 1$ , and for two layers:

$$R_2 = \frac{\varepsilon_2}{sh(kb_1 h_2)} S_2 \quad (22)$$

I.e. for two layers the electric boundary condition has the following view:

$$i \sum_{n=1}^{n_0} C_n \left( e_{3jk} \alpha_j^{(n)} b_k^{(n)} - \varepsilon_{3j} \alpha_4^{(n)} b_j^{(n)} \right)_0 = \frac{b_1 \varepsilon_1 \varepsilon_0}{sh(kb_1 h_1)} \left[ ch(kb_1 h_1) - \frac{\varepsilon_1}{\varepsilon_1 ch(kb_1 h_1) + \frac{\varepsilon_2 sh(kb_1 h_1)}{sh(kb_1 h_2)} S_2} \right] \sum_{n=1}^{n_0} C_n (\alpha_4^{(n)})_0 \quad (23a)$$

where:

$$S_2 = ch(kb_1 h_2) - \frac{\varepsilon_2}{\varepsilon_2 ch(kb_1 h_2) + R_3 sh(kb_1 h_2)} \quad (23b)$$

The recurrent coefficient  $R_3$  gives possibility to obtain the equation for three layers from equation for two layers:

$$R_3 = \frac{\varepsilon_3}{sh(kb_1 h_3)} S_3 \quad (24)$$

For three layers:

$$S_3 = ch(kb_1 h_3) - \frac{\varepsilon_3}{\varepsilon_3 ch(kb_1 h_3) + R_4 sh(kb_1 h_3)} \quad (25)$$

For three layers  $R_4 = 1$ , and for more than three:

$$R_4 = \frac{\varepsilon_4}{sh(kb_1 h_4)} S_4 \quad (26)$$

And so on, i.e. the equation of electric boundary conditions for  $m + 1$  layers may be obtained from the equation for  $m$  layers by using the recurrent coefficient  $R_{m+1}$  ( $R_{M+1} = 1$ , if  $M$  is the total number of layers). To obtain the equation for  $M$  layers one must write equation for one layer, then for two layers and so on until the equation for  $M$  layers will be obtained.

If one of the boundary surfaces  $x_3 = x_3^{(m)}$  is short circuited (metalized), then electric conditions of all the further boundaries are unimportant, because the electric field outside





For two metal layers (or the first layer is metal and the second layer is an arbitrary nonpiezoelectric material, or two arbitrary nonpiezoelectric layers with shorted bottom surface of the first layer):

$$\begin{aligned}
 & \left. \begin{aligned} a_{qn} &= (\alpha_j^{(n)})_0 & n=1, \dots, 4 \\ a_{qn} &= -(\alpha_j^{(n-4)})_1 & n=5, \dots, 10 \\ a_{qn} &= 0 & n=11, \dots, 16 \end{aligned} \right\} \begin{aligned} & q=1, 2, 3 \\ & j=q \\ & \end{aligned} & \left. \begin{aligned} a_{qn} &= (c_{3jkl} \alpha_k^{(n)} b_l^{(n)} + e_{k3j} \alpha_4^{(n)} b_k^{(n)})_0 & n=1, \dots, 4 \\ a_{qn} &= - (c_{3jkl} \alpha_k^{(n-4)} b_l^{(n-4)})_1 & n=5, \dots, 10 \\ a_{qn} &= 0 & n=11, \dots, 16 \end{aligned} \right\} \begin{aligned} & q=4, 5, 6 \\ & j=q-3 \end{aligned} \\
 & \left. \begin{aligned} a_{qn} &= 0 & n=1, \dots, 4 \\ a_{qn} &= (\alpha_j^{(n-4)})_1 \exp[ik(b_3^{(n-4)})_1 h_1] & n=5, \dots, 10 \\ a_{qn} &= -(\alpha_j^{(n-10)})_2 \exp[ik(b_3^{(n-10)})_2 h_1] & n=11, \dots, 16 \end{aligned} \right\} \begin{aligned} & q=7, 8, 9 \\ & j=q-6 \end{aligned} \\
 & \left. \begin{aligned} a_{qn} &= 0 & n=1, \dots, 4 \\ a_{qn} &= (c_{3jkl} \alpha_k^{(n-4)} b_l^{(n-4)})_1 \exp[ik(b_3^{(n-4)})_1 h_1] & n=5, \dots, 10 \\ a_{qn} &= - (c_{3jkl} \alpha_k^{(n-10)} b_l^{(n-10)})_2 \exp[ik(b_3^{(n-10)})_2 h_1] & n=11, \dots, 16 \end{aligned} \right\} \begin{aligned} & q=10, 11, 12 \\ & j=q-9 \end{aligned} \\
 & \left. \begin{aligned} a_{qn} &= 0 & n=1, \dots, 10 \\ a_{qn} &= (c_{3jkl} \alpha_k^{(n-10)} b_l^{(n-10)})_2 \exp[ik(b_3^{(n-10)})_2 (h_1 + h_2)] & n=11, \dots, 16 \end{aligned} \right\} \begin{aligned} & q=13, 14, 15 \\ & j=q-12 \end{aligned} \\
 & \left. \begin{aligned} a_{qn} &= (\alpha_4^{(n)})_0 & n=1, \dots, 4 \\ a_{qn} &= 0 & n=5, \dots, 16 \end{aligned} \right\} q=16
 \end{aligned} \tag{30}$$

The first six strings represent continuity of the displacements ( $q = 1, 2, 3$ ) and the stresses ( $q = 4, 5, 6$ ) on the bottom surface of the first layer, the second six strings - continuity of the displacements ( $q = 7, 8, 9$ ) and stresses ( $q = 10, 11, 12$ ) on the bottom surface of the second layer, the strings up 13 to 15 - zero stress on the top surface of the second (top) layer, and the last string ( $q = 16$ ) - zero potential on the bottom surface of the first layer.

The next examples are the isotropic dielectric layers on the piezoelectric substrate.

For one isotropic dielectric layer with both open surfaces the first 9 strings of the boundary conditions determinant are the same as in (29) and the last string is:

$$\left. \begin{aligned} a_{qn} &= i \left( e_{3jk} \alpha_j^{(n)} b_k^{(n)} - \varepsilon_{3j} \alpha_4^{(n)} b_j^{(n)} \right)_0 - \frac{b_1 \varepsilon_1 \varepsilon_0}{sh(kb_1 h_1)} S_1 (\alpha_4^{(n)})_0 & n=1, \dots, 4 \\ a_{qn} &= 0 & n=5, \dots, 10 \end{aligned} \right\} q=10 \tag{31}$$

where  $S_1$  is represented by (21b) at  $R_2 = 1$ .

For one isotropic dielectric layer with the open bottom surface and the shorted top surface the expression (31) is valid, but  $S_1 = ch(kb_1 h_1)$ .

For one isotropic dielectric layer with bottom shorted surface the boundary conditions determinant coincides with (29) completely.

For two isotropic dielectric layers with all open surfaces the first 15 strings of the boundary conditions determinant are the same as in (30) and the last string is:

$$\left. \begin{aligned} a_{qn} &= i \left( e_{3jk} \alpha_j^{(n)} b_k^{(n)} - \varepsilon_{3j} \alpha_4^{(n)} b_j^{(n)} \right)_0 - \frac{b_1 \varepsilon_1 \varepsilon_0}{sh(kb_1 h_1)} S_1 (\alpha_4^{(n)})_0 \quad n=1, \dots, 4 \\ a_{qn} &= 0 \quad n=5, \dots, 16 \end{aligned} \right\} q=16 \quad (32)$$

where one must use (21b) for  $S_1$ , (22) for  $R_2$ , and (23b) for  $S_2$  ( $R_3 = 1$  must be set in (23b)).

For two isotropic dielectric layers with the top shorted surface of the top layer (all other boundaries are open) the expression (32) is valid, but  $S_2 = ch(kb_1 h_2)$  instead of (23b).

For two isotropic dielectric layers with the bottom shorted surface of the top layer the expression (32) is valid, but  $S_1 = ch(kb_1 h_1)$  instead of (21b), and (22), (23b) are not needed.

If the bottom surface of the first layer is shorted, the boundary conditions determinant coincides with (30) completely.

And now we will consider some examples with piezoelectric layers.

For one piezoelectric layer with open surfaces the boundary conditions determinant contains 12 strings and 12 columns and elements of this determinant are:

$$\left. \begin{aligned} a_{qn} &= (\alpha_j^{(n)})_0 \quad n=1, \dots, 4 \\ a_{qn} &= -(\alpha_j^{(n-4)})_1 \quad n=5, \dots, 12 \end{aligned} \right\} \begin{aligned} q=1, 2, 3 \\ j=q \end{aligned} \quad \left. \begin{aligned} a_{qn} &= (c_{3jkl} \alpha_k^{(n)} b_l^{(n)} + e_{k3j} \alpha_4^{(n)} b_k^{(n)})_0 \quad n=1, \dots, 4 \\ a_{qn} &= -(c_{3jkl} \alpha_k^{(n-4)} b_l^{(n-4)} + e_{k3j} \alpha_4^{(n-4)} b_k^{(n-4)})_1 \quad n=5, \dots, 12 \end{aligned} \right\} \begin{aligned} q=4, 5, 6 \\ j=q-3 \end{aligned}$$

$$\left. \begin{aligned} a_{qn} &= (\alpha_4^{(n)})_0 \quad n=1, \dots, 4 \\ a_{qn} &= -(\alpha_4^{(n-4)})_1 \quad n=5, \dots, 12 \end{aligned} \right\} q=7 \quad \left. \begin{aligned} a_{qn} &= (e_{3jk} \alpha_j^{(n)} b_k^{(n)} - \varepsilon_{3j} \alpha_4^{(n)} b_j^{(n)})_0 \quad n=1, \dots, 4 \\ a_{qn} &= -(e_{3jk} \alpha_j^{(n-4)} b_k^{(n-4)} - \varepsilon_{3j} \alpha_4^{(n-4)} b_j^{(n-4)})_1 \quad n=5, \dots, 12 \end{aligned} \right\} q=8$$

$$\left. \begin{aligned} a_{qn} &= 0 \quad n=1, \dots, 4 \\ a_{qn} &= (c_{3jkl} \alpha_k^{(n-4)} b_l^{(n-4)} + e_{k3j} \alpha_4^{(n-4)} b_k^{(n-4)})_1 \exp[ik(b_3^{(n-4)})_1 h_1] \quad n=5, \dots, 12 \end{aligned} \right\} \begin{aligned} q=9, 10, 11 \\ j=q-8 \end{aligned} \quad (33)$$

$$\left. \begin{aligned} a_{qn} &= 0 \quad n=1, \dots, 4 \\ a_{qn} &= \left\{ i \left( e_{3jk} \alpha_j^{(n-4)} b_k^{(n-4)} - \varepsilon_{3j} \alpha_4^{(n-4)} b_j^{(n-4)} \right)_1 - b_1 \varepsilon_0 (\alpha_4^{(n-4)})_1 \right\} \exp[ik(b_3^{(n-4)})_1 h_1] \quad n=5, \dots, 12 \end{aligned} \right\} q=12$$

Here the first three strings ( $q = 1, 2, 3$ ) represent the continuity of the three components ( $j = 1, 2, 3$ ) of mechanical displacements on the substrate surface ( $x_3^{(0)} = 0$ ), the next three strings ( $q = 4, 5, 6$ ) are the continuity of the three normal components ( $j = 1, 2, 3$ ) of the mechanical stress on the substrate surface ( $x_3^{(0)} = 0$ ), the next string ( $q = 7$ ) - continuity of the electric potential on the same surface, then ( $q = 8$ ) - continuity of the normal component of the electric displacement on the substrate surface ( $x_3^{(0)} = 0$ ), the next three strings ( $q = 9, 10, 11$ ) are three ( $j = 1, 2, 3$ ) zero normal components of the mechanical stress on the top surface of the layer ( $x_3^{(1)} = h_1$ ), and the last string ( $q = 12$ ) expresses the continuity of the normal component of the electric displacement on the open top surface of the layer ( $x_3^{(1)} = h_1$ ).

For one piezoelectric layer with shorted bottom surface and open top one the expressions (33) are valid, excepting the strings 7 and 8 ( $q = 7$  and 8), which must be replaced with:

$$\left. \begin{array}{ll} a_{qn} = (\alpha_4^{(n)})_0 & n=1, \dots, 4 \\ a_{qn} = 0 & n=5, \dots, 12 \end{array} \right\} q=7 \quad \left. \begin{array}{ll} a_{qn} = 0 & n=1, \dots, 4 \\ a_{qn} = (\alpha_4^{(n-4)})_1 & n=5, \dots, 12 \end{array} \right\} q=8 \quad (34a)$$

These expressions represent the zero electric potential of the bottom surface of the layer (the substrate surface).

For one piezoelectric layer with shorted top surface and open bottom one the expressions (33) are valid, excepting the last string ( $q = 12$ ), which must be replaced with:

$$\left. \begin{array}{ll} a_{qn} = 0 & n=1, \dots, 4 \\ a_{qn} = (\alpha_4^{(n-4)})_1 \exp[ik(b_3^{(n-4)})_1 h_1] & n=5, \dots, 12 \end{array} \right\} q=12 \quad (34b)$$

which corresponds to the zero electric potential of the top surface of the layer.

For one piezoelectric layer with both shorted surface one can use expressions (33), in which strings 7 and 8 must be replaced with (34a) and string 12 – with (34b).

For two piezoelectric layers on the piezoelectric substrate with all open surfaces the boundary conditions determinant contains the following 20 strings:

$$\left. \begin{array}{ll} a_{qn} = (\alpha_j^{(n)})_0 & n=1, \dots, 4 \\ a_{qn} = -(\alpha_j^{(n-4)})_1 & n=5, \dots, 12 \\ a_{qn} = 0 & n=13, \dots, 20 \end{array} \right\} \begin{array}{l} q=1, 2, 3 \\ j=q \end{array} \quad \left. \begin{array}{ll} a_{qn} = (c_{3jkl} \alpha_k^{(n)} b_l^{(n)} + e_{k3j} \alpha_4^{(n)} b_k^{(n)})_0 & n=1, \dots, 4 \\ a_{qn} = -(c_{3jkl} \alpha_k^{(n-4)} b_l^{(n-4)} + e_{k3j} \alpha_4^{(n-4)} b_k^{(n-4)})_1 & n=5, \dots, 12 \\ a_{qn} = 0 & n=13, \dots, 20 \end{array} \right\} \begin{array}{l} q=4, 5, 6 \\ j=q-3 \end{array}$$

$$\left. \begin{array}{ll} a_{qn} = (\alpha_4^{(n)})_0 & n=1, \dots, 4 \\ a_{qn} = -(\alpha_4^{(n-4)})_1 & n=5, \dots, 12 \\ a_{qn} = 0 & n=13, \dots, 20 \end{array} \right\} q=7 \quad \left. \begin{array}{ll} a_{qn} = (e_{3jk} \alpha_j^{(n)} b_k^{(n)} - \varepsilon_{3j} \alpha_4^{(n)} b_j^{(n)})_0 & n=1, \dots, 4 \\ a_{qn} = -(e_{3jk} \alpha_j^{(n-4)} b_k^{(n-4)} - \varepsilon_{3j} \alpha_4^{(n-4)} b_j^{(n-4)})_1 & n=5, \dots, 12 \\ a_{qn} = 0 & n=13, \dots, 20 \end{array} \right\} q=8$$

$$\left. \begin{array}{ll} a_{qn} = 0 & n=1, \dots, 4 \\ a_{qn} = (\alpha_j^{(n-4)})_1 \exp[ik(b_3^{(n-4)})_1 h_1] & n=5, \dots, 12 \\ a_{qn} = -(\alpha_j^{(n-12)})_2 \exp[ik(b_3^{(n-12)})_2 h_1] & n=13, \dots, 20 \end{array} \right\} q=9, 10, 11 \quad j=q-8$$

$$\left. \begin{array}{ll} a_{qn} = 0 & n=1, \dots, 4 \\ a_{qn} = (c_{3jkl} \alpha_k^{(n-4)} b_l^{(n-4)} + e_{k3j} \alpha_4^{(n-4)} b_k^{(n-4)})_1 \exp[ik(b_3^{(n-4)})_1 h_1] & n=5, \dots, 12 \\ a_{qn} = -(c_{3jkl} \alpha_k^{(n-12)} b_l^{(n-12)} + e_{k3j} \alpha_4^{(n-12)} b_k^{(n-12)})_2 \exp[ik(b_3^{(n-12)})_2 h_1] & n=13, \dots, 20 \end{array} \right\} q=12, 13, 14 \quad j=q-11$$

$$\left. \begin{array}{ll} a_{qn} = 0 & n=1, \dots, 4 \\ a_{qn} = (\alpha_4^{(n-4)})_1 \exp[ik(b_3^{(n-4)})_1 h_1] & n=5, \dots, 12 \\ a_{qn} = -(\alpha_4^{(n-12)})_2 \exp[ik(b_3^{(n-12)})_2 h_1] & n=13, \dots, 20 \end{array} \right\} q=15 \quad (35)$$

$$\left. \begin{aligned} a_{qn} &= 0 & n &= 1, \dots, 4 \\ a_{qn} &= \left( e_{3jk} \alpha_j^{(n-4)} b_k^{(n-4)} - \varepsilon_{3j} \alpha_4^{(n-4)} b_j^{(n-4)} \right)_1 \exp[ik(b_3^{(n-4)})_1 h_1] & n &= 5, \dots, 12 \\ a_{qn} &= - \left( e_{3jk} \alpha_j^{(n-12)} b_k^{(n-12)} - \varepsilon_{3j} \alpha_4^{(n-12)} b_j^{(n-12)} \right)_2 \exp[ik(b_3^{(n-12)})_2 h_1] & n &= 13, \dots, 20 \end{aligned} \right\} q = 16$$

$$\left. \begin{aligned} a_{qn} &= 0 & n &= 1, \dots, 12 \\ a_{qn} &= \left( c_{3jkl} \alpha_k^{(n-12)} b_l^{(n-12)} + e_{k3j} \alpha_4^{(n-12)} b_k^{(n-12)} \right)_2 \exp[ik(b_3^{(n-12)})_2 (h_1 + h_2)] & n &= 13, \dots, 20 \end{aligned} \right\} \begin{aligned} q &= 17, 18, 19 \\ j &= q - 16 \end{aligned}$$

$$\left. \begin{aligned} a_{qn} &= 0 & n &= 1, \dots, 12 \\ a_{qn} &= \left\{ i \left( e_{3jk} \alpha_j^{(n-12)} b_k^{(n-12)} - \varepsilon_{3j} \alpha_4^{(n-12)} b_j^{(n-12)} \right)_2 - b_1 \varepsilon_0 (\alpha_4^{(n-12)})_2 \right\} \times \\ & \times \exp[ik(b_3^{(n-12)})_2 (h_1 + h_2)] & n &= 13, \dots, 20 \end{aligned} \right\} q = 20$$

Here the first three strings ( $q = 1, 2, 3$ ) represent the continuity of the three components ( $j = 1, 2, 3$ ) of mechanical displacements on the substrate surface ( $x_3^{(0)} = 0$ ), the next three strings ( $q = 4, 5, 6$ ) are the continuity of the three normal components ( $j = 1, 2, 3$ ) of the mechanical stress on the substrate surface ( $x_3^{(0)} = 0$ ), the next string ( $q = 7$ ) - continuity of the electric potential on the same surface, then ( $q = 8$ ) - continuity of the normal component of the electric displacement on the substrate surface ( $x_3^{(0)} = 0$ ), strings 9, 10, 11 - the continuity of the three components ( $j = 1, 2, 3$ ) of mechanical displacements on the surface between the first and the second layers ( $x_3^{(1)} = h_1$ ), strings 12, 13, 14 - the continuity of the three components ( $j = 1, 2, 3$ ) of mechanical stress on the surface between the first and the second layers ( $x_3^{(1)} = h_1$ ), the next string ( $q = 15$ ) - continuity of the electric potential on the same surface, then ( $q = 16$ ) - continuity of the normal component of the electric displacement on the same surface, the next three strings ( $q = 17, 18, 19$ ) are three ( $j = 1, 2, 3$ ) zero normal components of the mechanical stress on the top surface of the top layer ( $x_3^{(2)} = h_1 + h_2$ ), and the last string ( $q = 20$ ) expresses the continuity of the normal component of the electric displacement on the open top surface of the top layer ( $x_3^{(2)} = h_1 + h_2$ ).

For two piezoelectric layers on the piezoelectric substrate with shorted bottom surface of the first layer and with the open other surfaces strings number 7 and 8 in expressions (35) must be replaced with:

$$\left. \begin{aligned} a_{qn} &= (\alpha_4^{(n)})_0 & n &= 1, \dots, 4 \\ a_{qn} &= 0 & n &= 5, \dots, 20 \end{aligned} \right\} q = 7$$

$$\left. \begin{aligned} a_{qn} &= 0 & n &= 1, \dots, 4 \\ a_{qn} &= (\alpha_4^{(n-4)})_1 & n &= 5, \dots, 12 \\ a_{qn} &= 0 & n &= 13, \dots, 20 \end{aligned} \right\} q = 8 \quad (36a)$$

For two piezoelectric layers on the piezoelectric substrate with shorted bottom surface of the second layer and with open other surfaces strings number 15 and 16 in expressions (35) must be replaced with:

$$\left. \begin{aligned} a_{qn} &= 0 & n &= 1, \dots, 4 \\ a_{qn} &= (\alpha_4^{(n-4)})_1 \exp[ik(b_3^{(n-4)})_1 h_1] & n &= 5, \dots, 12 \\ a_{qn} &= 0 & n &= 13, \dots, 20 \end{aligned} \right\} q=15 \quad (36b)$$

$$\left. \begin{aligned} a_{qn} &= 0 & n &= 1, \dots, 12 \\ a_{qn} &= (\alpha_4^{(n-12)})_2 \exp[ik(b_3^{(n-12)})_2 h_1] & n &= 13, \dots, 20 \end{aligned} \right\} q=16$$

For two piezoelectric layers on the piezoelectric substrate with shorted top surface of the second layer and with open other surfaces the string number 20 in expressions (35) must be replaced with:

$$\left. \begin{aligned} a_{qn} &= 0 & n &= 1, \dots, 12 \\ a_{qn} &= (\alpha_4^{(n-12)})_2 \exp[ik(b_3^{(n-12)})_2 (h_1 + h_2)] & n &= 13, \dots, 20 \end{aligned} \right\} q=20 \quad (36c)$$

If two surfaces of three are shorted, then two corresponding expressions of (36a) – (36c) must be used for replacing the corresponding expressions of (35), taking into account, that (36a) “short-circuits” the first surface (the substrate surface), (36b) – the second surface, and (36c) – the third one (the top surface of the top layer).

If all three surfaces are shorted, all expressions (36a) – (36c) must be used for replacing the corresponding expressions in (35).

All the examples, considered above, allow to understand how to form the boundary conditions determinant and for more complicated structures with three, four, five etc. layers, if necessary.

Thus, the determinant of the boundary conditions is formed. Now we have to solve the equation (28). This means we need to find a value of wave velocity (or velocity and attenuation coefficient for the pseudo-surface wave), for which the boundary conditions determinant vanishes. The solution of equation (28) can be found by any available iterative procedure. In our case, we apply our own algorithm to search the global extremum of function of several variables (Dvoesherstov et. al., 1999). Solution corresponds to the global minimum of the function, which is the square of the absolute value of the boundary conditions determinant.

Another widely used method of finding solution is to calculate the effective dielectric permittivity (Adler, 1994):

$$\varepsilon_{eff} = \frac{D_3^{(m)}}{kb_1 \varphi^{(m)}} \quad (37)$$

Here  $\varphi^{(m)}$  and  $D_3^{(m)}$  - the potential and electric displacement on the top surface of the layer  $m$ . Corresponding string of the boundary conditions determinant is used for expression (37). For example, for top surface of the top layer under condition that this layer is piezoelectric, the effective permittivity technique gives the follow equation, which expresses continuity of the dielectric permittivity:

$$\frac{i \sum_{n=N_{M-1}+1}^{N_M} C_n \left( e_{3jk} \alpha_j^{(n)} b_k^{(n)} - \varepsilon_{3j} \alpha_4^{(n)} b_j^{(n)} \right) \exp[ik b_3^{(n)} x_3^{(M)}]}{b_1 \varepsilon_0 \sum_{n=N_{M-1}+1}^{N_M} C_n \alpha_4^{(n)} \exp[ik b_3^{(n)} x_3^{(M)}]} = \begin{cases} \varepsilon_0 \\ \infty \end{cases} \quad (38)$$



The top value in the right part of this equation corresponds to the open surface, the bottom value ( $\infty$ ) – to short-circuited one. One can see that coefficients  $C_n$  are needed for using of this technique. These coefficients are obtained by solving the equations system (27), from those the equation, corresponding to the surface number  $m$ , is excluded. For example, in our case one must exclude the last equation of this system (corresponding to the last string of the boundary conditions determinant). The system (27) is uniform and its solution is defined with an accuracy up to an arbitrary coefficient. Therefore after excluding one of the equation from this system we can set any  $C_n$  of any value, for example  $C_N = 1$  and then solve the  $N-1$  power nonuniform system and to obtain all the coefficients  $C_n$  for using the equation (38). This procedure is repeating for different values of the wave velocity (or the velocity and the attenuation coefficients) until the equation (38) is satisfied. We used the global search procedure for equation (38) solving (Dvoesherstov et. al., 1999). Calculations by using the boundary conditions determinant (solving the system (27) in this case is not required) and by using the effective dielectric permittivity are mathematically equivalent each other and give the same result. But in some cases one technique gives result with better reliability than another, and in other cases – contrary. Our soft contains both techniques and one can easily switch from one to another by the single mouse click. When the wave velocity (or the velocity and the attenuation coefficient) is obtained, one can calculate all the coefficients  $C_n$  by solving the equation system (27) and then the wave amplitudes for any  $x_3$  coordinate in any medium by substitution  $C_n$  into (11) and (12).

After the calculation of the wave phase velocity one can obtain all the wave propagation characteristics: an electromechanical coupling coefficient, a temperature coefficient of delay, a power flow angle, a diffraction parameter. Dependences of the layers thickness and theirs mass density on a temperature, which are needed for temperature coefficient of delay calculations, one can find, for example in (Shimizu et. al., 1976).

All the propagation characteristics can be modified by proper choice of the layer parameters. For example, Fig. 2 shows dependences of the temperature coefficient of delay ( $TCD$ ) on quartz with single Al and Au layer on the second Euler angle and on the relative layer thickness. Material constants for quartz are taken from (Shimizu and Yamamoto, 1980), for

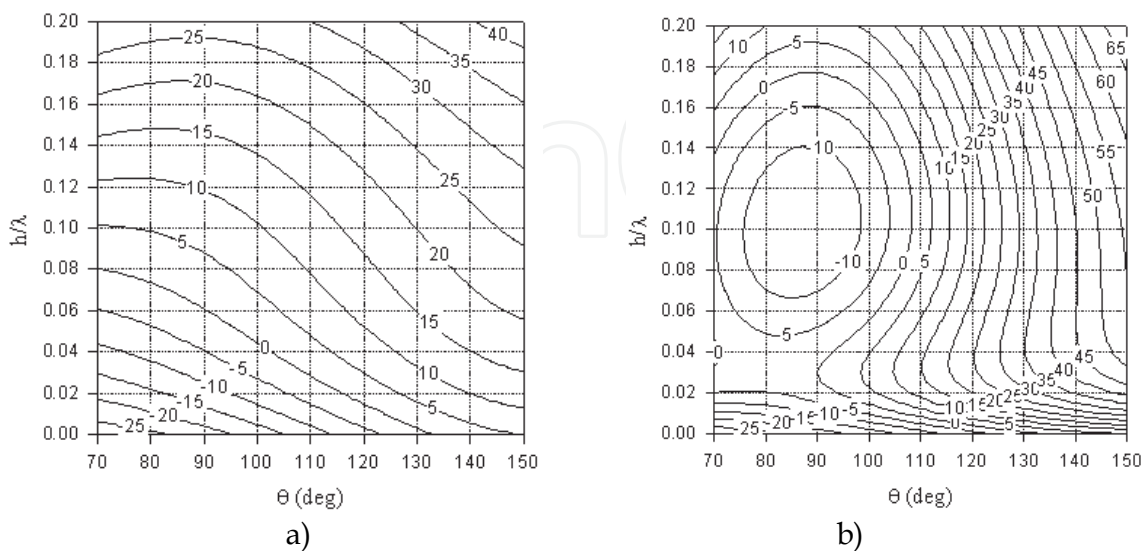


Fig. 2. Dependence of  $TCD$  (ppm/°C) on the 2<sup>nd</sup> Euler angle  $\theta$  and on the relative layer thickness  $h/\lambda$  for Al (a) and Au (b). The first and third Euler angles are equal to zero.



Al and Au – from (Ballandras et. al., 1997). One can see in Fig. 2, that negative values of  $TCD$  can be compensated by metallic layer. For example, orientation YX-quartz ( $0^\circ, 90^\circ, 0^\circ$ ) becomes thermostable if  $h/\lambda = 0.061$  for Al layer and YX-quartz keeps the temperature stability in range  $0.027 \leq h/\lambda \leq 0.032$  for Au layer.

So, multilayer structures can be used both for protection against external undesired influence and for improvement of the wave propagation characteristics, i.e. the SAW device properties. All these possibilities can be evaluated by means of calculation technique, described here.

### 3. Bulk acoustic waves in multilayer structures

Bulk acoustic waves are used in film bulk acoustic resonators. The simplest such resonator contains at least three layers, namely an active piezoelectric layer, in which transformation of the electric signal into the acoustic wave takes place, and two metallic (usually aluminum) electrodes, connected to the source of the electric signal. The structure of such resonator (named membrane type resonator) is schematically shown in Fig. 3a.

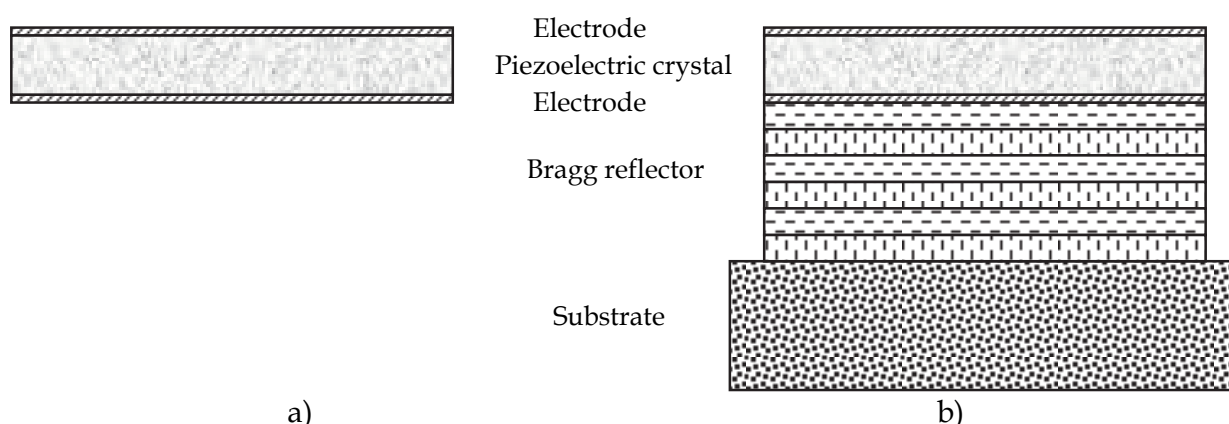


Fig. 3. Schematic view of the membrane type film bulk acoustic wave resonator (a) and of the SMR resonator (b).

FBAR resonators are used in the ultra high frequency range (several GHz and higher), therefore a thickness of the active layer is very small (microns and less). There are some problems with mounting of such small structures on the solid massive and relatively thick substrate. It is impossible to place membrane type FBAR on the substrate directly, because in this case the useful signal will be deformed by multiple spurious oscillation modes due to an acoustic interaction of the resonator and the substrate. To prevent this interaction more complicated constructions are required. In particular, an air gap between the bottom electrode and the substrate must be provided or cavity in substrate under a bottom electrode must be etched. These variants require rather complex technological processes application. Another possibility is mounting the multilayer Bragg reflector directly on the substrate and then mounting of the resonator directly on this reflector. Such construction is named a solid mounted resonator (SMR). The structure of such resonator schematically is shown in Fig. 3b.

The Bragg reflector contains several (3 – 5) pairs of two materials with different acoustic properties. The thickness of each layer in the reflector must be equal to a quarter of the

wavelength in its material. Such construction provides attenuation of the wave and prevents an acoustic interaction of the active zone of the resonator and the substrate.

Transversal sizes of the resonator are usually much larger than its total thickness, therefore an analysis of all the main properties may be performed in the one-dimensional approach. The most rigorous one-dimensional theory of such multilayer structures is presented in (Nowotny and Benes, 1987). The following description is based on this theory, some modified for expansion of its possibilities.

The wave equations, describing processes in the solid piezoelectric medium, are the same as for surface acoustic waves – see (1) and (2). Assuming that all the values depend only on the single spatial coordinate  $x_1$  (mechanical displacements  $u_i$  along all the coordinates  $x_i$  take place in this case nevertheless), we can write simpler form of these equations:

$$c_{1jk1} \frac{\partial^2 u_k}{\partial x_1^2} + e_{11j} \frac{\partial^2 \varphi}{\partial x_1^2} = \rho \frac{\partial^2 u_j}{\partial t^2} \quad j, k = 1, 2, 3 \quad (39)$$

$$e_{11k} \frac{\partial^2 u_k}{\partial x_1^2} - \varepsilon_{11} \frac{\partial^2 \varphi}{\partial x_1^2} = 0 \quad (40)$$

Complex material constants (with real and imaginary parts) can be used for modeling of electro-acoustic losses in the medium.

The solution for the electric potential  $\varphi$  can be obtained from (40) in such form:

$$\varphi = \frac{e_{11k}}{\varepsilon_{11}} u_k + \phi_1 x_1 + \phi_0 \quad (41)$$

Here  $\phi_0$  and  $\phi_1$  are arbitrary unknown constants.

Substitution (41) into (39) gives:

$$\bar{c}_{1jk1} \frac{\partial^2 u_k}{\partial x_1^2} = \rho \frac{\partial^2 u_j}{\partial t^2} \quad (42)$$

Here  $\bar{c}_{1jk1}$  are the stiffened elastic constants:

$$\bar{c}_{1jk1} = c_{1jk1} + \frac{e_{11j} e_{11k}}{\varepsilon_{11}} \quad (43)$$

We will seek the solution of these equations ( $j = 1, 2, 3$ ) as a sinusoidal wave, propagating along the  $x_1$  axis with the velocity  $v$ :

$$u_k(x_1, t) = \beta_k e^{i\omega \left( \frac{x_1}{v} - t \right)} = \beta_k e^{i\omega(\alpha x_1 - t)}, \quad (44)$$

where  $\alpha = 1/v$  is a slowness.

Substitution of (44) into the equations (42) transforms them into the linear algebraic equations system:

$$\bar{c}_{1jk1} \beta_k = \bar{c} \beta_j, \quad (45)$$

where

$$\bar{c} = \frac{\rho}{\alpha^2} = \rho v^2 \quad (46)$$

In more detailed form the system (45) has the following view:

$$\begin{aligned} (\bar{c}_{1111} - \bar{c})\beta_1 + \bar{c}_{1121}\beta_2 + \bar{c}_{1131}\beta_3 &= 0 \\ \bar{c}_{1211}\beta_1 + (\bar{c}_{1221} - \bar{c})\beta_2 + \bar{c}_{1231}\beta_3 &= 0 \\ \bar{c}_{1311}\beta_1 + \bar{c}_{1321}\beta_2 + (\bar{c}_{1331} - \bar{c})\beta_3 &= 0 \end{aligned} \quad (47)$$

This is a system of linear equations for the three amplitudes  $\beta_1, \beta_2, \beta_3$ . This system can have a nontrivial solution only if the determinant of its coefficients is equal to zero:

$$\begin{vmatrix} \bar{c}_{1111} - \bar{c} & \bar{c}_{1121} & \bar{c}_{1131} \\ \bar{c}_{1211} & \bar{c}_{1221} - \bar{c} & \bar{c}_{1231} \\ \bar{c}_{1311} & \bar{c}_{1321} & \bar{c}_{1331} - \bar{c} \end{vmatrix} = 0 \quad (48)$$

It gives the third power polynomial equation for  $\bar{c}$ , i.e. for  $\rho v^2$ . Three roots of this equation will represent the three eigenvalues  $\bar{c}^{(n)}$  ( $n = 1, 2, 3$ ), giving three values of the bulk wave velocity  $v^{(n)}$  or three values of the slowness  $\alpha^{(n)}$ .

Three values  $\beta_k^{(n)}$  ( $k = 1, 2, 3$ ) correspond to each value  $\bar{c}^{(n)}$ . These values  $\beta_k^{(n)}$  are obtained by solving the system (47) for each value  $\bar{c}^{(n)}$  and represent the eigenvector. System (47) is homogeneous, so its solution is determined up to an arbitrary factor. Consequently, we can normalize each eigenvector by its modulus, and work further with the normalized dimensionless vector. The three normalized eigenvectors are complete and orthogonal:

$$\beta_k^{(n)} \beta_k^{(m)} = \delta_{nm}, \quad \sum_n \beta_k^{(n)} \beta_l^{(n)} = \delta_{kl} \quad (\delta_{kl} \text{ is the Kronecker symbol}) \quad (49)$$

The general solution of the equations system (42) we will seek in such view:

$$u_k(x_1, t) = u_k(x_1) e^{-i\omega t}, \quad (50)$$

where  $u_k(x_1)$  is the linear combination of three bulk waves, obtained from equations (47) and (48):

$$u_k(x_1) = \sum_{n=1}^3 \beta_k^{(n)} [A^{(n)} \cos(\alpha^{(n)} \omega x_1) + B^{(n)} \sin(\alpha^{(n)} \omega x_1)] \quad (51)$$

Here  $A^{(n)}$  and  $B^{(n)}$  are six unknown coefficients of the linear combination. Together with  $\phi_0$  and  $\phi_1$  we have the eight unknown coefficients to be defined further.

We need the eight boundary conditions for obtaining the eight unknown coefficients. We will use three normal components of the stress tensor, three components of the mechanical displacement, the normal component of the electric displacement and the electric potential for some concrete coordinate  $x_1$ , for example for  $x_1 = 0$ , as boundary values for unknown coefficients determination.

The mechanical displacements and the electric potential are determined by expressions (51) and (41) respectively, and for the stress tensor and for electric displacement the following expressions are valid:

$$T_{1j} = c_{1jk1} \frac{\partial u_k}{\partial x_1} + e_{11j} \frac{\partial \varphi}{\partial x_1} = \sum_n \beta_j^{(n)} \bar{c}^{(n)} \alpha^{(n)} \omega [-A^{(n)} \sin(\alpha^{(n)} \omega x_1) + B^{(n)} \cos(\alpha^{(n)} \omega x_1)] + e_{11j} \phi_1 \quad (52)$$

$$D_1 = e_{11k} \frac{\partial u_k}{\partial x_1} - \varepsilon_{11} \frac{\partial \varphi}{\partial x_1} = -\varepsilon_{11} \phi_1 \quad (53)$$

Substituting  $x_1 = 0$  into (41) and (51) – (53), we get the following eight equations for determination of  $A^{(n)}$ ,  $B^{(n)}$ ,  $\phi_0$ , and  $\phi_1$ :

$$u_j(0) = \sum_n \beta_j^{(n)} A^{(n)} \quad T_{1j}(0) = \sum_n \beta_j^{(n)} \bar{c}^{(n)} \alpha^{(n)} \omega B^{(n)} + e_{11j} \phi_1 \quad (54)$$

$$D_1(0) = -\varepsilon_{11} \phi_1 \quad \varphi(0) = \frac{e_{11k}}{\varepsilon_{11}} u_k(0) + \phi_0 \quad (55)$$

Solving this system (taking into account the completeness and the orthogonality conditions (49)), we can get all the unknown coefficients:

$$A^{(n)} = \beta_k^{(n)} u_k(0) \quad B^{(n)} = \frac{1}{\bar{c}^{(n)} \alpha^{(n)} \omega} \beta_j^{(n)} \left[ T_{1j}(0) + \frac{e_{11j}}{\varepsilon_{11}} D_1(0) \right] \quad \phi_0 = \varphi(0) - \frac{e_{11k}}{\varepsilon_{11}} u_k(0) \quad \phi_1 = -\frac{1}{\varepsilon_{11}} D_1(0) \quad (56)$$

These coefficients (with using (41), (51) – (53)) give the possibility to obtain all the values  $u_j$ ,  $T_{1j}$ ,  $D_1$ , and  $\varphi$  for any coordinate  $x_1$ , if these values are known for  $x_1 = 0$  coordinate.

Let us consider in particular the single layer of thickness  $l$ , infinite in lateral directions – see Fig. 4.

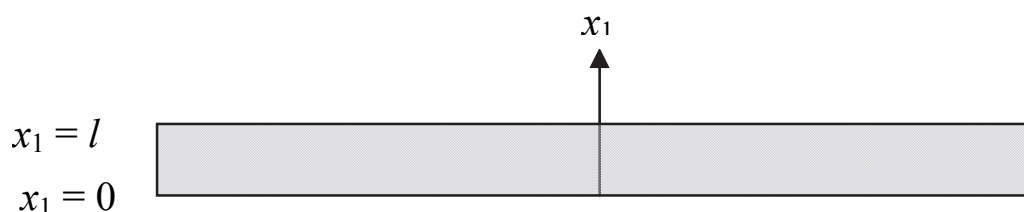


Fig. 4. The single layer of thickness  $l$ .

All the values  $u_j$ ,  $T_{1j}$ ,  $D_1$ , and  $\varphi$  for coordinate  $x_1 = l$  can be expressed as a linear combination of these values for coordinate  $x_1 = 0$  in the following matrix form:

$$\begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ T_{11} \\ T_{12} \\ T_{13} \\ \varphi \\ D_1 \end{pmatrix}_{x_1=l} = \begin{pmatrix} M_{11}^{uu} & M_{12}^{uu} & M_{13}^{uu} & M_{11}^{uT} & M_{12}^{uT} & M_{13}^{uT} & 0 & M_1^{uD} \\ M_{21}^{uu} & M_{22}^{uu} & M_{23}^{uu} & M_{21}^{uT} & M_{22}^{uT} & M_{23}^{uT} & 0 & M_2^{uD} \\ M_{31}^{uu} & M_{32}^{uu} & M_{33}^{uu} & M_{31}^{uT} & M_{32}^{uT} & M_{33}^{uT} & 0 & M_3^{uD} \\ M_{11}^{Tu} & M_{12}^{Tu} & M_{13}^{Tu} & M_{11}^{TT} & M_{12}^{TT} & M_{13}^{TT} & 0 & M_1^{TD} \\ M_{21}^{Tu} & M_{22}^{Tu} & M_{23}^{Tu} & M_{21}^{TT} & M_{22}^{TT} & M_{23}^{TT} & 0 & M_2^{TD} \\ M_{31}^{Tu} & M_{32}^{Tu} & M_{33}^{Tu} & M_{31}^{TT} & M_{32}^{TT} & M_{33}^{TT} & 0 & M_3^{TD} \\ M_1^{\varphi u} & M_2^{\varphi u} & M_3^{\varphi u} & M_1^{\varphi T} & M_2^{\varphi T} & M_3^{\varphi T} & 1 & M^{\varphi D} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ T_{11} \\ T_{12} \\ T_{13} \\ \varphi \\ D_1 \end{pmatrix}_{x_1=0} = \mathbf{M} \cdot \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ T_{11} \\ T_{12} \\ T_{13} \\ \varphi \\ D_1 \end{pmatrix}_{x_1=0} \quad (57)$$

Here 8x8 matrix  $\mathbf{M}$  is the transfer matrix of the single layer. This matrix allows to calculate the values  $u_j$ ,  $T_{1j}$ ,  $D_1$ , and  $\varphi$  on one surface of the layer via these values on another surface. The elements of the transfer matrix are defined by wave equations solutions (i.e. by material properties of the layer) by such a manner:

$$M_{ij}^{uu} = M_{ij}^{TT} = \sum_n \beta_i^{(n)} \beta_j^{(n)} \cos(\alpha^{(n)} \omega l) \quad M_{ij}^{uT} = \frac{1}{\rho \omega} \sum_n \beta_i^{(n)} \beta_j^{(n)} \alpha^{(n)} \sin(\alpha^{(n)} \omega l) \quad (58)$$

$$M_{ij}^{Tu} = -\rho \omega \sum_n \beta_i^{(n)} \beta_j^{(n)} v^{(n)} \sin(\alpha^{(n)} \omega l) \quad M_i^{uD} = M_i^{\varphi T} = \frac{1}{\omega \sqrt{\rho \varepsilon_{11}}} \sum_n \beta_i^{(n)} k^{(n)} \sin(\alpha^{(n)} \omega l) \quad (59)$$

$$M_i^{TD} = M_i^{\varphi u} = -2 \sqrt{\frac{\rho}{\varepsilon_{11}}} \sum_n \beta_i^{(n)} k^{(n)} v^{(n)} \sin^2 \frac{\alpha^{(n)} \omega l}{2} \quad M^{\varphi D} = -\frac{l}{\varepsilon_{11}} \left[ 1 - \frac{1}{\omega l} \sum_n k^{(n)2} v^{(n)} \sin(\alpha^{(n)} \omega l) \right] \quad (60)$$

Here

$$k^{(n)} = \frac{\beta_j^{(n)} e_{11j}}{\sqrt{c} \varepsilon_{11}} \quad (61)$$

In expressions (58) – (61)  $i, j = 1, 2, 3$  (a number of the coordinate axis),  $n = 1, 2, 3$  (a number of the partial solution of the wave equations). The values  $k^{(n)}$ , given by (61), are the dimensionless scalar coupling coefficients ( $k^{(n)}$  are nonzero only for piezoelectric medium). One can see from the previous equations that the transfer matrix approaches to the unit matrix if the layer thickness  $l \rightarrow 0$ .

If a layer is nonpiezoelectric dielectric, all the elements of its transfer matrix, containing the value  $k^{(n)}$ , are zero, excepting  $M^{\varphi D}$ , and the transfer matrix of the nonpiezoelectric dielectric layer has a simpler form:

$$\mathbf{M} = \begin{pmatrix} M_{11}^{uu} & M_{12}^{uu} & M_{13}^{uu} & M_{11}^{uT} & M_{12}^{uT} & M_{13}^{uT} & 0 & 0 \\ M_{21}^{uu} & M_{22}^{uu} & M_{23}^{uu} & M_{21}^{uT} & M_{22}^{uT} & M_{23}^{uT} & 0 & 0 \\ M_{31}^{uu} & M_{32}^{uu} & M_{33}^{uu} & M_{31}^{uT} & M_{32}^{uT} & M_{33}^{uT} & 0 & 0 \\ M_{11}^{Tu} & M_{12}^{Tu} & M_{13}^{Tu} & M_{11}^{TT} & M_{12}^{TT} & M_{13}^{TT} & 0 & 0 \\ M_{21}^{Tu} & M_{22}^{Tu} & M_{23}^{Tu} & M_{21}^{TT} & M_{22}^{TT} & M_{23}^{TT} & 0 & 0 \\ M_{31}^{Tu} & M_{32}^{Tu} & M_{33}^{Tu} & M_{31}^{TT} & M_{32}^{TT} & M_{33}^{TT} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & M^{\varphi D} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \tag{62}$$

For a metal layer in an electrostatic approximation the electric potential is always the same on both its surfaces, therefore  $M^{\varphi D} = 0$  for metal layer and the transfer matrix of the metal layer has the simplest form:

$$\mathbf{M} = \mathbf{M}_{Em} = \begin{pmatrix} M_{11}^{uu} & M_{12}^{uu} & M_{13}^{uu} & M_{11}^{uT} & M_{12}^{uT} & M_{13}^{uT} & 0 & 0 \\ M_{21}^{uu} & M_{22}^{uu} & M_{23}^{uu} & M_{21}^{uT} & M_{22}^{uT} & M_{23}^{uT} & 0 & 0 \\ M_{31}^{uu} & M_{32}^{uu} & M_{33}^{uu} & M_{31}^{uT} & M_{32}^{uT} & M_{33}^{uT} & 0 & 0 \\ M_{11}^{Tu} & M_{12}^{Tu} & M_{13}^{Tu} & M_{11}^{TT} & M_{12}^{TT} & M_{13}^{TT} & 0 & 0 \\ M_{21}^{Tu} & M_{22}^{Tu} & M_{23}^{Tu} & M_{21}^{TT} & M_{22}^{TT} & M_{23}^{TT} & 0 & 0 \\ M_{31}^{Tu} & M_{32}^{Tu} & M_{33}^{Tu} & M_{31}^{TT} & M_{32}^{TT} & M_{33}^{TT} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \tag{63}$$

The designation “ $\mathbf{M}_{Em}$ ” will be explained further.  
Now we can consider a multilayer system. Fig. 5 shows a multilayer structure with arbitrary quantity N of arbitrary layers.

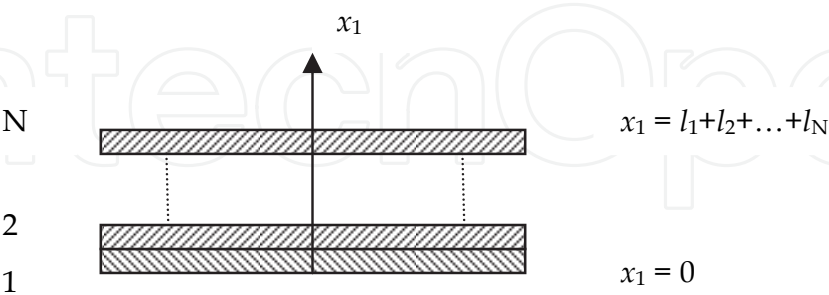


Fig. 5. Multilayer structure.

For multilayer structure the “output” values  $u_j$ ,  $T_{1j}$ ,  $D_1$  and  $\varphi$  of the first layer are the “input” values for the second layer and so on. Therefore the transfer matrix of the multilayer structure is a multiplication of the transfer matrices of each layer:

$$\mathbf{M} = \mathbf{M}_N \cdot \ldots \cdot \mathbf{M}_2 \cdot \mathbf{M}_1 \tag{64}$$

The factors sequence must be namely such, as in (64), any transposition is impossible in general case, because  $A \cdot B \neq B \cdot A$  for a matrices multiplication in general case. The matrix  $\mathbf{M}$  in (64) transfers the values  $u_j$ ,  $T_{1j}$ ,  $D_1$  and  $\varphi$  from the surface  $x_1 = 0$  (bottom) to the surface  $x_1 = l_1 + l_2 + \dots + l_N$  (top).

All the layers may be arbitrary (piezoelectric, dielectric, metal), but if the layer is used as an electrode, its transfer matrix differs from matrices, described above. It is obviously, that only the metal layer can be used as an electrode. Therefore all the mechanical values and the electric potential of the electrode are transferred by the matrix (63). If the metal layer is not connected to the electric source and is electrically neutral, the matrix (63) transfer the normal component of the electric displacement correctly too, i.e.  $(D_1)_{x_1=l} = (D_1)_{x_1=0}$  (but not inside the metal layer, where  $D_1 = 0$ ). But if the metal layer is connected to the electric source and is used as an electrode, a discontinuity of the value  $D_1$  takes place which is not represented in the matrix (63).

Therefore the special consideration is needed for electrodes. Fig. 6 shows two electrodes, connected to an external harmonic voltage source with an amplitude  $V$  and a frequency  $\omega$ .

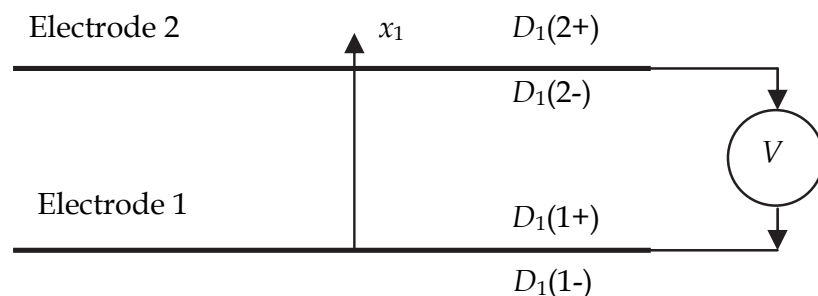


Fig. 6. Two electrodes, connected to an external harmonic voltage source with amplitude  $V$  and frequency  $\omega$ .

First we will consider electrodes of zero thickness. Therefore all the mechanical values are transferred without changes (electric potential is transferred without changes always by metal layer of any thickness).

Values  $D_1(1-)$  and  $D_1(1+)$  on both sides of the first electrode are different, for the second electrode analogously. The difference  $D_1(1+) - D_1(1-)$  is equal to the electric charge per unit area of the electrode (in the SI system). A time derivative of this value is the current density. Its multiplication on the electrode area  $A$  gives the total electrode current. For a harmonic signal the time derivative equivalent to a multiplication on  $i\omega$ . As a result the following expression takes place for a current  $I_1$  of the electrode 1:

$$I_1 = i\omega A[D_1(1+) - D_1(1-)] \quad (65)$$

For electrode 2 analogously. If there are only two electrodes connected to one electric source, then  $I = I_1 = -I_2$  and:

$$I = VY, \quad (66)$$

where  $V = \varphi_1 - \varphi_2$  ( $\varphi_1$  and  $\varphi_2$  are electrode potentials) and  $Y$  is an admittance of two electrodes for the external electric source.

We are free in determining the zero point of the electric potential  $\varphi$  and we can choose it so:

$$\varphi_1 + \varphi_2 = 0, \quad \text{i.e. } V = 2\varphi_1 = -2\varphi_2 \quad (67)$$



As a result, we can obtain from (65) and (66):

$$D_1(1+)=\frac{2Y}{i\omega A}\varphi_1+D_1(1-)\tag{68}$$

which expresses the value of  $D_1$  at the upper side of the electrode as a linear function of the values of  $\varphi$  and  $D_1$  at the lower side ( $\varphi$  has the same value on both sides of an electrode). It means that the transfer matrix of the electrode of zero thickness (an ideal electrode) has a following form:

$$\mathbf{M}_{\text{Ee}}=\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{2Y}{i\omega A} & 1 \end{pmatrix}\tag{69}$$

The metal electrode of a finite thickness (a real electrode) can be presented as a combination of two layers, one of which is the metal electrode of a zero thickness (an ideal electrode), transferring only electric values, and another one is a layer of a finite thickness, transferring only the mechanical values (mechanical layer) - see Fig. 7.

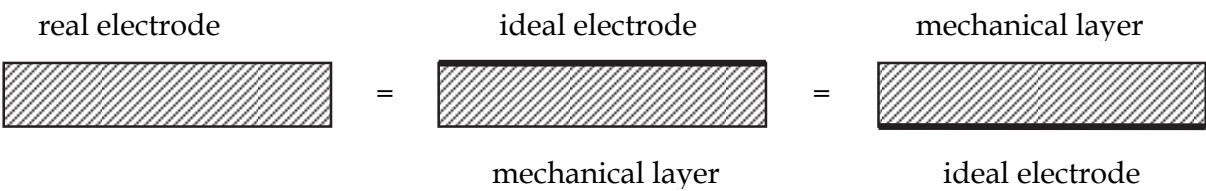


Fig. 7. Representation of a real electrode as a combination of an ideal electrode and a mechanical layer.

Therefore we can obtain the whole transfer matrix of the real electrode as a multiplication of a matrix of the ideal electrode (69) and a matrix, transferring only mechanical values and presented by expression (63):

$$\mathbf{M}_{\text{E}}=\mathbf{M}_{\text{Ee}}\cdot\mathbf{M}_{\text{Em}}=\mathbf{M}_{\text{Em}}\cdot\mathbf{M}_{\text{Ee}}\tag{70}$$

As it was mentioned above, the matrices don't obey the commutative law in general case, but in this concrete case one can transpose these two matrices, what can be checked by direct multiplication. This means, in particular, that an ideal electrode can be placed on any side of the read electrode, as shown in Fig. 7. Physically more correctly to place the ideal electrode on the side which is a face of contact with the interelectrode space. As a result, the multilayer bulk acoustic wave resonator, containing arbitrary quantity of arbitrary layers, but only with two electrodes, has a view, presented in Fig. 8.

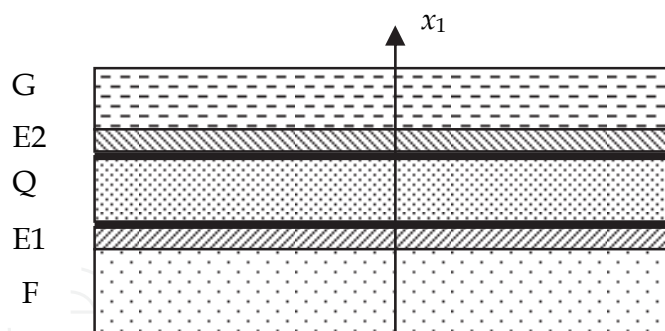


Fig. 8. Multilayer bulk acoustic wave resonator with two electrodes.

Here F is a combination of arbitrary quantity of arbitrary layers under electrodes, G is the same above electrodes, Q is the same between electrodes (at least one of layers in Q must be piezoelectric), E1 and E2 are the two electrodes of a finite thickness.

All the eight values  $u_j$ ,  $T_{1j}$ ,  $D_1$  and  $\varphi$  are transferring from a lower surface of the whole construction to its upper surface by the whole transfer matrix, which is the multiplication of transfer matrices of each elements:

$$\mathbf{M}_{FE1QE2G} = \mathbf{M}_G \cdot \mathbf{M}_{E2} \cdot \mathbf{M}_Q \cdot \mathbf{M}_{E1} \cdot \mathbf{M}_F \quad (71)$$

Transfer matrices  $\mathbf{M}_F$ ,  $\mathbf{M}_Q$ ,  $\mathbf{M}_G$  are calculated by (64) and matrices  $\mathbf{M}_{E1}$  and  $\mathbf{M}_{E2}$  – by (70).

Because of electrodes presence the total transfer matrix of the whole resonator  $\mathbf{M}_{FE1QE2G}$  does not have generally the special form with 0 and 1 in the 7<sup>th</sup> column and the 8<sup>th</sup> row (as in (57)), but it is of the most general form:

$$\mathbf{M}_{FE1QE2G} = \begin{pmatrix} M_{11}^{uu} & M_{12}^{uu} & M_{13}^{uu} & M_{11}^{uT} & M_{12}^{uT} & M_{13}^{uT} & M_1^{u\varphi} & M_1^{uD} \\ M_{21}^{uu} & M_{22}^{uu} & M_{23}^{uu} & M_{21}^{uT} & M_{22}^{uT} & M_{23}^{uT} & M_2^{u\varphi} & M_2^{uD} \\ M_{31}^{uu} & M_{32}^{uu} & M_{33}^{uu} & M_{31}^{uT} & M_{32}^{uT} & M_{33}^{uT} & M_3^{u\varphi} & M_3^{uD} \\ M_{11}^{Tu} & M_{12}^{Tu} & M_{13}^{Tu} & M_{11}^{TT} & M_{12}^{TT} & M_{13}^{TT} & M_1^{T\varphi} & M_1^{TD} \\ M_{21}^{Tu} & M_{22}^{Tu} & M_{23}^{Tu} & M_{21}^{TT} & M_{22}^{TT} & M_{23}^{TT} & M_2^{T\varphi} & M_2^{TD} \\ M_{31}^{Tu} & M_{32}^{Tu} & M_{33}^{Tu} & M_{31}^{TT} & M_{32}^{TT} & M_{33}^{TT} & M_3^{T\varphi} & M_3^{TD} \\ M_1^{\varphi u} & M_2^{\varphi u} & M_3^{\varphi u} & M_1^{\varphi T} & M_2^{\varphi T} & M_3^{\varphi T} & M^{\varphi\varphi} & M^{\varphi D} \\ M_1^{Du} & M_2^{Du} & M_3^{Du} & M_1^{DT} & M_2^{DT} & M_3^{DT} & M^{D\varphi} & M^{DD} \end{pmatrix} \quad (72)$$

The expressions, obtained above, allow to calculate the admittance of the resonator  $Y$  which is its main work characteristic.

The zero boundary conditions for  $T_{1j}$  and  $D_1$  on the external free lower and upper surfaces of the construction are used for these calculations:

$$T_{11} = 0, T_{12} = 0, T_{13} = 0, D_1 = 0 \quad \text{on free surfaces} \quad (73)$$

The normal components of a stress tensor are equal to zero because lower and upper surfaces are free, the electric displacement is zero because the electric field of the external source is concentrated only between two electrodes (between their inner surfaces).

Let us denote the mechanical displacements and the electric potential on the lower free surface as  $u_1^{(1)}, u_2^{(1)}, u_3^{(1)}, \varphi^{(1)}$  and the same values on the upper free surface as  $u_1^{(2)}, u_2^{(2)}, u_3^{(2)}, \varphi^{(2)}$ . Then with taking into account (73) these values will be connected each other by the transfer matrix  $\mathbf{M}_{\text{FE1QE2G}}$  by the following expression:

$$\begin{pmatrix} u_1^{(2)} \\ u_2^{(2)} \\ u_3^{(2)} \\ 0 \\ 0 \\ 0 \\ \varphi^{(2)} \\ 0 \end{pmatrix} = \begin{pmatrix} M_{11}^{uu} & M_{12}^{uu} & M_{13}^{uu} & M_{11}^{uT} & M_{12}^{uT} & M_{13}^{uT} & M_1^{u\varphi} & M_1^{uD} \\ M_{21}^{uu} & M_{22}^{uu} & M_{23}^{uu} & M_{21}^{uT} & M_{22}^{uT} & M_{23}^{uT} & M_2^{u\varphi} & M_2^{uD} \\ M_{31}^{uu} & M_{32}^{uu} & M_{33}^{uu} & M_{31}^{uT} & M_{32}^{uT} & M_{33}^{uT} & M_3^{u\varphi} & M_3^{uD} \\ M_{11}^{Tu} & M_{12}^{Tu} & M_{13}^{Tu} & M_{11}^{TT} & M_{12}^{TT} & M_{13}^{TT} & M_1^{T\varphi} & M_1^{TD} \\ M_{21}^{Tu} & M_{22}^{Tu} & M_{23}^{Tu} & M_{21}^{TT} & M_{22}^{TT} & M_{23}^{TT} & M_2^{T\varphi} & M_2^{TD} \\ M_{31}^{Tu} & M_{32}^{Tu} & M_{33}^{Tu} & M_{31}^{TT} & M_{32}^{TT} & M_{33}^{TT} & M_3^{T\varphi} & M_3^{TD} \\ M_1^{\varphi u} & M_2^{\varphi u} & M_3^{\varphi u} & M_1^{\varphi T} & M_2^{\varphi T} & M_3^{\varphi T} & M^{\varphi\varphi} & M^{\varphi D} \\ M_1^{Du} & M_2^{Du} & M_3^{Du} & M_1^{DT} & M_2^{DT} & M_3^{DT} & M^{D\varphi} & M^{DD} \end{pmatrix} \begin{pmatrix} u_1^{(1)} \\ u_2^{(1)} \\ u_3^{(1)} \\ 0 \\ 0 \\ 0 \\ \varphi^{(1)} \\ 0 \end{pmatrix} \quad (74)$$

From here we can write for the 4<sup>th</sup> – 6<sup>th</sup> rows separately and for the 8<sup>th</sup> row separately:

$$\begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} M_{11}^{Tu} & M_{12}^{Tu} & M_{13}^{Tu} \\ M_{21}^{Tu} & M_{22}^{Tu} & M_{23}^{Tu} \\ M_{31}^{Tu} & M_{32}^{Tu} & M_{33}^{Tu} \end{pmatrix} \cdot \begin{pmatrix} u_1^{(1)} \\ u_2^{(1)} \\ u_3^{(1)} \end{pmatrix} + \begin{pmatrix} M_1^{T\varphi} \\ M_2^{T\varphi} \\ M_3^{T\varphi} \end{pmatrix} \cdot \varphi^{(1)} \quad 0 = (M_1^{Du} \quad M_2^{Du} \quad M_3^{Du}) \cdot \begin{pmatrix} u_1^{(1)} \\ u_2^{(1)} \\ u_3^{(1)} \end{pmatrix} + M^{D\varphi} \cdot \varphi^{(1)} \quad (75)$$

We can obtain the vector  $u_1^{(1)}, u_2^{(1)}, u_3^{(1)}$  from the first equation (75) (using the standard inverse matrix designation):

$$\begin{pmatrix} u_1^{(1)} \\ u_2^{(1)} \\ u_3^{(1)} \end{pmatrix} = - \begin{pmatrix} M_{11}^{Tu} & M_{12}^{Tu} & M_{13}^{Tu} \\ M_{21}^{Tu} & M_{22}^{Tu} & M_{23}^{Tu} \\ M_{31}^{Tu} & M_{32}^{Tu} & M_{33}^{Tu} \end{pmatrix}^{-1} \cdot \begin{pmatrix} M_1^{T\varphi} \\ M_2^{T\varphi} \\ M_3^{T\varphi} \end{pmatrix} \cdot \varphi^{(1)} \quad (76)$$

Now we can substitute this into the second equation (75) and obtain:

$$0 = - (M_1^{Du} \quad M_2^{Du} \quad M_3^{Du}) \cdot \begin{pmatrix} M_{11}^{Tu} & M_{12}^{Tu} & M_{13}^{Tu} \\ M_{21}^{Tu} & M_{22}^{Tu} & M_{23}^{Tu} \\ M_{31}^{Tu} & M_{32}^{Tu} & M_{33}^{Tu} \end{pmatrix}^{-1} \cdot \begin{pmatrix} M_1^{T\varphi} \\ M_2^{T\varphi} \\ M_3^{T\varphi} \end{pmatrix} \cdot \varphi^{(1)} + M^{D\varphi} \cdot \varphi^{(1)} \quad (77)$$

In an arbitrary case  $\varphi^{(1)} \neq 0$ , therefore we obtain from (77) the follow scalar equation:

$$(M_1^{Du} \quad M_2^{Du} \quad M_3^{Du}) \cdot \begin{pmatrix} M_{11}^{Tu} & M_{12}^{Tu} & M_{13}^{Tu} \\ M_{21}^{Tu} & M_{22}^{Tu} & M_{23}^{Tu} \\ M_{31}^{Tu} & M_{32}^{Tu} & M_{33}^{Tu} \end{pmatrix}^{-1} \cdot \begin{pmatrix} M_1^{T\varphi} \\ M_2^{T\varphi} \\ M_3^{T\varphi} \end{pmatrix} - M^{D\varphi} = 0 \quad (78)$$

This is the main equation of the problem. It connects the resonator admittance  $Y$  with the frequency  $\omega$ , because  $Y$  value is contained in the transfer matrices of electrodes. We can set

the concrete value of  $\omega$  and calculate from (78) the corresponding value of  $Y$ , i.e. we can obtain the frequency response of the resonator – its main work characteristic. Matrix elements in (78) are elements of the total transfer matrix of the whole device – see (72).

In an arbitrary case the equation (78) cannot be solved analytically. The solution can be found only by some numerical method. We used our own algorithm of searching for the global extremum of a function of several variables (Dvoesherstov et. al., 1999). Solution corresponds to the global minimum of the square of the absolute value of the left part of the equation (78). Two arguments of this function are the real and imaginary parts of the admittance  $Y$  (for each given frequency).

If there is not any piezoelectric layer in the packets  $F$  and  $G$  outside the electrodes, the transfer matrices of these packets have the simpler form (62) and the equation (78) can be solved analytically in the following view:

$$\frac{i\omega A}{Y} = (M_Q^{\phi T} \cdot M_F'' + M_Q^{\phi u}) \cdot [M_G'' \cdot M_Q^{uu} + M_Q^{TT} \cdot M_F'' + M_Q^{Tu} + M_G'' \cdot M_Q^{uT} \cdot M_F'']^{-1} \cdot (M_G'' \cdot M_Q^{uD} + M_Q^{TD}) - M_Q^{\phi D} \quad (79)$$

Here the compressed form of matrices is used for compactness. For example,  $M_Q^{uu}$  means the 3x3 matrix including the first 3 columns and the first 3 rows of the 8x8 matrix,  $M_Q^{uT}$  means the 3x3 matrix including the columns 4 – 6 and the first 3 rows of the 8x8 matrix,  $M_Q^{\phi T}$  means the 1x3 matrix including the columns 4 – 6 and the 7th row of the 8x8 matrix, and so on. Index  $Q$  means that all these elements are taken from transfer matrix of the  $Q$  packet (not for the whole device).  $M_F''$  and  $M_G''$  are 3x3 matrices, obtained as follows:

$$M_F'' = (M_{E1m} \cdot M_F)^{Tu} \cdot [(M_{E1m} \cdot M_F)^{uu}]^{-1} \quad M_G'' = [(M_G \cdot M_{E2m})^{TT}]^{-1} \cdot (M_G \cdot M_{E2m})^{Tu} \quad (80)$$

In these expressions the lower indexes  $F$  and  $G$  also designate the corresponding packets,  $M_F$  and  $M_G$  are the whole 8x8 matrices of the corresponding packets,  $M_{E1m}$  and  $M_{E2m}$  – the “mechanical” parts of the electrodes 8x8 matrices and upper indexes  $uu$ ,  $Tu$ ,  $uT$  and  $TT$  means that corresponding 3x3 matrices are taken from whole 8x8 matrices.

Practically all the concrete FBAR devices do not contain piezoelectric layers outside the electrodes, i.e. practically for all these devices the frequency response can be calculated with expressions (79) – (80).

But not only the frequency response can be calculated by the technique, described here. The expression (57) allows to calculate all eight values  $u_j$ ,  $T_{1j}$ ,  $D_1$  and  $\phi$  not only on the second surface of the layer but also for any coordinate  $x_1$  inside the layer, if these eight values are known for the first “input” surface of this layer. These values on the second “output” surface of the first layer can be used as “input” values for the second layer for the same calculations for any coordinate  $x_1$  inside the second layer and so on, i.e. the spatial distribution of all eight values inside the whole multilayer system can be obtained. As was mentioned above, the values on the first “input” surface of the first layer must be known for such calculations (for frequency response calculations all eight values on the first surface of the first layer are not needed).

Four of eight values, namely,  $T_{1j}$  and  $D_1$  are known, they are zero – see (73). The absolute value of the electric potential is not essential from point of view of the spatial distribution of all eight values. We can set any (but not zero) value of the electric potential on the first surface of the first layer, for instance  $\phi^{(1)} = -1$  V. Then we can obtain all three values of the mechanical displacements  $u_1^{(1)}, u_2^{(1)}, u_3^{(1)}$  from the equation (76). So all eight values on the

first surface of the first layer are determined and the spatial distribution of all these values can be obtained for any multilayer resonator with two electrodes. The admittance  $Y$  for given frequency  $\omega$  must be calculated preliminary, because both these values are needed for the spatial distribution calculation.

The spatial distribution gives a possibility to obtain some information about physical wave processes those take place inside the multilayer structure, in particular - how the Bragg reflector “works”.

Fig. 9 shows the frequency response of the membrane type resonator (as in Fig. 3a), obtained by technique, described above. The mass density of all the materials are taken in a form  $(1 + i\delta)\rho$ , where  $\delta = -0.001$  in this case. The frequency response is calculated for two variants of the Al electrode thickness - zero and  $0.1\text{ }\mu\text{m}$ .

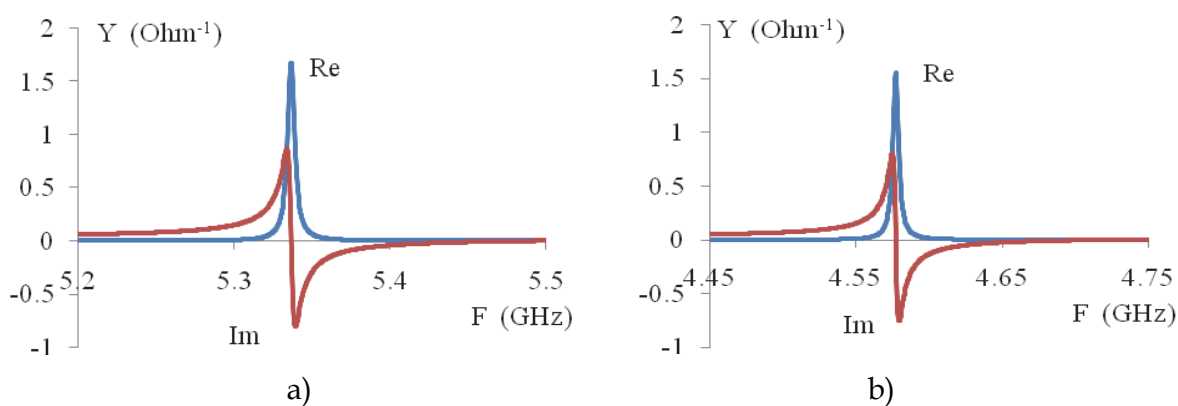


Fig. 9. Frequency response of the membrane type resonator. Active layer - AlN, thickness  $1\text{ }\mu\text{m}$ . a) - zero electrode thickness,  $F_{\text{res}} = 5.337\text{ GHz}$ , b) - Al electrode thickness  $0.1\text{ }\mu\text{m}$ ,  $F_{\text{res}} = 4.577\text{ GHz}$ . Electrode area  $0.01\text{ mm}^2$ .

Fig. 9 illustrates an influence of the electrode thickness on a resonance frequency (this frequency is obtained directly from a graphic as coordinate of a maximum of a  $Y$  real part). The resonance frequency is decreased by the electrodes of a finite thickness, because the whole device with more total thickness corresponds to more half-wavelength. This illustrates Fig. 10 in which the spatial distribution of the  $T_{11}$  component of the stress tensor is shown, obtained also by a technique, described above.

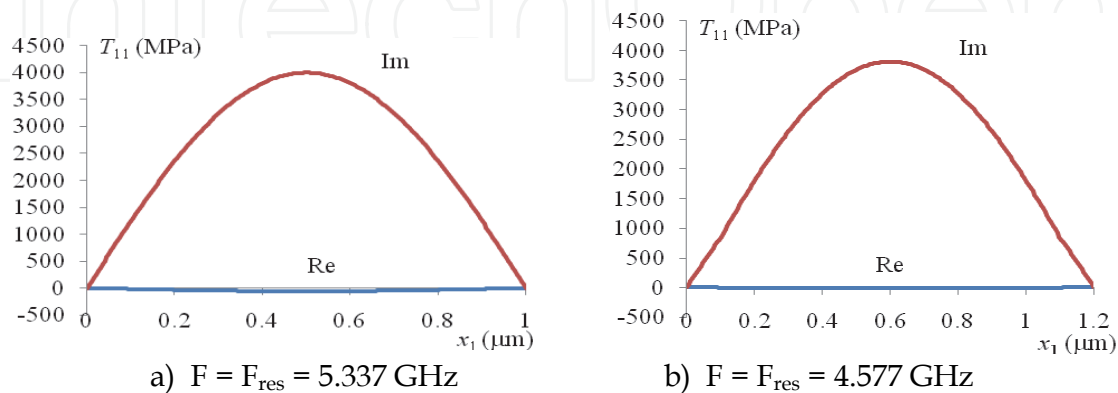


Fig. 10. Spatial distribution of  $T_{11}$  component of the stress tensor for two variants, shown in Fig. 9.  $F = F_{\text{res}}$  in both cases.

A half-wavelength corresponds to a distance between neighbouring points with zero stress. In a case a) this distance is  $1\text{ }\mu\text{m}$  and corresponds to a resonance frequency  $5.337\text{ GHz}$ , whereas in a case b) a half-wavelength is equal to  $1.2\text{ }\mu\text{m}$  and corresponds to a lower frequency  $4.577\text{ GHz}$ . This gives a possibility to control the resonance frequency by changing of the top electrode thickness. For example, Fig. 11 shows dependences of the resonance frequency on a top electrode thickness for two materials of this electrode – Al and Au. The bottom electrode is Al of a thickness  $0.1\text{ }\mu\text{m}$  in both cases.

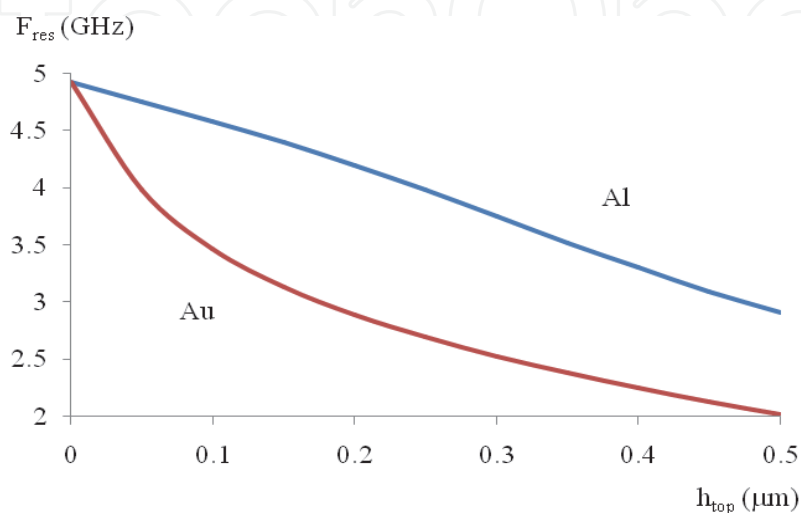


Fig. 11. Dependences of the resonance frequency on the top electrode tickness for Al and Au. The bottom electrode is Al ( $0.1\text{ }\mu\text{m}$ ) in both cases. The thickness of AlN is  $1\text{ }\mu\text{m}$ .

For displaying of the possibilities of the described method Fig. 12 shows also the spatial distributions of the longitudinal component of the displacement  $u_1$  and the electric potential  $\varphi$  for the membrane type resonator, corresponding to Figs. 9b and 10b.

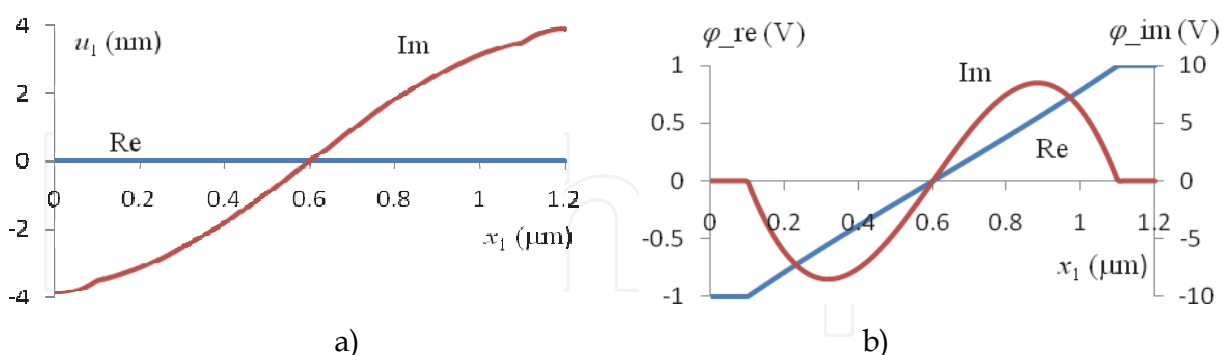


Fig. 12. Spatial distribution of the longitudinal component of the displacement  $u_1$  (a) and the electric potential  $\varphi$  (b) for the membrane type resonator with Al electrodes of finite thickness  $0.1\text{ }\mu\text{m}$ .

Distribution of  $D_1$  is not shown here because it is very simple –  $D_1 = \text{const}$  between the electrodes and equal to zero outside the inner surfaces of the electrodes.

If membrane type resonator is placed on the substrate of not very large thickness, then multiple modes appear, and this resonator can be a multi-frequency resonator, as shown in Fig. 13a.

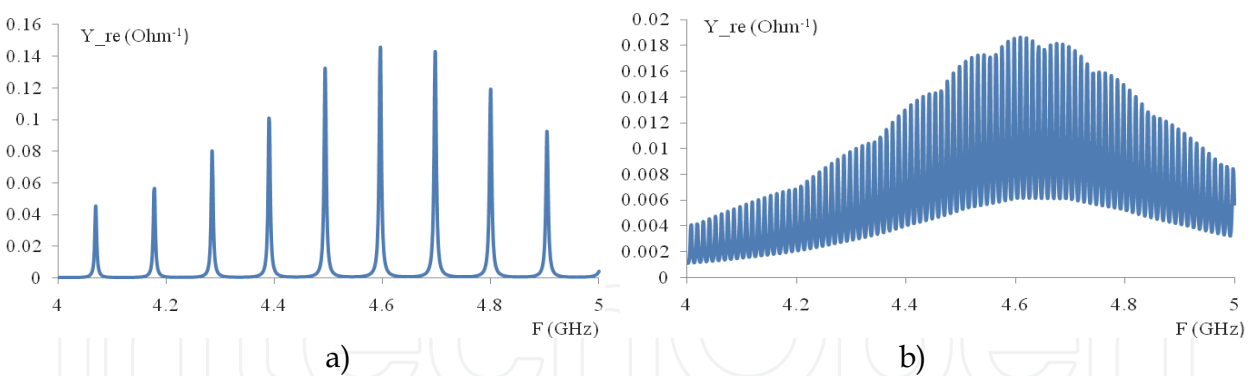


Fig. 13. FBAR membrane type resonator on a Si substrate of thickness  $100\ \mu\text{m}$  (a) and  $1000\ \mu\text{m}$  (b). Electrodes – Al, thickness  $0.1\ \mu\text{m}$ , active layer – AlN, thickness  $1\ \mu\text{m}$ .

But if the substrate is too thick, there are too many modes and the resonator transforms from multi-mode actually into a “not any mode” resonator, as one can see in Fig. 13b. So, the membrane type resonator cannot be placed on the massive substrate directly because of an acoustic interaction with this substrate. One must to provide an acoustic isolation between an active zone of the resonator and a substrate. One of techniques of such isolation is a Bragg reflector between the active zone and the substrate (as shown in Fig. 3b). This reflector contains several pairs of materials with different acoustic properties. The difference of the acoustic properties of two materials in a pair must not be small. Acoustic properties of materials, used for Bragg reflector, are characterized by a value  $\rho V$ , where  $\rho$  is a mass density and  $V$  is a velocity. Values  $\rho V$  are shown in Fig. 14 for some isotropic materials. Material constants are taken from (Ballandras et. al., 1997).

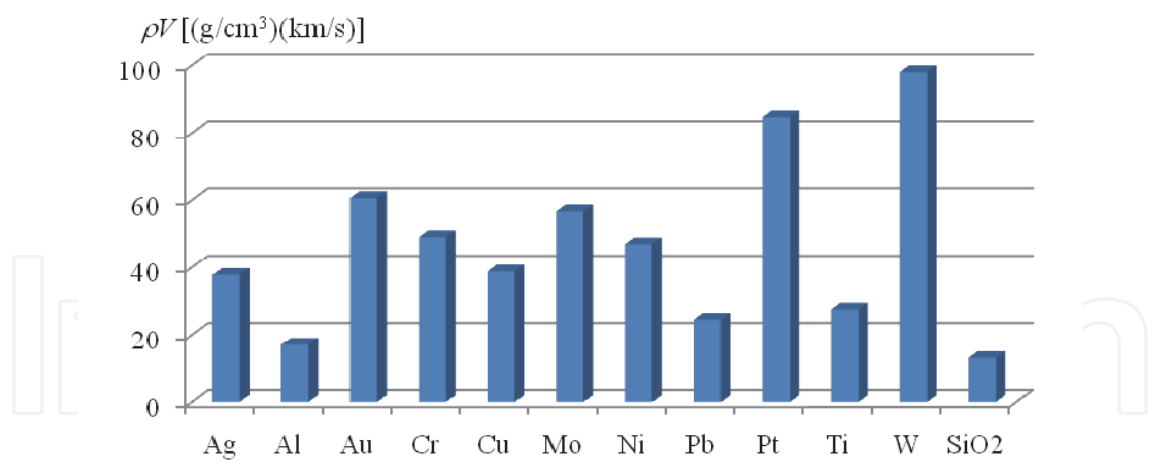


Fig. 14. The value  $\rho V$  for some isotropic materials.

As one can see in Fig. 14, the best combination for a Bragg reflector is SiO<sub>2</sub>/W. A pair Ti/W is good too, and a combination Ti/Mo also can be used successfully (combinations of Au or Pt with other materials also can be not bad, but not cheap). The thickness of each layer of the reflector must be equal to a quarter-wavelength in a material of the layer for a resonance frequency. As it was mentioned above, the resonance frequency is defined mainly by the active layer thickness and can be adjusted by proper choice of the top electrode thickness.



The computation technique, based on the described here rigorous solution of the wave equations, allows to calculate any bulk wave resonators with any quantity of any layers, including the resonators with Bragg reflector. For example, Fig. 15a shows a frequency response of the resonator, containing an AlN active layer (1  $\mu\text{m}$ ), two Al electrodes (both 0.2  $\mu\text{m}$ ), three pairs of layers SiO<sub>2</sub>/W, and a Si substrate (1000  $\mu\text{m}$ ).

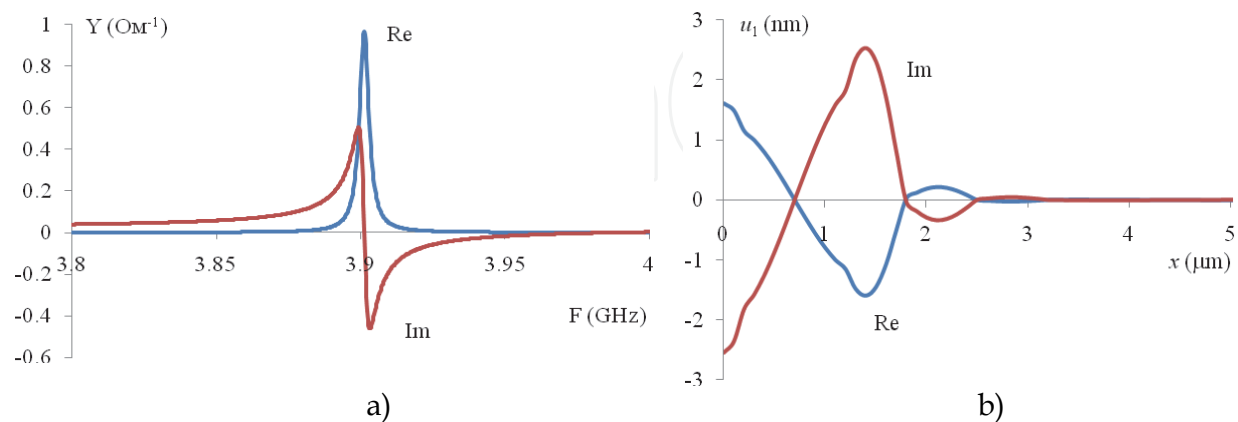


Fig. 15. A frequency response (a) and a distribution of  $u_1$  (b) for a resonator with a Bragg reflector, containing three pairs of layers SiO<sub>2</sub>/W.

A thickness of a Bragg reflector layer is 0.38  $\mu\text{m}$  for SiO<sub>2</sub> and 0.33  $\mu\text{m}$  for W (a quarter-wavelength in a corresponding material for a resonance frequency). Fig. 15a shows, that three pairs of SiO<sub>2</sub>/W combination is quite enough for full acoustic isolation of an active zone and a substrate. A spatial distribution of a wave amplitude illustrates an influence of the Bragg reflector on a wave propagation, for example, Fig. 15b shows this distribution for a longitudinal component of a mechanical displacement. A coordinate axis  $x$  here is directed from a top surface of a top electrode ( $x = 0$ ) towards a substrate. One can see in Fig. 15b that a wave rapidly attenuates in the Bragg reflector and does not reach the substrate. Calculation results show, that the first layer after an electrode must be one with lower value  $\rho V$  – the SiO<sub>2</sub> layer in this case. In a contrary case a reflection will not take place.

If difference of values  $\rho V$  of two layers of each pair is not large enough, then three pairs may not be sufficient for effective reflection. For example, calculations show that three or even four pairs of Ti/Mo layers are not sufficient for suppressing the wave in the substrate. Only five pairs give a desired effect in this case and provide results similar shown in Fig. 15 for SiO<sub>2</sub>/W layers.

So, the described technique allows to calculate any multilayer FBAR resonators, containing any combinations of any quantity of any layers. The main results of these calculations are a frequency response of a resonator and spatial distributions of physical characteristics of the wave (displacement, stress, electric displacement and potential).

In addition this technique gives a possibility to calculate a thermal sensitivity of the resonator too, i.e. an influence a temperature on a resonance frequency. A resonance frequency always changes in general case when a temperature changes. This change is characterized by a temperature coefficient of a frequency:

$$TCF = \frac{1}{F_r} \frac{dF_r}{dT} \quad (81)$$

Here  $T$  is a temperature,  $F_r$  is a resonance frequency.

A computation technique, used here, allows to apply this expression for  $TCF$  calculation directly and to calculate this value by numerical differentiation.

A temperature influence on a resonance frequency is due to three basic causes:

1. A temperature dependence of material constants (stiffness, piezoelectric, dielectric tensors) -  $TCF_c$
2. A temperature dependence of a mass density -  $TCF_p$
3. A temperature dependence of a layer thickness -  $TCF_h$

A temperature dependence of material constants is described by temperature coefficients of these constants, a temperature dependence of a mass density is described by three linear expansion coefficients or by a single bulk expansion coefficient, a temperature dependence of a thickness is described by a linear expansion coefficient along a thickness direction. All these coefficients can be found in a literature, for example, for materials, usually used for FBAR resonators, one can see corresponding values in (Ivira et al., 2008).

First we will consider the simplest variant – a membrane type FBAR resonator with a single AlN layer and infinite thin electrodes. For typical values of AlN temperature coefficients we can easily obtain:

$$TCF = TCF_c + TCF_p + TCF_h = (-29.639 + 7.343 - 5.268) \cdot 10^{-6} / ^\circ\text{C} = -27.564 \cdot 10^{-6} / ^\circ\text{C}$$

One can check by a direct calculation, that this result does not depend on a thickness of AlN layer (for this variant with electrodes of finite thickness and for any multilayer structure with layers of finite thickness it is not so).  $TCF_p$  value is always positive,  $TCF_h$  value is always negative. A sign of  $TCF_c$  is defined mainly by a sign of temperature coefficients of stiffness constants. If temperature coefficients of stiffness constants are negative (for most materials, including AlN), then  $TCF_c$  is negative, if temperature coefficients of some stiffness constants are positive (rare case, for example quartz), then  $TCF_c$  can be positive and a total  $TCF$  can be zero.

For AlN a  $TCF$  value is always negative. Al electrodes aggravate this position, because temperature coefficients of Al stiffness constants are negative too. From this point of view Mo electrodes are more preferable, because absolute values of temperature coefficients of its stiffness constants are significantly less than ones for Al (althouth they are also negative). For example, the concrete membrane type resonator Al/AlN/Al with an Al thickness  $0.2 \mu\text{m}$  and an AlN thickness  $1.1 \mu\text{m}$  we can obtain:  $TCF = -44.23 \cdot 10^{-6} / ^\circ\text{C}$  ( $F_r = 3.648 \text{ GHz}$ ), and for Mo/AlN/Mo resonator with the same geometry:  $TCF = -33.76 \cdot 10^{-6} / ^\circ\text{C}$  ( $F_r = 2.615 \text{ GHz}$ ).

For most applications a resonator must be thermostable, i.e.  $TCF$  must be equal to zero. The single possibility to compensate the negative  $TCF$  of AlN and of electrodes and to provide a total zero  $TCF$  is to add some additional layer with positive temperature coefficients of stiffness constants. Such material is, for example  $\text{SiO}_2$ . Fig. 16 shows dependences of  $TCF$  of membrane type resonator with Mo electrodes on a thickness  $h_t$  of a  $\text{SiO}_2$  layer for two cases:  $\text{SiO}_2$  layer is placed together with AlN layer between electrodes (structure Mo/ $\text{SiO}_2$ /AlN/Mo) and  $\text{SiO}_2$  layer is placed outside the electrodes (structure  $\text{SiO}_2$ /Mo/AlN/Mo). Corresponding dependences of a resonance frequency are presented in Fig. 16 too.

Fig. 16 shows that a  $\text{SiO}_2$  layer more effectively influences on both  $TCF$  and a resonance frequency, when it is placed between electrodes.

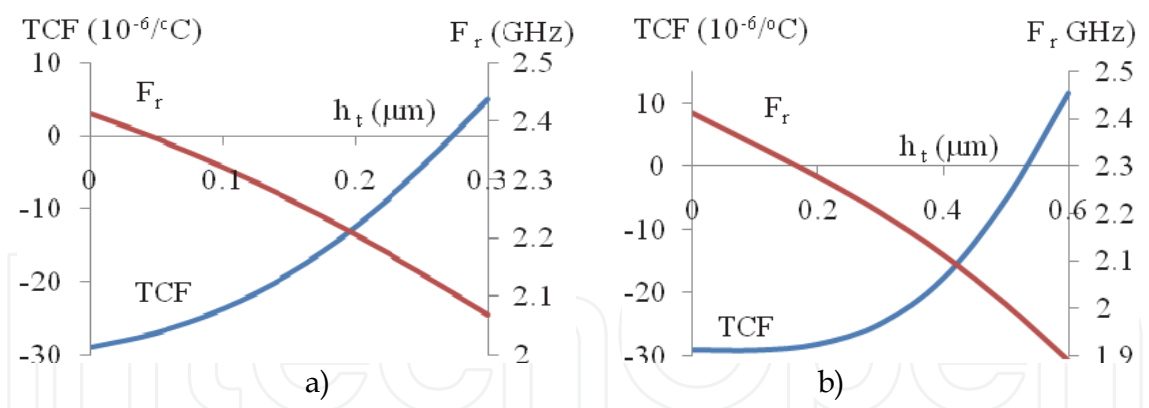


Fig. 16. Dependences of TCF and a resonance frequency on a SiO<sub>2</sub> layer thickness  $h_t$  for cases, when SiO<sub>2</sub> is placed between electrodes (a) and when SiO<sub>2</sub> is placed outside electrodes (b). A thickness of Mo electrodes is 0.06  $\mu\text{m}$ , a thickness of AlN is 1.9  $\mu\text{m}$ .

Calculations show that a Bragg reflector does not change a resonance frequency of the corresponding membrane type resonator, if a thickness of each layer of the reflector is exactly equal to a quarter-wavelength. But a Bragg reflector influences on a TCF. For this reason it is reasonable to choose SiO<sub>2</sub> as one material of a reflector. In this case a thickness of an additional compensating SiO<sub>2</sub> layer can be reduced. For example, a thickness of SiO<sub>2</sub> layer outside electrodes, corresponding to  $TCF = 0$ , is equal about 0.53  $\mu\text{m}$  for variant, shown in Fig. 16b for membrane type resonator. A resonance frequency is about 2.11 GHz for this case. The Bragg reflector with three pairs of SiO<sub>2</sub>/Mo, corresponding this frequency, does not change this frequency, but a TCF becomes positive due to SiO<sub>2</sub> material presense in the reflector. One must reduce a thickness of an additional compensating SiO<sub>2</sub> layer to return a TCF to zero. But then a resonance frequency will increase. We must either increase an AlN layer thickness to return a resonance frequency or to change thickness of a Bragg reflector layers to adjust the reflector to a new resonance frequency. In any case several steps of sequential approximation are necessary. The technique, described here, allows to do this without problem. For example, presented in Fig. 16b, full thermocompensation can be obtained for  $h_t = 0.4$   $\mu\text{m}$  (instead of 0.53  $\mu\text{m}$  for membrane type resonator) and for thickness of SiO<sub>2</sub> and Mo layers in a Bragg reflector 0.71  $\mu\text{m}$  and 0.75  $\mu\text{m}$  respectively. The AlN layer thickness remains 1.9  $\mu\text{m}$  and a resonance frequency slightly shifts remaining in the vicinity of 2.1 GHz.

In many cases a presentation of FBAR resonator by means of some equivalent circuit is convenient – see for example (Hara et. al., 2009). The simplest variant of an equivalent circuit is shown in Fig. 17.

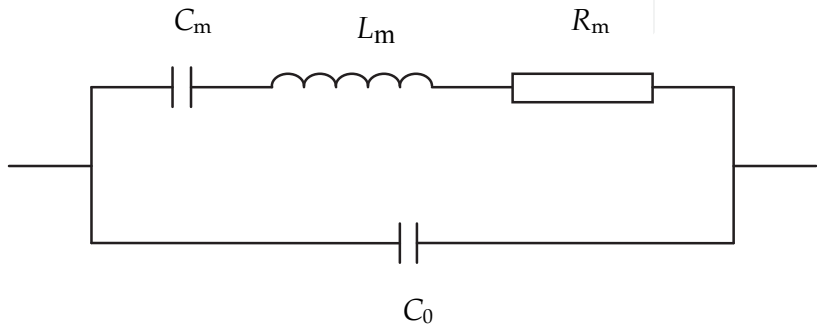


Fig. 17. An equivalent circuit of FBAR resonator.

Here  $C_0$  is a static capacitance of a resonator – a real physical value, which can be calculated by the geometry of the resonator and the dielectric properties of the layers between the electrodes:

$$C_0 = \left( \frac{1}{\varepsilon_0 A} \sum_{i=1}^m \frac{l_i}{\varepsilon_i} \right)^{-1} \quad (82)$$

where  $\varepsilon_i$  and  $l_i$  is a relative dielectric permittivity (element  $\varepsilon_{11}$  of a tensor) of a layer number  $i$  and its thickness,  $\varepsilon_0 = 8.854 \cdot 10^{-12}$  F/m – the dielectric constant,  $A$  is an area of a resonator electrode,  $m$  is a quantity of layers between electrodes.

Values  $C_m$ ,  $L_m$ , and  $R_m$  are equivalent dynamic capacitance, inductance and resistance of the resonator – values, which can not be determined from any physical representation – only by comparison with experimental frequency response or with response, obtained by some exact theory. Theory, described here, allows to obtain these values.

An admittance of the equivalent circuit, shown in Fig. 17, can be calculated by following expressions:

$$Y_e = \left( j\omega L_m + \frac{1}{j\omega C_m} + R_m \right)^{-1} + j\omega C_0 = Y_{Rm} + Y_{Im} + j\omega C_0 \quad (83)$$

Here

$$Y_{Rm} = \frac{R_m}{\left( \frac{1}{\omega C_m} - \omega L_m \right)^2 + R_m^2} \quad Y_{Im} = j \frac{\frac{1}{\omega C_m} - \omega L_m}{\left( \frac{1}{\omega C_m} - \omega L_m \right)^2 + R_m^2} \quad (84)$$

$Y_{Rm}$  and  $Y_{Im}$  are an active and reactive components of a dynamic admittance of the resonator,  $j\omega C_0$  is an admittance of the static capacitance.

Comparison of admittance, calculated by (83) and (84), with admittance, calculated by a rigorous theory, described here, allows to obtain the unique values  $C_m$ ,  $L_m$ , and  $R_m$ , which give a frequency response, equivalent to the response, given by the rigorous theory.

The resonance frequency of the equivalent circuit, shown in Fig. 17, is defined as:

$$\omega_r = 2\pi F_r = \frac{1}{\sqrt{L_m C_m}} \quad (85)$$

The value  $R_m$  corresponds to a maximum of the active component of the admittance (see (84)):

$$R_m = \frac{1}{(Y_{Rm})_{\max}} \quad (86)$$

We can find a quality-factor from curve of a active component of the admittance:

$$Q = \frac{F_r}{\Delta F} \quad (87)$$

Here  $\Delta F$  is a full width of the curve at a level 0.5 of a maximum.

Then we can calculate an equivalent dynamic inductance:

$$L_m = \frac{QR_m}{2\pi F_r} \quad (88)$$

At last we can calculate an equivalent dynamic capacitance with help of (85):

$$C_m = \frac{1}{L_m(2\pi F_r)^2} \quad (89)$$

All these calculations the computer program performs automatically and shows obtained results in corresponding windows of the program interface (a program is made in a Borland C++ Builder medium and provides automatic transfer of main results into Excel worksheet). A frequency response, calculated by expressions (83) and (84) with values  $C_m$ ,  $L_m$ ,  $R_m$ , obtained by such a manner, practically coincides with a frequency response, calculated with rigorous theory, described here (if there is only one resonance peak in a frequency range). In a wide frequency range may be several resonance peaks. In this case one can connect required quantity of  $C_m$ ,  $L_m$ ,  $R_m$  circuits in parallel (but with only one  $C_0$  for all them) in Fig. 17.  $C_m$ ,  $L_m$ ,  $R_m$  values for every circuit can be determined by comparison with corresponding peak, given by a rigorous theory.

#### 4. Conclusion

General methods of surface and bulk acoustic wave in multilayer structures calculation are described in this chapter. Corresponding equations are formulated. These equations allow to calculate all the main wave propagation characteristics and the device parameters. A phase velocity, an electromechanical coupling coefficient, a temperature coefficient of delay, a power flow angle and others for surface wave devices and a frequency response, a spatial distribution of the wave characteristics, a resonance frequency, a temperature coefficient of frequency, parameters of an equivalent circuit for bulk acoustic resonators are available for calculations by described techniques. Obtained results allow better to understand processes taking place in these devices and to improve their characteristics. Corresponding algorithms and computer programs can be used for design of surface and bulk acoustic wave devices.

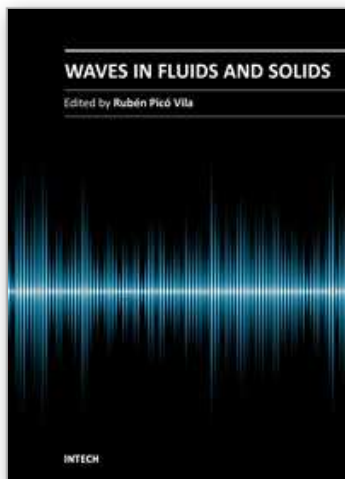
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## **Waves in Fluids and Solids**

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Acoustics is an discipline that deals with many types of fields wave phenomena. Originally the field of Acoustics was consecrated to the sound, that is, the study of small pressure waves in air detected by the human ear. The scope of this field of physics has been extended to higher and lower frequencies and to higher intensity levels. Moreover, structural vibrations are also included in acoustics as a wave phenomena produced by elastic waves. This book is focused on acoustic waves in fluid media and elastic perturbations in heterogeneous media. Many different systems are analyzed in this book like layered media, solitons, piezoelectric substrates, crystalline systems, granular materials, interface waves, phononic crystals, acoustic levitation and soft media. Numerical methods are also presented as a fourth-order Runge-Kutta method and an inverse scattering method.

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