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INFLUENCE OF A BIASING STRESS ON THE SAW VELOCITY ON PIEZOELECTRIC SUBSTRATE

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The nonlinear differential equations and boundary conditions in small-field variables, for small fields superposed on large static biasing states, are obtained from general invariant nonlinear electroelastic equations. The influence on Surface Acoustic Wave (SAW) velocity of prestress (six independent tensor coefficients) is analyzed. Biasing stress tensor is involved directly into equations of motion, and the linearization about the static state is done. Change of mass density as well as the effective elastic constants of the piezoelectric substrate as a consequence of prestress is taken into account. Numerical results, given SAW velocity on prestressed substrate for different direction of stress and wave propagation are obtained for lithium niobate.

Developed theory and numerical program may be useful for analyzing and designing SAW sensors of temperature, pressure, acceleration and stress.

1. Introduction

In recent years, a number of workers [3, 5, 6, 7,9–12, 15, 17, 20, 21] have analysed and measured the change in acoustic surface wave (SAW) velocity due to applied static biasing stresses. The problem is interesting from three points of view. First, this effect can be easily used in SAW sensors of pressure, acceleration, force, temperature, gas existence and others [6, 12, 15, 16, 17]. Second, the main sources of frequency instabilities of SAW oscillators and other devices are temperature and forces effects [6, 16, 20]. Therefore it can be useful to describe stress sensitivity of SAW velocity. Third, the stress or strain may be utilized to control the performance of SAW devices for example selectivity of filters [6, 9] or temperature compensation of the devices.

In this paper a system of nonlinear electroelastic equations for small fields superposed on a bias [1, 2, 3, 13, 18, 21] is applied to the determination of the velocity of SAW in prestressed piezoelectric substrate. The influence of the biasing stress appears in the boundary conditions as well as the differential equations. The equations in the paper are written in the reference frame, connected with the material coordinates to make the boundary conditions easy to formulate, so the stress tensor is the Piola-Kirchhoff tensor [13, 18]. Although the electric, electroelastic and elastic nonlinearities are included in the basic equations, only the elastic nonlinearities are included in the calculation, because the rest of coefficients and higher order constants can be negligible and have the second order meaning in the considered problem [13, 20].

Nonlinear system of equations is linearized involving decomposition of the stress and other field quantities into two parts, static biasing one, and dynamic connected with SAW. After that the well-known procedure is used to obtain final results and computer algorithm [19]. Numerical results for Y cut lithium niobate are presented using the published values of the second and third order elastic, piezoelectric and dielectric constants.

2. Nonlinear electroelastic equations

Velocity of SAW, having a harmonic form below

$$e^{-jbX_2} \cdot e^{j\omega(t - X_1/v)} \qquad (\mathrm{Im}\{b\} < 0) \tag{1}$$

on the surface of the piezoelectric halfspace is searched. The halfspace is under initial stress. The structure considered and used coordinate system is depicted in Fig. 1. The denotations are as follow: ω — angular frequency, v — wave velocity, b — decay constant of SAW, X_i — material coordinates.

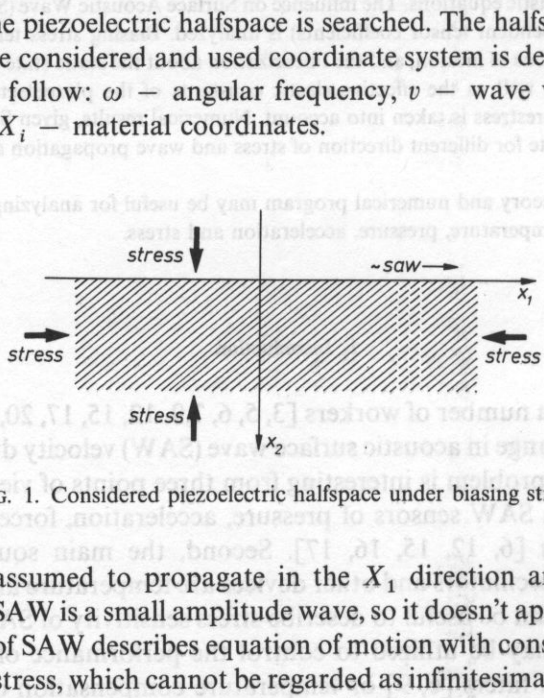

FIG. 1. Considered piezoelectric halfspace under biasing stress

The wave is assumed to propagate in the X_1 direction and decay in the X_2 direction and also SAW is a small amplitude wave, so it doesn't appreciably modify the bias. Propagation of SAW describes equation of motion with constitutive relations. In the case of biasing stress, which cannot be regarded as infinitesimally small, the general nonlinear equations should be taken into consideration as a starting point. They are written below in the reference frame with material coordinates (Lagrange's description), so stress tensor T is the Piola-Kirchhoff tensor [13, 18, 21]

$$\varrho \ddot{u}_j = \frac{\partial T_{ij}}{\partial X_i}, \tag{2}$$

$$T_{ij} = c_{ijkl}u_{k,l} + \gamma_{ijklmn}u_{k,l}u_{m,n} - e_{kij}E_k, \tag{3}$$

$$D_j = e_{jkl}u_{k,l} + \varepsilon_{ji}E_i. \tag{4}$$

In equation (2) ϱ is the mass density, and u is the displacement vector. It should be noted that ϱ is a function of stress $\varrho = \varrho(T)$ and this effect will be taken into account later. Constitutive relation (3) for a Piola-Kirchhoff stress tensor is composed of three parts. First component is linear elastic term with second order elastic tensor c_{ijkl} in the unprestressed state.The second is nonlinear elastic term with the third order effective (because in actual frame) elastic tensor γ_{ijklmn} and the third part is the piezoelectric term with the electroelastic tensor (linear only) e_{ijk}. The second constitutive relation (4) is usual for piezoelectrics and contains linear term of electroelasticity and electricity.

Effective elastic tensor γ_{ijklmn} can be obtained on the strength of thermodynamical considerations in the reference frame and has the form [13, 18, 21]

$$\gamma_{ijklmn} = c_{inkl}\delta_{jm} + 0.5c_{ijnl}\delta_{km} + 0.5c_{ijklmn}. \tag{5}$$

It depends on elastic material tensors of the second and third order given in tables of crystals [4, 13], δ is the identity tensor.

It should be noted that in equations (2)–(4) the nonlinearities between T and E, D and u, and also D and E are neglected. Dropt components have the second order meaning in comparison to elastic nonlinearity because of the character of piezoelectric phenomena [13, 20].

3. Boundary conditions

Presented system of equations (2)–(4) is valid for a piezoelectric space. For the case of SAW on the halfspace surface, to close mathematically the problem the boundary conditions must be added to the propagation equations. Because every field quantity is defined in the actual frame, they are valid even then if the boundary surface is deformed under biasing stress. It allows to formulate boundary conditions formaly the same as in the unprestressed case [8, 13, 14, 18, 19].

Mechanical boundary condition is vanishing of the SAW stress components on the surface

$$T_{2j} = 0 \quad \text{for} \quad X_2 = 0 \tag{6}$$

and electric boundary condition is vanishing of the SAW either electric strength

$$\mathrm{E} = 0 \quad \text{for } X_2 = 0 \tag{7}$$

or electric displacement

$$\Delta D_{\perp} = 0 \quad \text{for } X_2 = 0 \tag{8}$$

depending on that if the surface is shorted (metalized) or free (vacuum) respectively.

Involving (3), condition (6) can be written as

$$c_{2jkl}u_{k,l}+\gamma_{2jklmn}u_{k,l}u_{m,n}-e_{k2j}E_k=0 \tag{9}$$

what is now more complicated relation then in the unprestressed case (nonlinear).

Propagation equations (2)–(4) with boundary conditions (9) and (7) or (8) stand complete system of equations describing propagation of SAW on prestressed piezoelectric substrate.

4. Procedure of linearization

Formulated problem has been solved by a few authors using many different methods, for example making Talor expansion about the gradient of the static displacement [6, 13], using polynomial approximation or a multi-scale method [13]. The most known method is the perturbation method [7, 10, 11, 12, 13, 15], which gives the integral relation for the velocity variation. The comparison of obtained results to perturbation theory will be given at the and of the paper.

To find the linearized form of the equations (2)–(4) the decomposition of every quantity appearing in these equations has been done. It is assumed that displacements in the substrate can be separated into two parts: biasing static (or quasi-static) displacement denoted by u_i^s resulting from biasing stress T_{ij}^s and dynamic displacement connected with the SAW u_i^d

$$\begin{aligned} u_i &= u_i^s+u_i^d = x_i-X_i,\\ u_i^s &= X_i^s-X_i,\\ u_i^d &= x_i-X_i^s. \end{aligned} \tag{10}$$

Analogously stress is decomposed into two components

$$T_{ij}=T_{ij}^s+T_{ij}^d \tag{11}$$

and additionally the static part is assumed to be homogeneous

$$T_{ij}^s=\mathrm{const}\,(X_i,t). \tag{12}$$

It should be written clearly now, that after biasing stress the mass density ϱ is changed into ϱ' because ϱ is a function of stress, so

$$\varrho'=\varrho\,(T_{ij}^s). \tag{13}$$

In piezoelectric substrate the initial electric field is conncted (because of nonzero tensor e) with the biasing stress. This effect gives some nonzero electric strength in the piezoelectric solid but doesn't perturb the SAW propagation, so it is neglected.

After substituting equations (10)–(13) into propagation equations (2)–(4) one can obtain separated relations for static biasing state and dynamic SAW propagation. The equation of motion

$$\varrho' \ddot{u}_j^d = \frac{\partial T_{ij}^d}{\partial X_i} \tag{14}$$

contains only the dynamical quantities and new mass density ϱ'. The constitutive equations can be written as follows

$$T_{ij}^s + T_{ij}^d = c_{ijkl}(u_{k,l}^s + u_{k,l}^d) - e_{kij}E_k + \gamma_{ijklmn}(u_{k,l}^s + u_{k,l}^d)(u_{m,n}^s + u_{m,n}^d) \tag{15}$$

$$D_j = e_{jkl}u_{k,l}^a + \varepsilon_{ji}E_i. \tag{16}$$

(as it was mentioned above the static biasing part of electric quantities are neglected). Equation (15) can be separated into two independent equations, one for static state

$$T_{ij}^s = c_{ijkl}u_{k,l}^s + \gamma_{ijklmn}u_{k,l}^s u_{m,n}^s \tag{17}$$

and the other for SAW

$$T_{ij}^d = c_{ijkl}u_{k,l}^d + \gamma_{ijklmn}u_{kl}^d u_{m,n}^d + \gamma_{ijklmn}u_{k,l}^s u_{m,n}^d + \gamma_{ijklmn}u_{k,l}^d u_{m,n}^s - e_{kij}E_k. \tag{18}$$

Equation (17) can be made a little bit easier, but the biasing state must be assumed small, small enough to neglect the square term in (17). And because SAW is assumed to be a small amplitude wave the square term $u_{k,l}^d u_{m,n}^d$ in (18) can be neglected also. These two assumption are written together, as

$$|u_{k,l}^d| \ll |u_{k,l}^s| \ll 1. \tag{19}$$

Of course the mixed terms $u_{k,l}^s u_{m,n}^d$ must stay in (18). The linear elastic constitutive relation for the biasing state is obtained from (17)

$$T_{ij}^s = c_{ijkl}u_{k,l}^s \tag{20}$$

and for SAW such a constitutive relation is derived from (18)

$$T_{ij}^d = c_{ijkl}u_{k,l}^d + (\gamma_{ijklmn} + \gamma_{ijmnkl})u_{m,n}^s u_{k,l}^d - e_{kij}E_k. \tag{21}$$

The last equation can be written in a form

$$T_{ij}^d = c'_{ijkl}u_{k,l}^d - e_{kij}E_k \tag{22}$$

which is the same as in linear piezoelectricity [8, 14, 18, 19]. The only change in c'_{ijkl} instead of c_{ijkl}, where

$$c'_{ijkl} = c_{ijkl} + (\gamma_{ijklmn} + \gamma_{ijmnkl})u_{m,n}^s. \tag{23}$$

Due to stress the mass density changes its value also, what has been mentioned by ϱ' in (19). This is because of the change of the volume of the substrate, and though [1]

$$\varrho' = \varrho/(1 + u_{m,m}^s). \tag{24}$$

Appearing in (23) and (24) quantity $u_{m,n}^s$ can be derived inverting the matrix equation (20)

$$u^s_{m,n} = c^{-1}_{stmn} T^s_{st}. \tag{25}$$

Concluding, making some additional assumptions such a linearized system of equations

$$\varrho' u^d_j = \frac{\partial T^d_{ij}}{\partial X_i} \tag{26}$$

$$T^d_{ij} = c'_{ijkl} u^d_{k,l} - e_{kij} E_k \tag{27}$$

$$D_j = e_{jkl} u^d_{k,l} + \varepsilon_{ji} E_i, \tag{28}$$

describing SAW propagation on prestressed piezoelectric substrate has been obtained. This system is formally identical to the system if the biasing stress doesn't exist. The coefficients are changed only: $c_{ijkl} \to c'_{ijkl}$ expressed in (23) with (25) $\varrho \to \varrho'$ expressed in (24), (25) and they are in fact functions of biasing stress.

The main advantage of presented reformulation is that one can use any well-known method or algorithm to solve the linear problem [8, 19] making small changes.

5. Numerical results

Taking ready made computer program for calculations SAW velocities on the unprestressed substrate surface, written by E. Danicki [19], and changing the algorithm (e.g. involving third order elastic constants and biasing stress tensor values as new parameters) the author can calculate SAW velocities for different directions of propagation and different tensor of prestress.

The results for lithium niobate Y-cut are presented as an example. First material data of $LiNbO_3$ are rewritten basing on literature:

1/ mass density [13]

$\varrho = 4.7 \cdot 10^3$ kg/m^3

2/ second order coefficients (in Voigt's notation) [13]

– independent elastic constants [GPa]

$c_{11} = 203$ $\quad c_{12} = 53$ $\quad c_{13} = 75$

$c_{33} = 245$ $\quad c_{44} = 60$ $\quad c_{14} = 9$

– the other nonvanishing elastic constants

$c_{22} = c_{11}$ $\quad c_{23} = c_{13}$ $\quad c_{24} = -c_{14}$

$c_{55} = c_{44}$ $\quad c_{56} = c_{14}$ $\quad c_{66} = 0.5(c_{11} - c_{12})$

– independent piezoelectric constants [C/m^2]

$e_{15} = 3.7$ $\quad e_{22} = 2.5$ $\quad e_{31} = 0.2$ $\quad e_{33} = 1.3$

– the other nonvanishing piezoelectric constants

$e_{16} = -e_{22}$ $e_{21} = -e_{22}$ $e_{24} = e_{15}$ $e_{32} = e_{31}$

– nonzero electric constants [pF]

$\varepsilon_{11} = 389$ $\varepsilon_{33} = 257$ $\varepsilon_{22} = \varepsilon_{11}$

3/ third order elastic constants [GPa] (average) [4, 13]

$c_{111} = -512$ $c_{123} = 719$ $c_{144} = -37$ $c_{344} = -540$

$c_{112} = 454$ $c_{124} = 55$ $c_{155} = -599$ $c_{444} = -41$

$c_{113} = 728$ $c_{133} = -34$ $c_{222} = -478$

$c_{114} = -410$ $c_{134} = -1$ $c_{333} = -363$

$c_{223} = c_{113}$ $c_{233} = c_{133}$ $c_{234} = -c_{134}$

$c_{244} = c_{155}$ $c_{255} = c_{144}$ $c_{455} = -c_{444}$

$c_{355} = c_{344}$ $c_{356} = c_{134}$ $c_{466} = c_{124}$

$c_{122} = c_{111} + c_{112} - c_{222}$ $c_{256} = 0.5(c_{114} - c_{124})$

$c_{156} = 0.5(c_{114} + c_{124})$ $c_{266} = 0.5(2c_{111} - c_{112} - c_{222})$

$c_{224} = -c_{114} - 2c_{124}$ $c_{166} = 0.5(-2c_{111} - c_{112} + 3c_{222}$

$c_{366} = 0.5(c_{113} - c_{123})$ $c_{456} = 0.5(-c_{144} + c_{155})$

The SAW velocity V [km/s] depending on the biasing stress T [GPa] in the case of free surface V_∞ and metalized surface V_0 for three direction of putting initial stress: along wave propagation X_1, perpendicularly to cut surface X_2 and perpendicularly to wave propagation in the cut plane X_3 are presented in Fig. 2 for $LiNbO_3$ *Y*-cut *Z*-propagation ($X_1 = Z$).

Normalized velocity

$$(V(T) - V(T=0))/(V(T=0))$$

in relation to zero biasing state are presented for $LiNbO_3$ *YZ* ($X_1 = Z$) in Fig. 3, and for $LiNbO_3$ YX ($X_1 = X$) in Fig. 4. It doesn't matter if the surface is metalized or free, because the prestress doesn't change the electromechanical coupling coefficient $(V_\infty - V_0)/V_0$ of the piezoelectric substrate (with the 0.0003 precision).

In the next two figures, Fig. 5 and Fig. 6, relative change of decay of SAW propagating on the stressed surface versus stress

$$(t(T) - t(T=0))/t(T=0) = \Delta t/t(T)$$

is presented for the same cuts of $LiNbO_3$. The SAW velocity change are taken into account not only, but also the change of the length (the path of propagation) under biasing stress.

Additionally, the change of SAW velocity versus the angle of propagation in relation to *Z* axis of $LiNbO_3$ Y-cut under biasing stress $T = 2$GPa put in the X_1 direction are illustrated in Fig. 7. The picture presents SAW velocity for unprestressed substrate also.

The last Fig. 8 is made in the polar coordinates on the cut surface *Y* of $LiNbO_3$. Four SAW velocity curves for zero biasing stress $T = 2$GPa stress putting in the three different directions are presented.

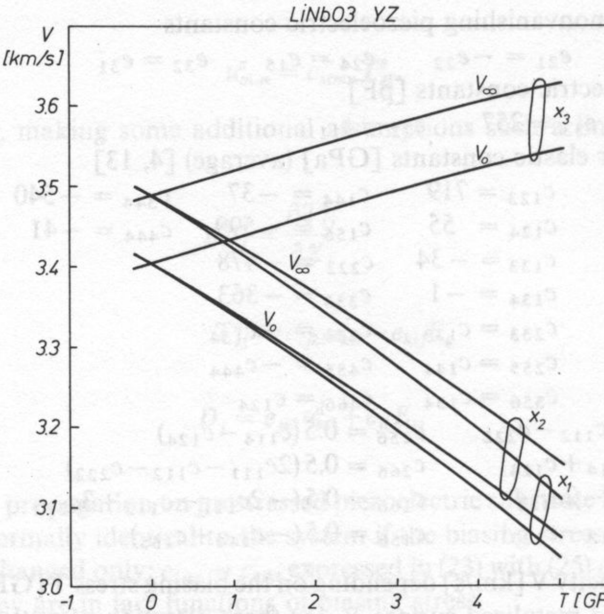

FIG. 2. SAW velocity as a function of prestress

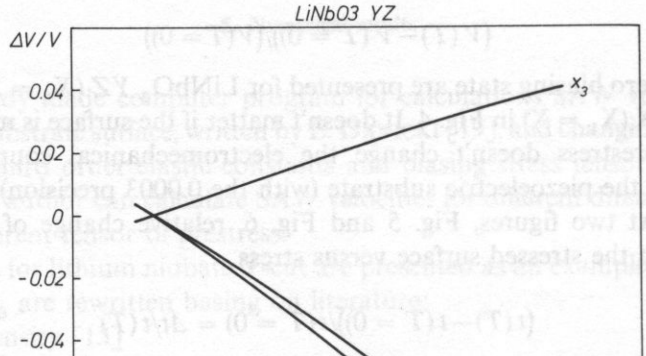

FIG. 3. Relative SAW velocity change versus static biasing stress

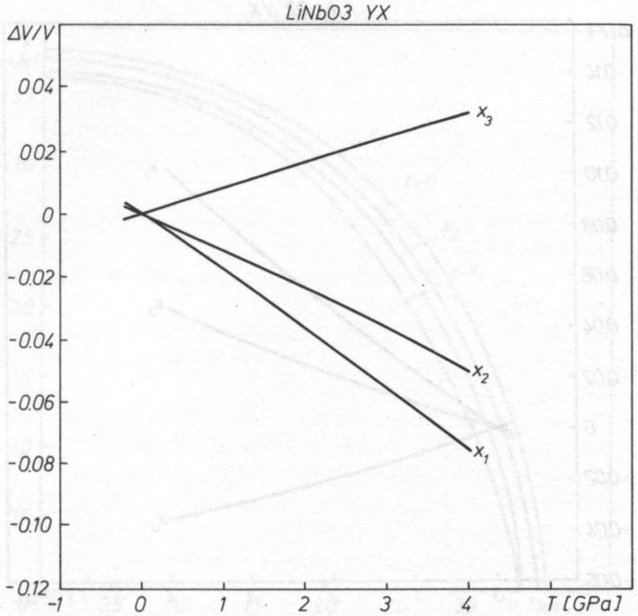

FIG. 4. Relative SAW velocity change versus static biasing stress

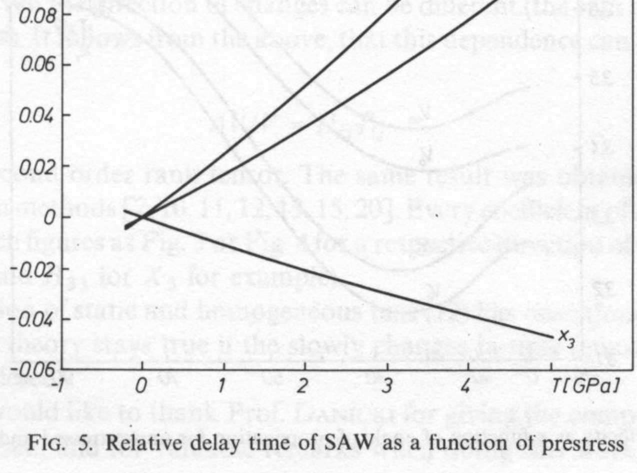

FIG. 5. Relative delay time of SAW as a function of prestress

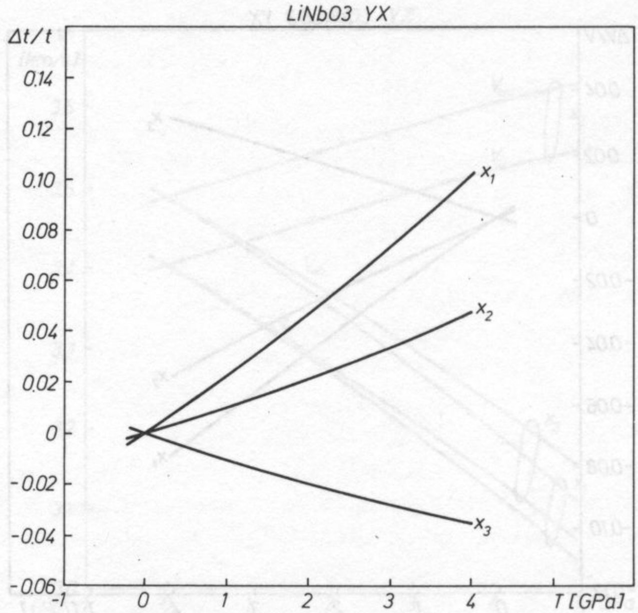

FIG. 6. Relative delay time of SAW as a function of prestress

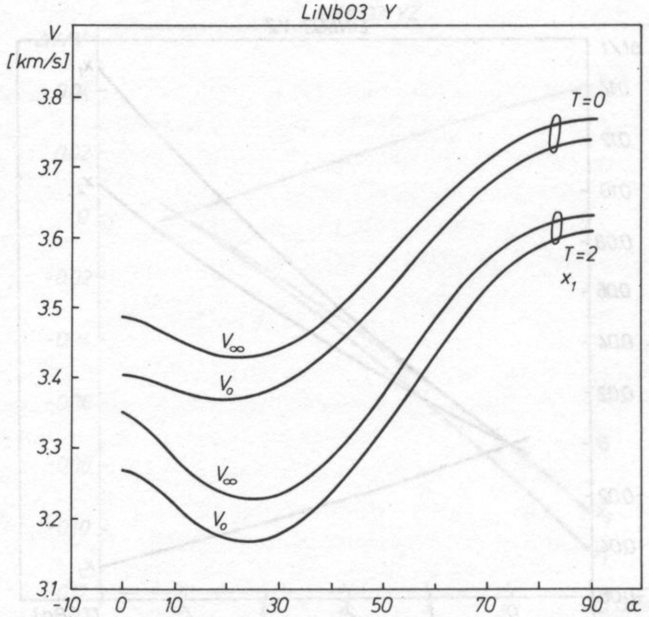

FIG. 7. SAW velocity as a function of angle of propagation for unprestressed and prestressed case

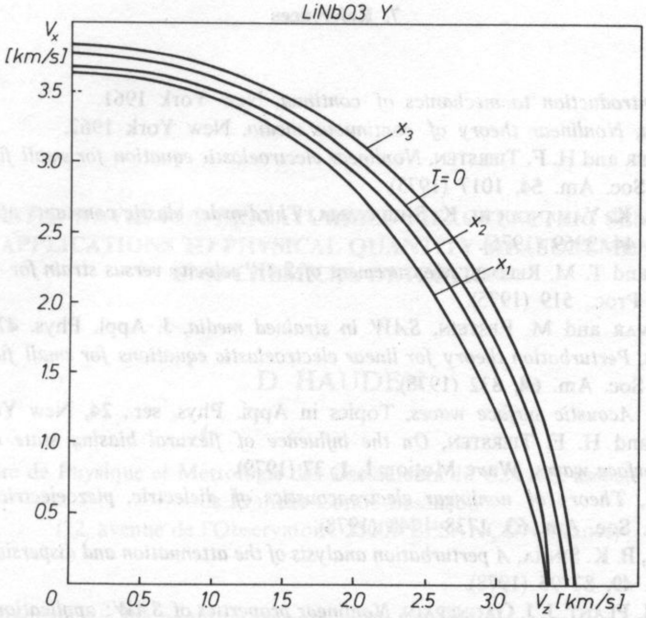

FIG. 8. SAW velocity as a function of angle of propagation for unprestressed and three directions of putting stress, in polar coordinates

6. Conclusions

Numerical results shows that the influence of the biasing stress on the SAW velocity is appreciable and linear (in tested range) and different for different direction of stress existence. Even the direction of changes can be different (the sign of curve slopes in Fig. 3 and Fig. 4). It follows from the above, that this dependence can be describe by the formula

$$\Delta V/V = H_{ij}T_{ij} \tag{29}$$

where H is the second order rank tensor. The same result was obtained by authors using perturbation methods [7, 10, 11, 12, 13, 15, 20]. Every coefficient of H_{ij} is the slope of the curve on such figures as Fig. 3 or Fig. 4 for a respective direction of stress (H_{11} for X_1, H_{22} for X_2 and H_{33} for X_3 for example).

The assumption of static and homogeneous bias (12) has been done in the paper, but the presented theory stays true if the slowly changes in time (quasistatics) of the prestress is considered.

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