SURFACE AND BULK WAVE VELOCITIES IN ARBITRARY ANISOTROPIC PIEZOELECTRIC MATERIALS

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Abstract

We present a numerical algorithm for the calculation of phase velocities of acoustic surface and bulk waves in anisotropic piezoelectric materials. The mathematical model is based on fundamental partial differential equations in three spatial dimensions which are the equations of motion and Poisson's equation. We present examples for $LiNbO_3$ and Quartz.

1. Introduction

In recent years modeling of wave propagation phenomena in anisotropic piezoelectric materials has become eminently important for surface acoustic wave device characterization and design. Most of the common computer programs for the analysis of the extrinsic device behaviour require on input the phase velocity of the surface wave [1]. In many cases the decay of the surface wave into bulk as well as the properties of the bulk waves in the sagittal plane are also of great interest. As experimental results are difficult to obtain for arbitrary crystal cuts the numerical calculation of phase velocities is an important tool for the investigation of less common materials and crystal cuts.

There exist some publications dealing with phase velocities of surface and bulk acoustic waves [2,3,4] but the authors in general postulate a pure exponential decay of the partial waves whose linear combination yield the surface wave. Our approximation is more rigorous as we do not anticipate the depth dependency in any way. For the calculation of the bulk modes we employ an abstract mathematical scheme rather than a wave-"ansatz".

Our computer program in which we have implemented the two methods is very flexible with respect to different materials and crystal cuts. The structure and the actual values of the material dependent tensors are stored in a database for most of the common materials. The input data are the type of material, the Euler's angles of the crystal cut and the kind of wanted calculation: either the surface wave solution or the plane bulk modes in the sagittal plane. In this paper a comparison is shown between the surface wave velocity and the velocities of the bulk shear modes on rotated Y-cut of $LiNbO_3$. Furthermore the bulk wave velocity curves for Quartz are demonstrated.

2. The Mathematical Model

The mathematical model is based on the partial differential equation system in three spatial dimensions ($j=1,2,3$) consisting of the equations of motion (1) and Poisson's equation (2). It is to be noted that standard tensor notation as well as Einstein's summation convention is used. The derivation of this system from the fundamental equations describing acoustic wave propagation in arbitrary piezoelectric materials can be found in [5].

$$c_{ijkl} \cdot \partial^2 u_k / \partial x_l \partial x_i -$$
$$- e_{kij} \cdot \partial^2 \varphi / \partial x_k \partial x_i = \varrho \cdot \partial^2 u_j / \partial t^2 \qquad (1)$$

$$e_{ikl} \cdot \partial^2 u_k / \partial x_l \partial x_i -$$
$$- \varepsilon_{ik} \cdot \partial^2 \varphi / \partial x_k \partial x_i = 0 \qquad (2)$$

u denotes the mechanical displacement, ϱ the mass density and φ the electric potential. The fourth rank tensor c is the elastic stiffness tensor, the third rank tensor e the piezoelectric tensor, and the second rank tensor ε the dielectric tensor in the actual i.e. rotated coordinate system.

Now we reduce the system to the two space dimensions $x=x_1$ and $z=x_3$ by assuming negligible derivation of all parameters in direction perpendicular to the sagittal plane and we define the solution vector s which includes the mechanical displacement vector u and the electric potential φ (4). This procedure leads to the following set of equations:

$$A \cdot s_{xx} + (B+B^T) \cdot s_{xz} + C \cdot s_{zz} = \Omega \cdot s_{tt}$$

$$t > 0, \quad x \in R, \quad z < 0 \qquad (3)$$

$$s = (u_1, u_2, u_3, \varphi)^T \qquad (4)$$

A, B, C, Ω are 4x4 matrices, A and C are symmetric, and B^T is the transpose of B. The matrix $B+B^T$ is obviously symmetric too. Ω is a diagonal matrix with the entries φ, φ, φ, 0.

3. The Surface Wave Velocity

We investigate surface acoustic waves on free surfaces. This is not a fundamental restriction because for metalized surfaces one has only to change the boundary conditions.

In the medium (air) above the surface the Poisson equation simplifies to the Laplace equation (5). The transition condition between crystal and air is given by the fact that there does not exist any charge on the interface. Thus, the divergency of the electric displacement has to vanish there (6). The component of the electric displacement perpendicular to the surface is called D_3 for the crystal and D_{air} for the air. The surface boundary conditions for the mechanical displacement result from the fact that all force components perpendicular to the surface have to vanish (7).

$$\Delta \varphi_{air} = 0 \qquad (5)$$

$$Div\ D = 0 \equiv D_3 = D_{air} \quad for\ z = 0 \quad (6)$$

$$T_{3j} = 0 \qquad for\ z = 0 \qquad (7)$$

By substituting the linear piezoelectric constitutive relations (8) and (9) into equations (6) and (7) one obtains the system of boundary conditions (10).

$$T_{ij} = c_{ijkl} \cdot S_{kl} - e_{nij} \cdot E_n \qquad (8)$$

$$D_m = e_{mkl} \cdot S_{kl} + \varepsilon_{mn} \cdot E_n \qquad (9)$$

$$B \cdot s_x + C \cdot s_z = (0,0,0,D_{air})^T \qquad (10)$$

Our model of the surface wave is a linear combination of partial waves (11). In contrast to other authors we do not assume a pure exponential decay of these partial waves into the depth but we allow a general function $g(z)$. (It should be mentioned that g is a vector with 4 components.)

$$s = e^{j(kx - \omega t)} \cdot g(z) \qquad (11)$$

First we have to eliminate the right hand side vector of equation (10). For that purpose we calculate the solution of the Laplace equation (12).

$$g_{air} = a_1 \cdot e^{kz} + a_2 \cdot e^{-kz} \qquad (12)$$

The constant a_1 must vanish because the limit of $g_{air}(z)$ for $z \to +\infty$ has to be zero. a_2 is estimated by a comparison of g_{air} with g_4 for $z = 0$ and we obtain an expression for D_{air} (13).

$$D_{air} = \varepsilon_{air} \cdot k \cdot \varphi \quad for\ z = 0 \qquad (13)$$

$$g(z) = f(\xi) = f(jkz) \qquad (14)$$

It is advantageous to make a transformation of the z-coordinate by introducing the new function f (14). Substituting equation (11) into (3),(10) and equation (13) into (10) yields a homogeneous system of four ordinary differential equations of second order (15) with the boundary conditions (16) and (17).

$$(A-v^2 \cdot \Omega) \cdot f + (B+B^T) \cdot f' + C \cdot f'' = 0 \quad (15)$$

$$(B+F) \cdot f(\xi) + C \cdot f'(\xi) = 0 \qquad for\ \xi = 0 \quad (16)$$

$$s(x,\xi,t) = 0 \qquad for\ \xi \to -j \cdot \infty \qquad (17)$$

The pure imaginary matrix F is coming from the dielectric displacement on the surface (13).

It is very important to state that the unknown phase velocity v is a parameter of the equation system (15). Therefore, an iterative algorithm must be applied: First, one has to give an initial guess for the phase velocity (a very good initial value is the phase velocity of the slower bulk shear mode); second, one must calculate the solution of the ordinary differential equation system, and third, one has to check if the boundary conditions can be satisfied with this solution. If the boundary conditions are not satisfied it is necessary to change the velocity and to repeat the whole procedure.

To solve the ordinary differential equation system we transform it into first order defining the solution vector h as follows:

$$h_1 = f$$

$$h_2 = (B+F) \cdot h_1 + C \cdot h_1' \qquad (18)$$

$$h' = H \cdot h \qquad with\ h = (h_1, h_2)^T \qquad (19)$$

$$H_{11} = -C^{-1} \cdot (B+F)$$

$$H_{12} = -C^{-1}$$

$$H_{21} = v^2 \cdot \mathbf{\Omega} - A + (B^T-F) \cdot C^{-1} \cdot (B+F)$$

$$H_{22} = -(B^T-F) \cdot C^{-1}$$

The first order system (19) is characterized by the complex 8x8 matrix H. H_{11}, H_{12}... denote the 4x4 submatrices of H.

The solution of the system (19) is given by equation (20) with the linear combination vector $\mathbf{\eta}$. Owing to the chosen first order transformation homogeneous boundary conditions (21) and (22) have to be satisfied by the solution.

$$h = e^{H \cdot \mathbf{\xi}} \cdot \mathbf{\eta} \qquad (20)$$

$$h_1 = 0 \qquad \text{for } \mathbf{\xi} \rightarrow -j \cdot \infty \qquad (21)$$

$$h_2 = 0 \qquad \text{for } \mathbf{\xi} = 0 \qquad (22)$$

Equation (20) is replaced by the spectral dissecton (23). The matrix G has as column vectors the eigenvectors of H and $\mathbf{\Lambda}$ is a diagonal matrix whose elements are given by the exponentials of the eigenvalues of H. (It should be mentioned that it is not absolutely necessary for $\mathbf{\Lambda}$ to be a diagonal but a Jordanian matrix. This is essential when H has multiple eigenvalues. This special case is included in our algorithm - as a lack of space it can not discussed here in detail.)

$$e^{H \cdot \mathbf{\xi}} = G \cdot \mathbf{\Lambda} \cdot \mathbf{\xi} \cdot G^{-1} \qquad (23)$$

At this stage the vector $\mathbf{\eta}$ in equation (20) is still not determined. The question is now if there exists an $\mathbf{\eta}$ such that the solution satisfies the boundary condition. For that purpose we have to investigate the eigenvalues of matrix H: eigenvalues with a positive imaginary part never can satisfy the boundary condition (21). If we arange the elements of the main diagonal of $\mathbf{\Lambda}$ in the way that we take first the eigenvalues with negative imaginary part it can be shown that the second four components of $\mathbf{\eta}$ must vanish (24). From boundary conditon (22) follows then straightforwardly that for an existing surface wave the 4x4 submatrix G_{21} has to be singular (25).

$$\mathbf{\eta}_2 = 0 \qquad (24)$$

$$G_{21} \cdot \mathbf{\eta}_1 = 0 \qquad (25)$$

The numerical effort for checking one given phase velocity to be the solution of the surface wave problem can be summarized as follows: assembling the complex 8x8 matrix H, estimating its eigenvalues and eigenvectors, and then calculating the determinant of the 4x4 matrix G_{21}.

4. The Bulk Wave Velocities

To obtain the plane bulk modes propagating in a given direction in the sagittal plane we transform equation (3) into polar coordinates $(r, \mathbf{\alpha})$ and form the limit for $r \rightarrow \infty$. This procedure yields a homogeneous system of four ordinary differential equations (26).

$$P \cdot s_{rr} = \mathbf{\Omega} \cdot s_{tt} \qquad (26)$$

$$P = A \cdot \cos^2 \mathbf{\alpha} + (B+B^T) \cdot \sin \mathbf{\alpha} \cdot \cos \mathbf{\alpha} + C \cdot \sin^2 \mathbf{\alpha}$$

Now we define the matrix Q by equation (27). Then, the eigenvalues of Q are the reciprocal squares of the phase velocities and the eigenvectors of Q are the corresponding displacement vectors of the bulk modes.

$$Q = P^{-1} \cdot \mathbf{\Omega} \qquad (27)$$

It should be noted that the fourth eigenvalue of Q is zero due to the quasi static approximation for the electric potential.

5. Results

Fig. 1 shows a comparison between the surface wave velocity curve (curve 1) and the velocity curves of the bulk shear modes (curves 2) for the 128° rotated Y-cut of $LiNbO_3$. It can clearly be seen that the surface velocity is stricly lower than the velocity of the slower bulk mode. As in the following drawings the scale in the middle represents the absolute value of the velocities in m/s. To present more details the center does not indicate zero but a defined minimum velocity.

Fig. 2 represents the velocity curves of the quasi longitudinal bulk modes for Quartz. The parameter of the curves (0, 30, 60,...) is the Euler's angle $\mathbf{\mu}$, i.e. the curve with the index 0 is the velocity curve in the sagittal plane (XZ-plane) of the unrotated crystal. The horizontal line indicates the X-direction of the crystal and the number on the end of each ray is the angle $\mathbf{\alpha}$ which defines the direction in the sagittal plane. As all curves are symmetric referring to the center the

curves for $0^\circ \le \psi \le 90^\circ$ are drawn only in the upper half and the curves for $90^\circ \le \psi \le 180^\circ$ in the lower half of the plot.
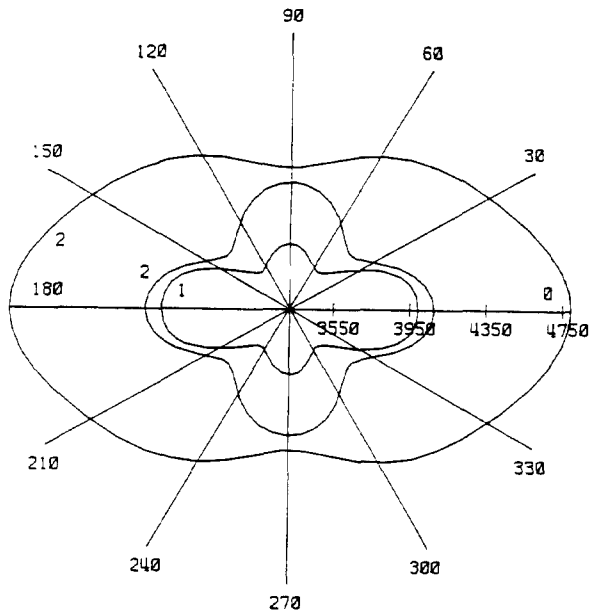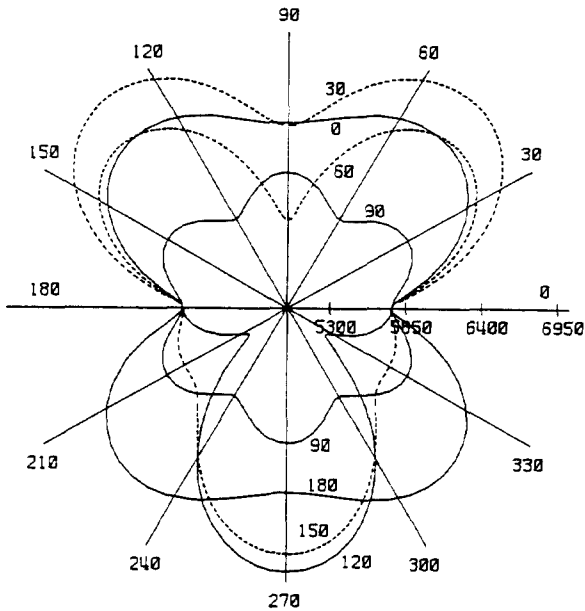

Fig. 1

Fig. 2

Fig. 3 shows the velocity curves of the bulk shear modes for Quartz in the same representation as Fig. 1. One can extract from this drawing that for the unrotated crystal ($\psi = 0^\circ$) the two shear modes in Z-direction ($\alpha = 90^\circ$) have the same phase velocity. Furthermore, one can see that the behaviour of the bulk

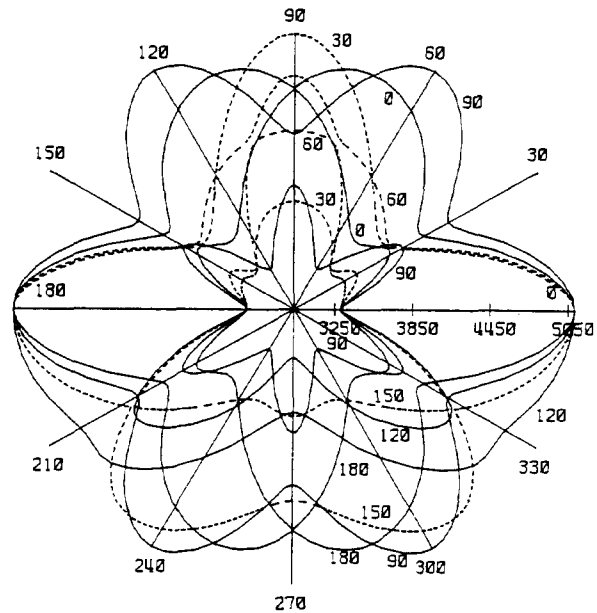modes is symmetric with regard to the YZ-plane.

Fig. 3

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Acknowledgement