SURFACE ACOUSTIC WAVE SENSITIVITY ON AN EXTERNAL MECHANICAL OR ELECTRICAL BIAS

D. GAFKA

Institute of Fundamental Technological Research
Polish Academy of Sciences
(00-049 Warszawa, ul. Świętokrzyska 21)

Using general rotationally invariant nonlinear electroelastic equations (energy balance equation and Gibbs function expansion) a derivation of constitutive equations for electroelastic media upon a mechanical or electrical bias has been presented. Bilinear constitutive relations for large quantities have been given and linear, but parametric, constitutive formulas for small-field variables have been derived in the reference or intermediate frame. Equations of motion and boundary conditions in the intermediate configuration required to solve the problem of SAW propagation are also reported. Basing on this theory, the velocity shifts of surface acoustic waves (SAW) for lithium niobate due to an external static stress or electric field are presented. Stress sensitivity is defined through six independent components of a second order symmetric tensor, and the electric field sensitivity is a vector of three components. Maps for different cuts of LiNbO₃ and a different direction of SAW propagation have been computed. These maps can be used to find new cuts of lithium niobate which has large or zero sensitivity either on the stress or electric field. This could be useful for special applications of the LiNbO₃ substrate in the technique of SAW devices.

1. Introduction

The change in surface acoustic wave (SAW) velocity due to applied static biasing stresses has been the subject of interest of many authors [5, 6, 7, 9, 10, 11, 12, 15, 19, 21]. The purpose of this paper is to present SAW velocity sensitivity on biasing, external stresses (whatever their origin: force, pressure, acceleration, thermoelastic effects) and also on external electric fields put to the crystal. Sensitivity has been calculated for different planes cuts and directions of SAW propagation.

This information can be useful in designing SAW devices of the kind as:
• transducers (IDT), delay lines (DL), filters, and oscillators [12], where the cut and direction of the smallest module of sensitivity should be chosen to minimize instabilities;
• sensors of pressure [12], acceleration [18, 19], force [27, 29], temperature [21], gas existence and so on, where the plane and direction of SAW propagation with the
highest module of sensitivity should be chosen such as to obtain suitable sensors for technical applications;

- SAW control devices where a stress, an electric field or a strain can be utilized to control the system, for example, selectivity of filters where the accurate plane and direction should be chosen [32].

Nonlinear electroelastic equations have already been considered since 1961 [1, 3, 4, 5]. Equations for small-field variable superposed on a large biasing state have also been reported by a few authors, for example [5, 7, 8, 14, 16, 17, 20, 22, 26, 28]. The fact that the nonlinear theory for small-field variables, obtained by only adding higher order terms in the linear constitutive equations, is inconsistent and gives wrong results is well known. So, in this paper we start in general from the internal energy balance to obtain proper nonlinear constitutive equations.

A theory will be given for any kind of electroelastic crystal, which is of course anisotropic, but homogeneous and nonconductive and nonsemiconductive. This means that we will not consider losses of any kind. As usual the electromagnetic part of the equations will be assumed in electrostatic approximation, so the magnetic field is not coupled with either the mechanical or electric field and need not be taken into account. Nonlinearity will be reduced to quadratic terms only, as they play the most important role in nonlinear phenomena or coupling between predeformation and small-field vibration (bilinear model).

Numerical results presenting SAW velocity sensitivity on different biases for lithium niobate have been calculated using the published values of the second and third order elastic, piezoelectric and dielectric constants [14, 16], and are reported at the end of the paper.

2. Nonlinear constitutive equations

Two basic configurations will be used. The reference frame connected with the material Cartesian coordinates, \( X_i, \ i=1, 2, 3 \), which will always be denoted by an uppercase letter and indices as well as every quantity given in this frame. The second is the actual configuration connected with the spatial Cartesian coordinates, \( x_i, \ i=1, 2, 3 \), which will be denoted by small letters and indices as well as every quantity given in this frame. Full advantage of well-known relations and tensor variables will be taken in the paper [2, 20]:

- mapping of the material point \( x_i=x_i(X_K, t) \);
- motion gradient \( F_{iK}=x_i,_{K} = \frac{\partial x_i}{\partial X_K}, J=\det F \);
- displacement gradient tensor \( H=\nabla U=F-I \), where \( I \) is the identity tensor and \( U_K=\delta_{K} x_i - X_K \);
- Cauchy strain tensor \( C=F^T F \);
- Lagrange strain tensor
\[ S = \frac{1}{2} (C - I) = \frac{1}{2} (H + H^T + H^T H); \]  

- velocity gradient tensor \( L = (\nabla V)^T \);
- rate of strain tensor \( D = \frac{1}{2} (L + L^T) \).

Also, we will denote electric strength in the actual frame by \( e = -\nabla \Phi \), electric polarization by \( p \), and the Maxwell stress tensor by

\[ t_{ij}^e = \varepsilon_0 e_i e_j + p_i e_j - 0.5 \varepsilon_0 e_k e_k \delta_{ij}, \]

which is not symmetric, but we can add the second term to the mechanical stress tensor, \( t_{ij}^m \) (nonsymmetric), and then they will both become symmetric as well as the total stress tensor

\[ t_{ij} = t_{ij}^m + t_{ij}^e = t_{ij}^{ms} + t_{ij}^{es}, \]

where

\[ t_{ij}^{es} = \varepsilon_0 e_i e_j - 0.5 \varepsilon_0 e_k e_k \delta_{ij}, \quad t_{ij}^{ms} = t_{ij}^m + p_i e_j. \]

The constitutive equations will be derived not in the actual frame like in [7], but in the reference frame like in [5, 14, 16, 20]. To solve equations for small-field variables superposed on a large biasing state, different authors have used different methods. The Taylor expansion about the intermediate state was exploited in [5, 14]. The multiple-scale technique was described in [14] and the perturbation method was used in [9, 10, 11, 22, 21] and mentioned in [14]. In this paper the straightforward substitution of the sum of the bias and small-field quantities will be performed to get small-field variables, parametric constitutive equations with coefficients depending on large quantities of the bias.

We will begin our considerations from the first law of thermodynamics, which is reproduced here for completeness. The global balance of energy stands that the change in time of the kinetic energy \( \mathcal{K} \) and the internal energy \( \mathcal{E} \) must be equated by the work \( \mathcal{W} \) done upon the body by external forces and heat \( \mathcal{Q} \) delivered to the body [8, 14, 20, 24]:

\[ \dot{\mathcal{K}} + \dot{\mathcal{E}} = \dot{\mathcal{W}} + \dot{\mathcal{Q}}. \]

In isothermal conditions the local balance equation, equivalent to the above, for electroelastic body can be written as [20]

\[ \rho \dot{\varepsilon} = \text{tr} \left( t^m L^T \right) + e \cdot p. \]

For the purpose of this paper it is more convenient to use instead of the internal energy density \( \varepsilon \) the scalar state function known as the Gibbs function, which can be obtained from by the Legendre transformation:

\[ \psi = \varepsilon - \frac{1}{\rho} e \cdot p, \]
so we can use the local energy balance in the form [20]

\[ \rho \dot{\psi} = \text{tr} (t^m L^T) - p \cdot \dot{e}. \]  

(8)

The internal energy \( \psi \) will be rotationally invariant if it is expressed in terms of material measures of the strain and electric field. We choose the Lagrange strain tensor \( S \), Eq. (1) and electric field convected to the reference frame, \( W=eF=-\nabla \Phi_f \), as independent variables. To get the Gibbs function in the form \( \psi = \psi (S, W) \), Eq. (8) must be rearranged to involve new variables. Differentiation of \( S \) and \( W \) in time gives

\[ \dot{S} = F^T DF, \quad \dot{e} = (\dot{W} - eLF) F^{-1}. \]  

(9)

Then

\[ \rho \dot{\psi} = \text{tr} (t^m L^T) - \text{tr} (pe^T) = \text{tr} (t^{ms} L^T) - \text{tr} (pF^{-1} \dot{W}^T). \]  

(10)

\( L^T \) can be decomposed into \( L^T = D - \Omega \), where \( \Omega = 0.5 (L - L^T) \) is the rate of the rotation tensor always skew-symmetric, so the product of \( t^{ms} \) and \( \Omega \) is always zero. We then get with the help of the inverse of the first of equations (9)

\[ \rho \dot{\psi} = \text{tr} (t^{ms} F^{-1} \dot{S}) - \text{tr} (pF^{-1} \dot{W}^T). \]  

(11)

The last equation rewritten in components is

\[ \rho \dot{\psi} = t_{ij} F^{-1}_{ik} F^{-1}_{jl} \dot{S}_{KL} + p_i e_j F^{-1}_{ik} F^{-1}_{jl} \dot{S}_{KL} - p_i F^{-1}_{ik} \dot{W}_K. \]  

(12)

To find the constitutive relations, we decompose \( \dot{\psi} \) into parts connected with nondependent variables

\[ \dot{\psi} = \frac{\partial \psi}{\partial S_{KL}} \frac{dS_{KL}}{dt} + \frac{\partial \psi}{\partial W_K} \frac{dW_K}{dt}. \]  

(13)

Multiplying Eq. (13) by \(-\rho\) and adding to Eq. (12) side by side, one can obtain

\[ \left( t^m_{ij} F^{-1}_{ik} F^{-1}_{jl} + p_i e_j F^{-1}_{ik} F^{-1}_{jl} - \rho \frac{\partial \psi}{\partial S_{KL}} \right) \dot{S}_{KL} - \left( p_i F^{-1}_{ik} + \rho \frac{\partial \psi}{\partial W_K} \right) \dot{W}_K = 0 \]  

(14)

Equation (14) must be hold for arbitrary nonzero time rotations of \( \dot{S}_{KL} \) and \( \dot{W}_K \), so it can be written separately as

\[ t^m_{ij} = \rho F^{-1}_{ik} F^{-1}_{jl} \frac{\partial \psi}{\partial S_{KL}} - p_i e_j = t^{ms}_{ij} - p_i e_j \]  

(15)

\[ p_i = -\rho F^{-1}_{ik} \frac{\partial \psi}{\partial W_K}. \]

There are still two quantities \( t^m_{ij}, p_i \) in the constitutive equations (15) given in the actual frame (spatial coordinates). It is obvious that if we want to apply constitutive relations
to practical problems, where we study the dynamical behaviour of a nonlinear elastic body of finite extent, it is much simpler to have these quantities convected to the reference frame (material coordinates). Then it will be easier to write the boundary conditions concerning either the mechanical displacement or stress, and either the electric potential or the electric displacement on the fixed surface in the reference frame instead of the deforming surface in the actual configuration.

So, we should briefly introduce \([5, 14, 16, 20]\):

- mechanical Piola—Kirchhoff stress tensor
  \[ T_{i j}^{m s} = J F^{-1}_{k l} t_{k j}^{m s}; \]  \hfill (16)

- Maxwell Piola—Kirchhoff stress tensor
  \[ T_{i j}^{e s} = J F^{-1}_{k l} e_{k j}^{s}; \]  \hfill (17)

- total Piola—Kirchhoff stress tensor
  \[ T_{i j} = T_{i j}^{m s} + T_{i j}^{e s} = J F^{-1}_{k l} t_{k j}; \]  \hfill (18)

- material polarization vector
  \[ P_{i} = J F^{-1}_{j l} p_{j}; \]  \hfill (19)

- material electric strength vector
  \[ E_{i} = J F^{-1}_{j l} e_{j}, \]  \hfill (20)

and of course the material electric displacement is \(D = \varepsilon_{0} E + P\).

It should be noted that \(E_{K}\) is not equal to \(-\Phi_{,K}\), because \(-\Phi_{,K}\) is \(W_{K}\), and \(E_{K}\) is only the transformed electric field from the actual to reference frame.

After substituting the second equation of (15) into Eq. (19) and using the conservation of mass equation in the form
\[ \rho^{F} = J \rho \]  \hfill (21)
(where \(\rho^{F}\) is the mass density in a free (undeformed) state, when the body is acted upon neither by force nor by electric field), one can obtain
\[ P_{i} = -\rho^{F} \frac{\partial \psi}{\partial W_{i}}. \]  \hfill (22)

Next, putting \(e = WF^{-1}\) into Eq. (20), it can be found that
\[ E_{i} = JC_{i k}^{-1} W_{k}. \]  \hfill (23)

With the help of the first equation of (15) and Eq. (16), we can express the mechanical Piola—Kirchhoff tensor as
\[ T_{i j}^{m s} = \delta_{i j} T_{i j}^{m s} = \rho^{F} F_{j l} \frac{\partial \psi}{\partial S_{i l}} \]  \hfill (24)
and taking into account Eq. (4) in Eq. (17), the Maxwell tensor can be expressed as
\[ T_{ij}^{e_0} = \delta_{ij} T_{ij}^{e_0} = J F_{kl}^{-1} (\varepsilon_0 F_{ik}^{-1} W_j F_{jk}^{-1} W_k - 0.5 \varepsilon_0 F_{il}^{-1} W_L F_{lk}^{-1} W_l \delta_{kj}) = \\
= J \varepsilon_0 W_j W_k (F_{ik}^{-1} F_{ij}^{-1} F_{jk}^{-1} - 0.5 F_{il}^{-1} F_{ik}^{-1} F_{kl}^{-1}). \] (25)

Equations (22), (23), (24) and (25) stand constitute relations in which every quantity is related to the reference frame.

3. Bilinear expansion of the Gibbs function

To obtain explicit forms (not with partial differentiation) of constitutive relations, we should expand the Gibbs thermodynamical function in terms of its independent variables in the reference frame. The expansion will be cut after the third order terms to get constitutive equations in a bilinear form. The linear and quadratic terms of constitutive relations play the most important role in describing nonlinear phenomena in electroelastic crystal [6, 13, 15, 16, 18, 19]. The other, higher order terms can be neglected. Let us introduce the expansion [14]

\[ \rho F \Psi = \frac{1}{2} c_{ijkl} s_{ij} s_{kl} + \frac{1}{6} c_{ijklmn} s_{ij} s_{kl} s_{mn} - \frac{1}{2} e_{ijkl} w_m s_{ij} s_{kl} + \\
- e_{miij} w_m s_{ij} - \frac{1}{2} \chi_{mn} w_m w_n - \frac{1}{6} \chi_{mnp} w_m w_n w_p - \frac{1}{2} l_{mni} w_m w_n s_{ij}, \] (26)

where:

- \( c_{ijkl} \) elastic tensor of the second order
- \( c_{ijklmn} \) elastic tensor of the third order
- \( e_{miij} \) piezoelectric tensor of the second order
- \( e_{ijkl} \) electroelastic tensor of the third order
- \( \chi_{mn} \) electric susceptibility tensor of the second order
- \( \chi_{mnp} \) electric susceptibility tensor of the third order
- \( l_{mni} \) electrostriction tensor of the third order.

Of course, in general, symmetry relations must be fulfilled [25]:

\[ c_{ijkl} = c_{ijlk} = c_{ijlk} = c_{klji} \]
\[ c_{ijklmn} = c_{ijklmn} = c_{ijlkmn} = c_{kljmni} = c_{mnklij} \]
\[ e_{miij} = e_{mij} \]
\[ e_{miij} = e_{mijkl} = e_{mijkl} = e_{mklij} \] (27)
\[ \chi_{mn} = \chi_{nm} \]
\[ \chi_{mnp} = \chi_{mpn} = \chi_{pnm} \]
\[ l_{mni} = l_{nmi} = l_{mni} \]

so we have only 21 independent coefficients of \( c_{ijkl} \), 56 of \( c_{ijklmn} \), 18 of \( e_{miij} \), 63 of \( e_{miijkl} \), 6 of \( \chi_{mn} \), 10 of \( \chi_{mnp} \) and 36 of \( l_{mni} \), what together gives 210 independent
material constants of crystals in the bilinear theory (45 in a linear one). But if a crystal has some symmetry points or axis or planes, what always happens, the number of material constants to be given is reduced further and is less than 210.

Additionally, we want to get expressions in the form like the form below:

\[ T = T(H,W) \quad D = D(H,W), \]  

(28)

where both \( W, H \) are gradients of the electric potential and mechanical displacement, respectively, \( W = -\nabla \Phi, H = \nabla U \), so we substitute now

\[ S = \frac{1}{2} (H + H^T + H^T H) \quad F = H + I, \]  

(29)

and [14]

\[ F^{-1} = I - H + H^T H + o(H^3) \quad J = 1 + \text{tr} \ H + \frac{1}{2} (\text{tr} \ H)^2 - \frac{1}{2} \text{tr} (H^T H) + o(H^3), \]  

(30)

where \( o(H^n) \) denotes the remaining terms of order higher than or equal to \( n \). After substitution of Eqs. (29) and (26) into Eq. (24) and dropping out higher terms, one can obtain

\[ T_{ij}^{ms} = c_{ijmn} H_{mn} + \left( c_{irnm} \delta_{jp} + \frac{1}{2} c_{ijrn} \delta_{pm} + c_{ijmnp} \right) H_{mn} H_{pr} + \]  

\[-(e_{pin} \delta_{jm} + e_{pilmn}) W_p W_{mn} - e_{pil} W_p - \frac{1}{2} l_{pril} W_p W_R. \]  

(31)

After substitution of Eq. (30) into Eq. (25), one can find

\[ T_{ij}^{m} = \frac{1}{2} \varepsilon_0 W_L W_K (\delta_{il} \delta_{jk} - \delta_{ik} \delta_{jl} - \delta_{ij} \delta_{kl}). \]  

(32)

Taking into account Eqs. (29) and (26), Eq. (22) can be rearranged as follows:

\[ P_I = e_{ikl} H_{kl} + \chi_{ij} W_J + \frac{1}{2} (e_{iklmn} + e_{inl} \delta_{km}) H_{kl} H_{mn} + \]  

\[ + \frac{1}{2} \chi_{ijk} W_J W_K + l_{ijkl} W_J H_{kl}. \]  

(33)

Next, substituting Eq. (30) into Eq. (23), one can obtain

\[ E_I = \delta_{ij} W_J + (\delta_{kl} \delta_{ij} - \delta_{il} \delta_{jk} - \delta_{ik} \delta_{jl}) W_J H_{kl}. \]  

(34)

Finally, we can join together \( T = T^{ms} + T^{es}, D = \varepsilon_0 E + P \), so the constitutive equations are obtained in the form
\[ T_{ij} = c_{ijkl} H_{kl} + c_{ijklmn} H_{kl} H_{mn} - e_{mi jkl} W_{m} H_{kl} - e_{mij} W_{m} - \frac{1}{2} l_{kl} W_{k} W_{l}, \]
\[ D_{i} = \varepsilon_{ij} W_{j} + \frac{1}{2} \varepsilon_{ijk} W_{j} W_{k} + l_{ijkl} W_{j} H_{kl} + \frac{1}{2} \epsilon_{iklmn} H_{kl} H_{mn} + e_{ikl} H_{kl}. \]

where the new tensors involved are

\[ l_{ijkl} = l_{ijkl} - \varepsilon_{0} (\delta_{il} \delta_{jk} + \delta_{ik} \delta_{jl} - \delta_{kl} \delta_{ij}) \]
\[ c_{ijklmn} = c_{inkl} \delta_{jm} + \frac{1}{2} c_{injl} \delta_{mk} + \frac{1}{2} c_{iklmn} \]
\[ e_{mi jkl} = e_{mij} \delta_{jk} + e_{mikl} \]
\[ \varepsilon_{iik} = \chi_{ijk} \]
\[ \varepsilon_{ij} = \varepsilon_{0} (\chi_{ij} + \delta_{ij}). \]

In the above equations, \( \varepsilon \) is the permittivity tensor of the crystal of the second order and \( \varepsilon \) is the permittivity tensor of the third order and \( l, c, e \) may be called third order effective tensors of electrostriction, elasticity and electroelasticity respectively. For these tensors the above symmetry relations are valid:

\[ l_{ijkl} = l_{ijlk} = l_{ijlk} \]
\[ c_{ijklmn} = c_{ijklmn} = c_{ijmnkl} \]
\[ e_{mi jkl} = e_{mij} \delta_{jk} + e_{mikl} \]
\[ \varepsilon_{ijk} = \varepsilon_{kij} = \varepsilon_{ijkl} \]
\[ \varepsilon_{ij} = \varepsilon_{ji}. \]

4. Parametric constitutive equations

The constitutive equations (35) are written in the reference frame. First, let us suppose, that the initial nonzero strain field as a result of external force or electric field exists in the body at first. Next, a small field is superposed to consider on this state. This means we now have a third, intermediate configuration of the body, in addition to the undisturbed reference configuration and actual one. The material point identified by the material coordinate \( X_{i} \) first moves to the intermediate coordinate \( X_{k} (X_{l}) \) by a large initial deformation and next to \( x_{k} (X_{l}) \) by a small alternating vibration. So every field quantity in the reference frame can be decomposed into two parts. The first is connected with the bias and the second, small, with SAW propagating in the body, for example. Let every time tilde denote quantities connected with the initial large state of deformation, whereas quantities without any indices denote SAW components. We have then, in the reference frame

\[ Z' = \tilde{Z} + Z, \quad \text{where} \quad Z = T, H, W, D, E, U, \Phi. \]
These total quantities must fulfil the constitutive equations (35), so

\[
\tilde{T}_{IJ} + T_{IJ} = \left\{ c_{IJKL} \tilde{H}_{KL} + c_{IJKLMN} \tilde{H}_{KL} \tilde{H}_{MN} - e_{MIJL} \tilde{W}_{M} \tilde{H}_{KL} - e_{MIJL} \tilde{W}_{M} + \frac{1}{2} l_{KLIJ} \tilde{W}_{K} \tilde{W}_{L} \right\} + \\
+ c_{IJKL} H_{KL} + c_{IJKLMN} H_{KL} \tilde{H}_{MN} + c_{IJMNKL} H_{KL} \tilde{H}_{MN} - e_{MIJL} W_{M} + \\
- e_{MIJL} W_{M} \tilde{H}_{KL} + \frac{1}{2} l_{KLIJ} W_{L} \tilde{W}_{K} + \frac{1}{2} l_{KLIJ} W_{L} \tilde{W}_{K} + \\
+ \left[ e_{IJKLMN} H_{KL} H_{MN} - e_{MIJL} W_{M} H_{KL} - \frac{1}{2} l_{KLIJ} W_{K} W_{L} \right] \right. 
\]

(39)

and

\[
\tilde{D}_{I} + D_{I} = \left\{ \varepsilon_{IJ} \tilde{W}_{J} + \frac{1}{2} \varepsilon_{JK} \tilde{W}_{J} \tilde{W}_{K} + l_{IJKL} \tilde{W}_{J} \tilde{H}_{KL} + \frac{1}{2} e_{IKLMN} \tilde{H}_{KL} \tilde{H}_{MN} + \\
+ e_{IK} \tilde{H}_{KL} \right\} + \varepsilon_{IJ} W_{J} + \frac{1}{2} \varepsilon_{JK} W_{J} \tilde{W}_{K} + \frac{1}{2} \varepsilon_{JK} W_{J} \tilde{W}_{K} + l_{IJKL} H_{KL} \tilde{W}_{J} + \\
+ l_{IJKL} W_{J} \tilde{H}_{KL} + \frac{1}{2} e_{IKLMN} H_{KL} \tilde{H}_{MN} + \frac{1}{2} e_{IMNKL} H_{KL} \tilde{H}_{MN} + e_{IK} H_{KL} + \\
+ \left[ \frac{1}{2} e_{JK} W_{J} W_{K} + l_{IJKL} W_{J} H_{KL} + \frac{1}{2} e_{IKLMN} H_{KL} H_{MN} \right]. 
\]

(40)

The terms in the last two formulas are regrouped in such a manner that the expressions in the first brackets can be said to be equal to the biasing quantities \( \tilde{T} \) and \( \tilde{D} \), respectively, while the terms in the square brackets can be neglected because they are second order terms of small-field quantities. After separation, one can obtain nonlinear constitutive equations for the large initial state in the form

\[
\tilde{T}_{IJ} = c_{IJKL} \tilde{H}_{KL} + c_{IJKLMN} \tilde{H}_{KL} \tilde{H}_{MN} - e_{MIJL} \tilde{W}_{M} \tilde{H}_{KL} - e_{MIJL} \tilde{W}_{M} - \frac{1}{2} l_{KLIJ} \tilde{W}_{K} \tilde{W}_{L}, 
\]

(41)

\[
\tilde{D}_{I} = \varepsilon_{IJ} \tilde{W}_{J} + \frac{1}{2} \varepsilon_{JK} \tilde{W}_{J} \tilde{W}_{K} + l_{IJKL} \tilde{W}_{J} \tilde{H}_{KL} + \frac{1}{2} e_{IKLMN} \tilde{H}_{KL} \tilde{H}_{MN} + e_{IK} \tilde{H}_{KL}, 
\]

and linear ones for a SAW small-field superposed on this biasing state

\[
T_{IJ} = c_{IJKL} H_{KL} - e_{MIJL} W_{M} 
\]

(42)

\[
D_{I} = \varepsilon_{IJ} W_{J} + e_{IKL} H_{KL}, 
\]

where the effective tensors are, of course, dependent on the biasing electric field and displacement gradient:
\[ c_{ijkl}^{\text{eff}} = c_{ijkl} + 2e_{ijklmn} \dot{H}_{mn} - e_{mijkl} \ddot{W}_m \]
\[ e_{ijkl}^{\text{eff}} = e_{ijkl} + e_{mijkl} \dot{H}_{kl} + l_{kmij} \ddot{W}_k \]
\[ e_{ij}^{\text{eff}} = e_{ij} + e_{ijk} \dot{W}_k + l_{ijkl} \ddot{H}_{kl}. \]  

(43)

5. SAW propagation description

The velocity of SAW, having the harmonic form below

\[ e^{-j\omega t} e^{j\omega (t - \frac{x_i}{V})} \quad \text{Im} \{b\} < 0 \]  

(44)
on the surface of the piezoelectric half-space, is searched now where \( \omega \) is the angular frequency, \( V \) is the wave velocity, and \( b \) is the decay constant of SAW. The wave is assumed to propagate in the \( X_1 \) direction and decay in the \( X_2 \) direction and also SAW is regarded as small amplitude wave, so it doesn’t appreciably modify the bias.

To calculate SAW velocity, the constitutive equations (42) must be joined with the equation of motion written in the frame after the bias \([5, 9, 16, 23, 28]\)

\[ T_{ij,i} = \rho \ddot{U}_j \]
\[ D_{j} = 0, \]  

(45)

where \( \rho = \rho \hat{F} / (\det \hat{F}) \) is the mass density after the biasing deformation. The boundary conditions on the surface of SAW propagation must be added to the above to close mathematically the problem. They are as follows \([5, 28]\):

\[ T_{ij} n_I = 0 \]

and for free surface

\[ D_I n_I = 0 \]
or metalized surface

\[ E_I \times n_I = 0, \]  

(6)

where \( n \) is the normal versor to the surface and two often exploited cases are described.

6. SAW sensitivity mapping

Using Eqs. (42), (45) and (46), the numerical program was developed to compute the SAW velocity on a piezoelectric substrate acted upon by either a stress or an electric field. The results are presented for one piezoelectric crystal, which is lithium niobate, as it is a well-known piezoelectric material, used as a substrate for many different surface acoustic wave (SAW) devices, linear ones and nonlinear as well.

The SAW velocity \( V \) [km/s] depending on the biasing stress \( T \) [GPa] in the case of the free surface \( V_\infty \) and metalized surface \( V_0 \) for three directions of putting initial
stress: along wave propagation $X_1$, perpendicularly to the cut surface $X_2$ and perpendicularly to the wave propagation direction in the cut plane $X_3$ are presented in Fig. 1 for LiNbO$_3$ Y-cut Z-propagation ($X_1 = Z$).

![Fig. 1. SAW velocity as a function of the prestress.](image)

It can be seen that SAW velocity is a linear function of a biasing stress, and generally it was found that the dependence of the relative change of SAW velocity due to the external stress is a linear tensor function of the form below:

$$\frac{\Delta V}{V_F} = \frac{V - V_F}{V_F} = \mathcal{H}_{ij} \tilde{T}_{ij},$$  \hspace{1cm} (47)

where $V_F$ is the SAW velocity on a free substrate (without any bias), $V$ is the velocity after bias, and $\mathcal{H}$ is the second order sensitivity tensor which has the same symmetry as $\tilde{T}$, so it has six independent components. This formula agrees well with the one obtained using the perturbation method [9, 11, 15, 28]. A similar equation can be written for the electric field sensitivity:

$$\frac{\Delta V}{V_F} = \frac{V - V_F}{V_F} = \mathcal{G}_{1E_1},$$  \hspace{1cm} (48)

where $\mathcal{G}$ is the first order sensitivity tensor (three components), so nine coefficients are necessary to describe completely the SAW velocity sensitivity on the external bias. It should be noted that the electromechanical coupling factor is much less sensitive on
both biases, so the same sensitivity can be used in the case of a metalized surface of lithium niobate as well as in the case of a free surface.

The results are presented for a lithium niobate crystal, and six independent stress sensitivity coefficients $\mathcal{H}_{11}$ are plotted as a contour-line mapping function of the cut angles of the plate and the propagation direction of the SAW. The homogeneous distribution of static biasing stresses is assumed, i.e. SAW is considered to propagate in a very small volume (with respect to the dimensions of the plate) — a local formulation.

The notation describing the lithium niobate crystal is defined according to the IEEE standard on piezoelectricity [31], i.e., the Euler triplet of angles is used: $\lambda$, $\mu$, $\theta$, where the first two describe the cut of the plate and $\theta$ is the propagation direction on this plane. The propagation direction is $X_1$ and the axis perpendicular to the cut plane is $X_2$. The tensors are related to the same coordinate system.

In the pictures below the angles are chosen as $\lambda = 0^\circ$ and $\mu \in [0,90^\circ]$, $\theta \in [0,90^\circ]$. This means that left lower corner of each picture is the ZX cut, left upper is the ZY cut, right lower is the YX cut, and right upper is the YZ cut of lithium niobate.

Figures 2—7 show contour-line characteristics of six components of the stress sensitivity for $\lambda = 0^\circ$. Figure 2 is for the normal stress acting along the propagation direction of SAW, Fig. 3 is for the normal stress acting on the propagation plane, Fig. 4 is for the normal stress acting along the direction perpendicular to SAW propagation direction and Figs 5, 6, 7 are for shear stresses respectively. The component of $\mathcal{H}_{11}$ has

![Fig. 2. Contour-line charts of the stress sensitivity $H_{11}$ in the $\mu - \theta$ plane. $\lambda = 0^\circ$. The unit of contour labels is $10^{-9}[\text{m}^2/\text{N}]$.](image)
Fig. 3. Contour-line charts of the stress sensitivity $H_{22}$ in the $\mu - \theta$ plane. $\lambda = 0^\circ$. The unit of contour labels is $10^{-9} [m^2/N]$.

Fig. 4. Contour-line charts of the stress sensitivity $H_{43}$ in the $\mu - \theta$ plane. $\lambda = 0^\circ$. The unit of contour labels is $10^{-9} [m^2/N]$.

[251]
Fig. 5. Contour-line charts of the stress sensitivity $H_1$ in the $\mu - \theta$ plane. $\lambda = 0^\circ$. The unit of contour labels is $10^{-9}$ [m²/N].

Fig. 6. Contour-line charts of the stress sensitivity $H_6$ in the $\mu - \theta$ plane. $\lambda = 0^\circ$. The unit of contour labels is $10^{-9}$ [m²/N].
its maximum near the YZ cut, $\mathcal{H}_{22}$ has two curves in the $\mu - \theta$ plane which are compensate regions for this kind of stress ($\mathcal{H}_{22} = 0$), while $\mathcal{H}_{33}$ has the maximum for about $\mu = 33^\circ$, $\theta = 0^\circ$. For shear stress sensitivities, one can also easily find minima, maxima and compensate regions in the $\mu - \theta$ plane. The unit of contour-lines is $10^{-9}$ [m²/N].

Three components, $\mathcal{H}_{11}$, $\mathcal{H}_{22}$, $\mathcal{H}_{33}$ are drawn together as a vector bar in Fig. 8. The longitude of the bar shows the magnitude of $\mathcal{H} = [\mathcal{H}_{11}, \mathcal{H}_{22}, \mathcal{H}_{33}]$ and the direction of the bar shows the most sensitive direction of putting the stress ($X_1$ is parallel to $\mu$, $X_2$ to $\theta$, and $X_3$ is perpendicular to the picture plane). Some contours of $\mathcal{H}_{11}$ are also drawn.

The results for three independent components of the sensitivity vector $\mathcal{G}$ are plotted as a contour-line mapping function of the same angles as in the above section. The electric field is also assumed to be homogeneous and static like the stress above. Figures 9 - 11 show the sensitivity of SAW velocity on the electric field put (Fig. 9) along the direction of propagation, Fig. 10 perpendicularly to the cut plane, and Fig. 11 perpendicularly to the propagation direction in the cut plane. The unit of contour-line is $10^{-12}$ [m/V]. The whole sensitivity vector is drawn as a bar in Fig. 12. The rules are the same as for Figs. 2 - 4 and 8.
Fig. 8. Vector $[H_{11}, H_{22}, H_{33}]$ bar graph for the normal stress sensitivity in the $\mu-\theta$ plane. $\lambda=0^\circ$.

Fig. 9. Contour-line charts of the electric field sensitivity $G_z$ in the $\mu-\theta$ plane, $\lambda=0^\circ$. The unit of contour labels is $10^{-12} [m/V]$. [254]
Fig. 10. Contour-line charts of the electric field sensitivity $G_2$ in the $\mu - \theta$ plane, $\lambda = 0^\circ$. The unit of contour labels is $10^{-12}$ [m/V].

Fig. 11. Contour-line charts of the electric field sensitivity $G_3$ in the $\mu - \theta$ plane, $\lambda = 0^\circ$. The unit of contour labels is $10^{-12}$ [m/V].

[255]
Fig. 12. Vector \([G_1, G_2, G_3]\) bar graph for the electric field sensitivity in the \(\mu-\theta\) plane, \(\lambda = 0^\circ\).

7. Conclusions

We have started, in general, from nonlinear equations to solve the nonlinear dynamical problem for small-field variables of SAW superposed on a large biasing state in an electrostatic body. Since we can see the final results, instead of solving nonlinear equations, we may solve linear ones, but with tensor coefficients being parametrically dependent on the bias.

Basing on the theory, a model describing the SAW velocity shift due to an external static electric field or a stress has been presented. The computed results for lithium niobate have been obtained and reported. It is easy to find the Euler angle triplet of minima and maxima or compensate regions (zero sensitivity), what is necessary for applications. The presented maps can be useful for the choice of locus and directions of propagation for LiNbO\(_3\) to obtain suitable ones. A balance between other SAW characteristics: the electromechanical coupling factor, the power flow angle should also be taken into account in designing SAW devices.
Acknowledgements

The author would like express his gratitude to Prof. K. YAMAOUCHI, and Prof. J. TANI, Tohoku University, for making available correct third order material tensors of lithium niobate [16] and for a useful discussion. Special thanks go to Prof. E. DANICKI, Institute of Fundamental Technological Research of the Polish Academy of Sciences for a valuable discussion and for giving the basic source code of the numerical program for SAW velocity calculations [30], which after some changes was used to produce computed results.

References


Received October 28, 1992