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Numerical Calculation of the Parameters of Surface and Pseudosurface Acoustic Waves in Multilayer Structures

V. I. Cherednick and M. Yu. Dvoesherstov

Lobachevski State University, Nizhni Novgorod, pr. Gagarina 23, 603950 Russia

e-mail: Cherednik@ichem.unn.ru, Dvoesh@rf.unn.ru

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Abstract—A method for numerically calculating the parameters of surface and pseudosurface electroacoustic waves propagating in multilayer piezoelectrics is suggested. The feasibility of wave parameter optimization by using various materials of the layers and piezoelectric substrate is demonstrated with particular examples. © 2003 MAIK “Nauka/Interperiodica”.

INTRODUCTION

The application of various layers on a piezoelectric substrate is a way of improving the parameters of propagating electroacoustic waves (EAWs). For example, a metal film of certain thickness may thermally suppress the EAW propagation when the orientation of the substrate provides a high piezoelectric coupling. Using the overlayer, one can vary the wave propagation velocity and, hence, the operating frequency of a piezoelectric device. The effect of the environment (gas or liquid) on the properties of the wave and overlayer is used in related sensors. Finally, the layer may protect the piezoelectric surface against undesired external impacts. One more advantage of multilayer compositions is the reduction of a velocity dispersion, which is observed in single-layer structures. Therefore, analysis and optimization of the EAW parameters in multilayer structures seems to be topical. Various aspects of this problem is discussed elsewhere [1–4].

In this paper, we formulate boundary conditions for insulating, metallic, and piezoelectric insulating overlayers and for a piezoelectric substrate of any crystal symmetry. Also, a general method for numerically calculating the parameters of EAWs propagating in multilayer piezoelectric crystal structures is reported.

STATEMENT OF THE PROBLEM AND BOUNDARY CONDITIONS

The parameters of EAWs propagating in the multilayer structures depend on the properties of the substrate and each of the layers. It is necessary to solve the set of piezoacoustic equations [5]

$$\rho \frac{\partial^2 u_j}{\partial t^2} - c_{ijkl} \frac{\partial^2 u_k}{\partial X_i \partial X_l} = e_{kij} \frac{\partial^2 \varphi}{\partial X_k \partial X_i}, \quad (1)$$

$$\varepsilon_{ik} \frac{\partial^2 \varphi}{\partial X_i \partial X_k} = e_{ikl} \frac{\partial^2 u_k}{\partial X_i \partial X_l}; \quad i, j, k, l = 1, 2, 3.$$

where X_i are coordinates; c_{ijkl} , e_{ijk} , and ε_{ij} are the tensors of the piezoelectric, elastic, and dielectric constants; ρ is the density of the medium; u_i are mechanical displacements; φ is the electrical potential; and t is time. The set of Eqs. (1) must be solved for each of the system's component (Fig. 1). A solution to set (1) is sought in the form

$$u_j = \alpha_j \exp(ikb_3 X_3) \exp[ik(b_1 X_1 - vt)],$$

$$\varphi = \alpha_4 \exp(ikb_3 X_3) \exp[ik(b_1 X_1 - vt)]; \quad (2)$$

$$j = 1, 2, 3.$$

Here, α_j are the mechanical displacement amplitudes, α_4 is the electric potential; k is the wavenumber; v is the wave velocity; and b_1 and b_3 are the coefficients that relate the wave amplitude to the coordinates X_1 and X_3 , respectively. In the general case, the coefficient b_1 may be represented as $b_1 = 1 + i\delta$, where δ is a real positive quantity that has the meaning of the decay of the wave along the propagation direction. For surface acoustic waves, the decay $\delta = 0$; for pseudosurface acoustic waves, $\delta > 0$ [6]. In the general case, substituting (2) into (1) yields a set of Christoffel equations, from which one, knowing the wave velocity V and the decay coefficient δ , can find eight complex roots $b_3(n)$ ($n = 1$ –

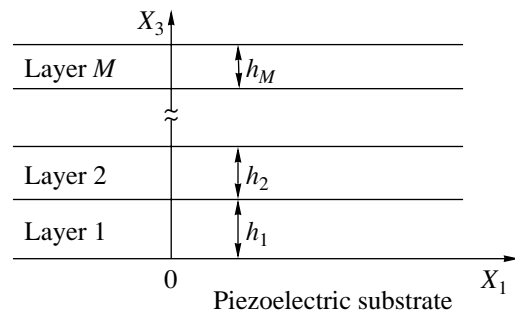


Fig. 1. Multilayer structure.

8) and the associated set of complex amplitudes $\alpha_1^{(n)}$, $\alpha_2^{(n)}$, $\alpha_3^{(n)}$, and $\alpha_4^{(n)}$. For each of the structure constituents, a general solution is represented as a linear combination of partial waves in this constituent:

$$\begin{aligned}
 u_j^{(m)} &= \sum_{n=N_{m-1}+1}^{N_m} C_n \alpha_j^{(n)} \exp[ik(b_i^{(n)} X_i - Vt)], \\
 \varphi^{(m)} &= \sum_{n=N_{m-1}+1}^{N_m} C_n \alpha_4^{(n)} \exp[ik(b_i^{(n)} X_i - Vt)]; \\
 & i, j = 1, 2, 3.
 \end{aligned}
 \tag{3}$$

Here, $b_1^{(n)} = 1 + i\delta$, $b_2^{(n)} = 0$, $b_3^{(n)}$ is a set of the roots of the polynomial equation (specific for each of the media), $N_m = n_0 + n_1 + \dots + n_m$, n_m is the number of partial modes in a medium of number m ($m = 0$ refers to the substrate; $m = 1$, to the first layer, etc.; $N_{0-1} = n_{0-1} = 0$), and C_n are unknown amplitude coefficients.

When analyzing surface or pseudosurface acoustic waves, one must properly select the roots $b_3^{(n)}$ for the substrate. For the layers, the rule of root selection is straightforward: for each of them, a solution must be constructed as a linear combination of partial modes. The unknown coefficients C_n of the linear combination in (3) are found from boundary conditions at the interfaces and at the outer boundary of the top layer. Unfortunately, general boundary conditions that are applicable to any combination of the substrate and layer materials cannot be stated in principle.

1. PIEZOELECTRIC LAYERS ON A PIEZOELECTRIC SUBSTRATE

In this case, three components of mechanical displacements u_j , three normal components of the mechanical stress tensor T_{3j} , the electrical potential φ , and the normal component of the electric field induction D_3 must satisfy the continuity conditions at the interfaces. The conditions at the boundary between m th and $(m + 1)$ th media are as follows:

$$\begin{aligned}
 & \sum_{n=N_{m-1}+1}^{N_m} C_n \alpha_j^{(n)} \exp[ikb_3^{(n)} X_3^{(m)}] \\
 & = \sum_{n=N_m+1}^{N_{m+1}} C_n \alpha_j^{(n)} \exp[ikb_3^{(n)} X_3^{(m)}],
 \end{aligned}
 \tag{4a}$$

$$\begin{aligned}
 & \sum_{n=N_{m-1}+1}^{N_m} C_n (c_{3jkl} \alpha_k^{(n)} b_l^{(n)} + e_{k3j} \alpha_4^{(n)} b_k^{(n)}) \exp[ikb_3^{(n)} X_3^{(m)}] \\
 & = \sum_{n=N_m+1}^{N_{m+1}} C_n (c_{3jkl} \alpha_k^{(n)} b_l^{(n)} + e_{k3j} \alpha_4^{(n)} b_k^{(n)}) \exp[ikb_3^{(n)} X_3^{(m)}],
 \end{aligned}
 \tag{4b}$$

$$\begin{aligned}
 & \sum_{n=N_{m-1}+1}^{N_m} C_n \alpha_4^{(n)} \exp[ik(b_3^{(n)} X_3^{(m)})] \\
 & = \sum_{n=N_m+1}^{N_{m+1}} C_n \alpha_4^{(n)} \exp[ik(b_3^{(n)} X_3^{(m)})],
 \end{aligned}
 \tag{4c}$$

$$\begin{aligned}
 & \sum_{n=N_{m-1}+1}^{N_m} C_n (c_{3jk} \alpha_j^{(n)} b_k^{(n)} - \epsilon_{3j} \alpha_4^{(n)} b_j^{(n)}) \exp[ikb_3^{(n)} X_3^{(m)}] \\
 & = \sum_{n=N_m+1}^{N_{m+1}} C_n (c_{3jk} \alpha_j^{(n)} b_k^{(n)} - \epsilon_{3j} \alpha_4^{(n)} b_j^{(n)}) \exp[ikb_3^{(n)} X_3^{(m)}]
 \end{aligned}
 \tag{4d}$$

Here, $m = 0, 1, 2, \dots, M - 1$, where M is the number of layers; $X_3^{(m)} = h_1 + h_2 + \dots + h_m$; and $X_3^{(0)} = 0$. Equations (4a)–(4d) are the continuity conditions for mechanical displacements, stresses, potential, and electric field induction.

If any surface $X_3 = X_3^{(m)}$ is covered by a metal layer of infinitesimal thickness and short-circuited, Eqs. (4c) and (4d) change. The right of (4c) and the left of (4d) vanish, and the right of (4d) is replaced by the right of (4c).

The potential $\varphi^{(f)}$ in free space must meet the Laplace equation and decrease down to zero with $X_3 \rightarrow \infty$. These conditions are satisfied if $\varphi^{(f)}$ is taken in the form

$$\varphi^{(f)} = \varphi^{(M)} e^{-kb_1(X_3 - X_3^{(M)})}, \quad X_3 \geq X_3^{(M)}. \tag{5}$$

Here, $\varphi^{(M)}$ is the potential at the outer boundary of the top layer ($X_3 = X_3^{(M)}$). Eventually, for the top surface uncovered, we obtain the electrical boundary condition

$$\begin{aligned}
 i \sum_{n=N_{M-1}+1}^{N_M} C_n (e_{3jk} \alpha_j^{(n)} b_k^{(n)} - \epsilon_{3j} \alpha_4^{(n)} b_j^{(n)}) \exp[ikb_3^{(n)} X_3^{(M)}] \\
 = b_1 \epsilon_0 \sum_{n=N_{M-1}+1}^{N_M} C_n \alpha_4^{(n)} \exp[ikb_3^{(n)} X_3^{(M)}].
 \end{aligned}
 \tag{6}$$

For the short-circuited top boundary, the electrical boundary condition may be derived from Eq. (4c) with $m = M$ and zero on the right.

When all the constituents of the system are piezoelectrics, the complete set of boundary conditions contains $n_0 + n_1 + n_2 + \dots + n_M$ equations for the same number of the unknowns C_n . For such a system, $n_0 = 4$ and $n_1 = n_2 = \dots = n_M = 8$ in the general case.

2. METALLIC LAYERS ON A PIEZOELECTRIC SUBSTRATE

The situation where the first layer is metallic and the others are either metallic or insulating in any combination may also be assigned to this case. Here, the mechanical boundary conditions at the interfaces remain the same as above and the electrical boundary conditions simplify to

$$\sum_{n=1}^{n_0} C_n \alpha_4^{(n)} = 0. \quad (7)$$

3. ISOTROPIC INSULATING LAYERS ON A PIEZOELECTRIC SUBSTRATE

Let a piezoelectric substrate support M isotropic insulating layers with permittivities ϵ_m . Then, electric boundary conditions become awkward, since any of the interfaces may be either open or short-circuited. In the general case, the electrical potential inside an m th layer depends on X_3 as follows:

$$\varphi^{(m)}(X_3) = A_m e^{-kb_1(X_3 - X_3^{(m-1)})} + B_m e^{kb_1(X_3 - X_3^{(m-1)})}, \quad (8)$$

$$X_3^{(m-1)} \leq X_3 \leq X_3^{(m)}.$$

Having defined all the coefficients A_m and B_m through the interfacial potentials, one then may, using the continuity conditions for the potential and normal component of the electric induction vector at each of the interfaces, eliminate the interfacial potentials and obtain the X_3 dependence of the potential $\varphi^{(1)}$ ($\varphi^{(1)}$ is the potential of the first layer) that involves only $\varphi^{(0)}(X_3 = 0)$, which is the potential on the substrate surface. The potential $\varphi^{(1)}$ appears in the expression for the normal component of the electric field induction in the first layer:

$$D_3^{(1)} = -\epsilon_1 \epsilon_0 \frac{d\varphi^{(1)}}{dX_3}. \quad (9)$$

The induction calculated by (9) for $X_3 = 0$ should now be set equal to the induction calculated for the substrate at the same X_3 . This yields a single electrical boundary condition for isotropic insulating layers on a

piezoelectric substrate. Its shape will depend considerably on the number of layers and on the electrical state of the interfaces (open or short-circuited).

(3a). All interfaces are open. If there is a single layer, electrical boundary conditions have the form

$$i \sum_{n=1}^{n_0} C_n (e_{3jk} \alpha_j^{(n)} b_k^{(n)} - \epsilon_{3j} \alpha_4^{(n)} b_j^{(n)}) = \frac{b_1 \epsilon_1 \epsilon_0}{\sinh(kb_1 n_1)} S_1 \sum_{n=1}^{n_0} C_n \alpha_4^{(n)}, \quad (10a)$$

where

$$S_1 = \cosh(kb_1 h_1) - \frac{\epsilon_1}{\epsilon_1 \cosh(kb_1 h_1) + R_2 \sinh(kb_1 h_1)}. \quad (10b)$$

In (10b),

$$R_2 = \frac{\epsilon_2}{\sinh(kb_1 h_2)} S_2, \quad (11)$$

is the recursive coefficient that makes it possible to derive a formula for two layers from the formula for one layer; that is, for two layers, the electrical boundary condition takes the form

$$i \sum_{n=1}^{n_0} C_n (e_{3jk} \alpha_j^{(n)} b_k^{(n)} - \epsilon_{3j} \alpha_4^{(n)} b_j^{(n)}) = \frac{b_1 \epsilon_1 \epsilon_0}{\sinh(kb_1 h_1)} \times \left[\cosh(kb_1 h_1) - \frac{\epsilon_1}{\epsilon_1 \cosh(kb_1 h_1) + \frac{\epsilon_2 \sinh(kb_1 h_2)}{\sinh(kb_1 h_2)} S_2} \right] \times \sum_{n=1}^{n_0} C_n \alpha_4^{(n)}, \quad (12a)$$

where

$$S_2 = \cosh(kb_1 h_2) - \frac{\epsilon_2}{\epsilon_2 \cosh(kb_1 h_2) + R_3 \sinh(kb_1 h_2)}. \quad (12b)$$

The recursive coefficient

$$R_3 = \frac{\epsilon_3}{\sinh(kb_1 h_3)} S_3, \quad (13)$$

allows one to obtain a formula for three layers from the formula for two layers; that is, for three layers, we have

combined into one quantity as [7]

$$\varepsilon_{\text{eff}} = \frac{D_3^{(M)}}{kb_{(1)}\phi^{(M)}}. \quad (16)$$

The wavenumber k here is added to match the dimensions of the left- and right-hand sides. The coefficient b_1 appears if pseudosurface waves are considered. In such a representation, the continuity condition for the induction or potential is replaced by the equivalent continuity condition for the effective permittivity. For an open surface, the effective permittivity is ε_0 ; for a short-circuited one, it is infinitely large (the permittivity of a metal). Having substituted potential (3) and induction (9) into (16), we arrive at

$$i \sum_{n=N_{M-1}+1}^{N_M} \frac{C_n(e_{3jk}\alpha_j^{(n)}b_k^{(n)} - \varepsilon_{3j}\alpha_4^{(n)}b_j^{(n)})\exp[ikb_3^{(n)}X_3^{(M)}]}{b_1\varepsilon_0 \sum_{n=N_{M-1}+1}^{N_M} C_n\alpha_4^{(n)}\exp[ikb_3^{(n)}X_3^{(M)}]} = \begin{cases} \varepsilon_0, \\ \infty. \end{cases} \quad (17)$$

The upper equality in (17) is totally equivalent to Eq. (6). The lower one is equivalent to Eq. (4c) if $m = M$ and the right-hand side is set equal to zero. The absolute value of (17) squared is used as an objective function in searching for the velocity V and the decay coefficient δ . For an open surface, the solution corresponds to the zero (minimum) of this function; for a short-circuited surface, to the pole. With piezoelectric layers, the use of the effective permittivity is valid not only for the outer surface of the top layer but also for any interface. In the latter case, when considering an open surface, one must take equal values of the effective permittivity on both sides of the surface. For a short-circuited surface, the potential of this surface should be set equal to zero. Then, for the construction of the effective permittivity, it is necessary to use the appropriate equation from set (15). An objective function for isotropic insulating layers can be constructed in the same way. In this case, we have only one equation of electrical boundary conditions, which is the continuity equation for the normal component of the induction on the substrate surface. This equation is found in view of the continuity of both electrical parameters (potential and field) on all other surfaces (for the open substrate surface) or in view of the zero potential on the short-circuited substrate surface.

COMPUTATIONAL RESULTS

Based on the above approach, we implemented an algorithm for computing the basic parameters of electroacoustic surface waves propagating in multilayer

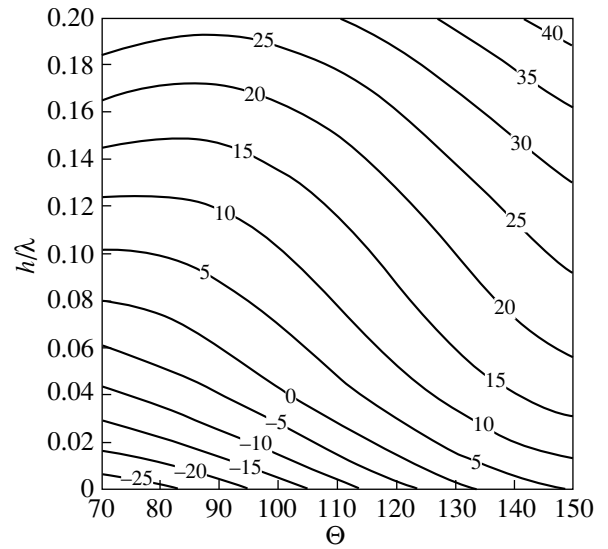


Fig. 2. Dependence of the tcd on Θ and reduced thickness h/λ of the aluminum layer on piez quartz ($\phi = 0$, $\Theta = 70$ – 150° , $\psi = 0$). The figures by the curves are tcd in $10^{-6} 1/^\circ\text{C}$.

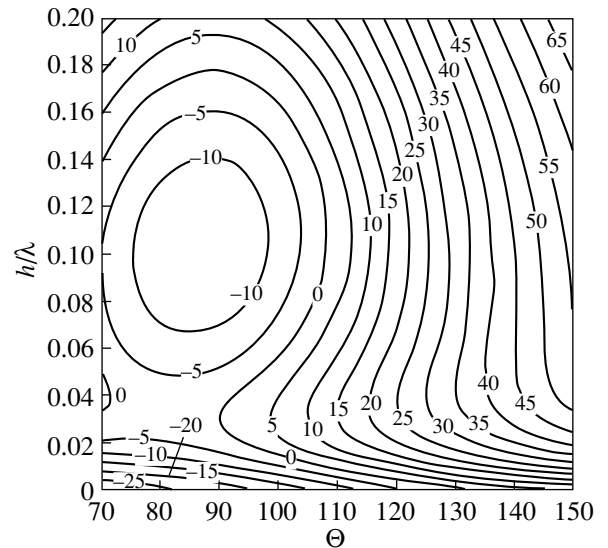


Fig. 3. The same as in Fig. 2 for gold on piez quartz.

structures. Figures 2 and 3 demonstrate the effect of individual layers of various metals on the temperature dependences of piez quartz with the second Eulerian angle Θ ranging from 70 to 150° and the first and third Eulerian angles being zero. These ranges of Eulerian angles correspond to piez quartz orientations (YX , $AT-X$, $ST-X$, et al.) that are most widely used in related devices. Specifically, the two-dimensional dependences of the temperature coefficient of delay (tcd) on Θ and on the normalized (to the wavelength λ) Al and Au layer thickness h are shown. The material constants for Al and Au were taken from [8]. From Figs. 2 and 3 it follows that negative values of tcd can be compen-

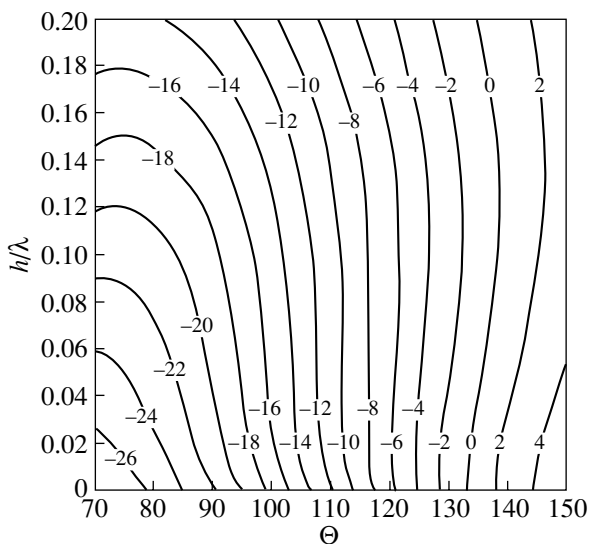


Fig. 4. The same as in Fig. 2 for an isotropic fused quartz layer on piez quartz.

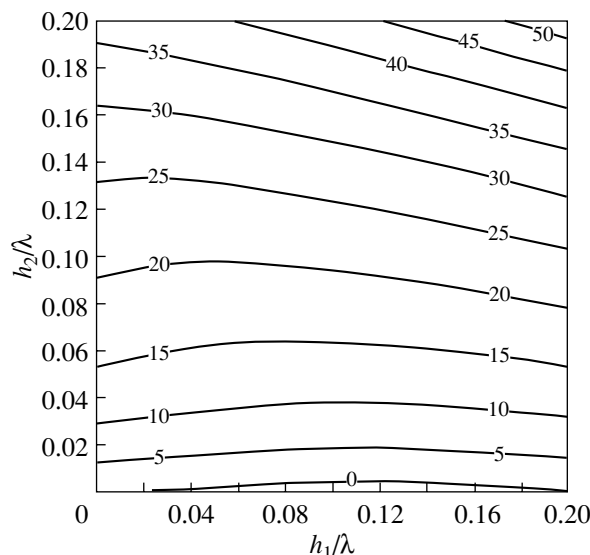


Fig. 5. Dependence of the *tcd* on the reduced thicknesses of isotropic fused quartz, h_1/λ , and aluminum layer, h_2/λ , on *ST-X* quartz (0, 132.75°, 0). The figures by the curves are *tcd* in $10^{-6} 1/^\circ\text{C}$.

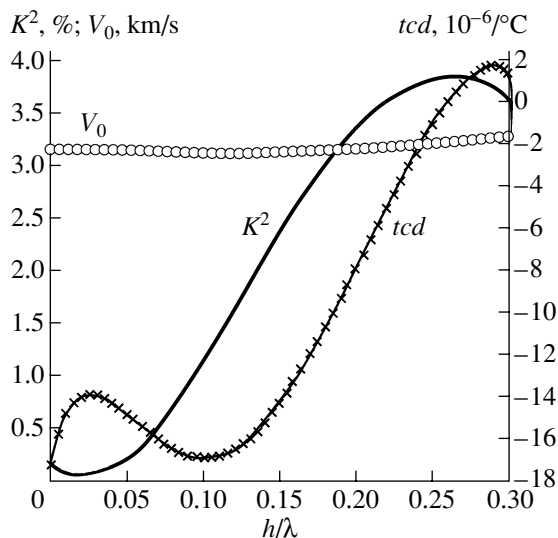


Fig. 6. *tcd*, K^2 , and V_0 vs. the thickness h/λ of LiNbO_3 (0, 38°, 0) on the quartz substrate (0, 100°, 0).

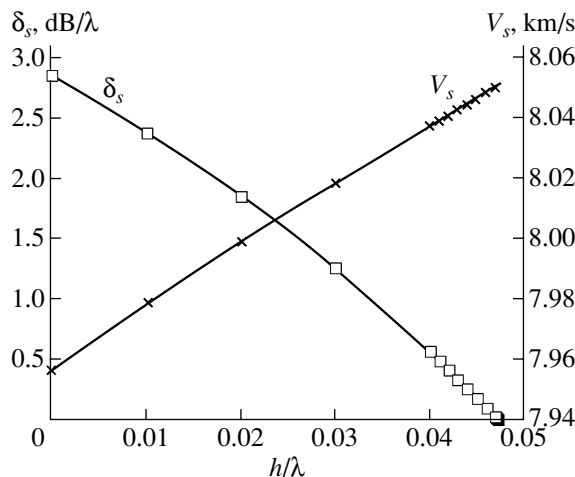


Fig. 7. Propagation losses δ_s and velocity V_s of the second-order pseudosurface wave vs. the thickness h/λ of the Al layer on the LiNbO_3 crystal surface (9, -49°, 0).

sated for by a metal layer of certain thickness. For example, the orientation YX ($\Theta = 90^\circ$) can be stabilized by applying an Al layer about 0.06λ thick on the quartz surface. Figure 4 shows the effect of an isotropic insulating fused quartz layer on the temperature behavior of the same crystal orientations. The effect is seen to be insignificant: the related isolines are arranged largely normally to the Θ axis. This means that fused quartz is promising as a protective layer against undesired environmental (mechanical and chemical) impacts that almost does not change the temperature properties of the system (in particular, the thermal stability of the ori-

entation *ST-X*, $\Theta = 132.75^\circ$, remains practically the same).

A thin metal layer applied on an isotropic insulator provides protection against electrical fields. The combined effect of an isotropic fused quartz layer covered by an aluminum layer is illustrated in Fig. 5, which shows the two-dimensional dependence of the *tcd* on the thicknesses of the fused quartz layer and aluminum overlayer in the crystal–fused quartz–aluminum system. The effect of the Al layer is significant; therefore, its thickness must be small so as not to break the thermal stability of the given orientation. Figure 6 plots the wave velocity V_0 , temperature coefficient of delay *tcd*,

and electromechanical coupling coefficient K^2 (an interdigital transducer on the surface) vs. the thickness of lithium niobate LiNbO_3 ($0, 38^\circ, 0$) applied on the open-surface quartz substrate ($0, 100^\circ, 0$). It is seen that K^2 reaches a value of 3.85% and tcd goes to zero near $h/\lambda = 0.26$. Thus, a LiNbO_3 layer on quartz may provide a combination of high K^2 , which is typical of lithium niobate, and a high thermal stability, which is inherent in quartz. Finally, let us consider the influence of a metal layer on the properties of pseudosurface waves propagating in LiNbO_3 ($0, -49^\circ, 0$). For this orientation, a second-order pseudosurface wave has the following parameters: $V_s = 7.9576$ km/s, $V_0 = 8.3144$ km/s, $\delta_s = 2.865$ dB/ λ , $\delta_0 = 0.531$ dB/ λ , and $K^2 = 8.58\%$. The subscripts 0 and s refer to the open and short-circuited surfaces, respectively. An aluminum layer of finite thickness decreases losses. The dependences of δ_s and V_s on the Al layer thickness are shown in Fig. 7. As h/λ grows from zero to 0.047, the losses decrease from 2.865 dB/ λ to about 10^{-3} dB/ λ . It appears that the metal layer changes the wave propagation conditions so that the angle at which the wave goes inward to the crystal diminishes.

CONCLUSIONS

A general method for numerically calculating the parameters of surface and pseudosurface acoustic waves propagating in multilayer structures is suggested. The structures involve piezoelectric, insulating,

and metal layers on a semi-infinite substrate of any crystal orientation. The effect of layers of different materials on electroacoustic surface wave propagation is studied. In a number of special cases, the thermal stability, electromechanical coupling coefficient, and propagation losses for pseudosurface waves may be improved. Various coatings in various combinations may improve considerably the characteristics of acoustoelectron devices.

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