The reflection of ultrasound from stressed piezoelectric crystals

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Abstract
A survey of the existing literature reveals research topics that span the whole range from interaction of ultrasound with isotropic materials to stressed general anisotropic materials on the one hand and unstressed piezoelectric materials on the other hand. As far as we know, besides one report dealing with BG waves, there are no reports available that describe the interaction of ultrasound with piezoelectric materials of general anisotropy under stress. The reason is probably the theoretical complexity of the subject.

The present paper reports how the interaction of ultrasound with single and multi layered piezoelectric materials under stress is described and highlights some of the peculiarities of the numerical results in the presence of stress compared to the unstressed case. This work may form the basic impetus for the future technology to manipulate properties of piezoelectric crystals by application of stress in order to produce better transducers and also for the study of the influence of pressure on the behavior of transducers in deep underwater applications.

1. Introduction
A description of the interaction of sound with stressed piezo-electric materials of general anisotropy is not quite simple. First of all there is the anisotropic effect which makes all the calculations complicated. Secondly there is the fact that the bias state is much larger than the additional sound fields. This means that the ‘small deformation’ approach does not work anymore and that classical nonlinear effects need to be incorporated. The bias force induces nonlinear effects and changes the properties of the material through which sound passes. Therefore it is necessary to relate the material properties to the bias state. Hence one has to deal with stress dependent material constants. Furthermore the symmetry of the crystal under consideration results in certain material constants becoming dependent on others. Finding those relationships is crucial because in the literature not all higher order material constants have been determined. Finally the problem of 4 bulk modes instead of only 3 in non-piezo materials forms an additional problem. In piezo materials there are three quasi acoustic waves and two quasi electromagnetic waves. Most often the piezo problem can be regarded as a quasi static problem whence only one quasi electromagnetic wave is left. Besides, this quasi electromagnetic waves propagates at least 10000 times faster than the quasi acoustic modes. This means that the generalized Christoffel equation becomes bad conditioned, which is yet another problem. In what follows, a short description is formulated of the basics of the theory. Final numerical results will be shown during the presentation itself.

2. Theoretical background
The free energy $W$ of a highly deformed crystal can be expressed by means of a Taylor series [1]

$$W = W_0 + \frac{1}{2} c_{klmnpq} e_{kl} e_{mn} e_{pq} + \frac{1}{3!} c_{klmnpqrs} e_{kl} e_{mn} e_{pq} e_{rs}$$

$$- \frac{1}{4!} c_{klmnpqrs} e_{kl} e_{mn} e_{pq} e_{rs} e_{ts}$$

$$- \frac{1}{2} e_{kl} E_k E_l - \frac{1}{2} \tilde{\xi}_{kl} E_k E_l E_j$$

$$- \frac{1}{6} e_{klm} E_k E_l E_m - \frac{1}{2} \gamma_{ijkl} E_k E_l E_m E_n + h.o.t$$

(1)

On the other hand, we also know that the constitutive equations for piezo electric materials are given by [2,3]

$$\sigma_{ij} - \sigma_{ij}^0 = \sigma_{ij}^M = \tilde{\xi}_{ijkl} (E_k - E_k^0)$$

$$D_k - D_k^0 = \varepsilon_{ij}^*(E_i - E_i^0) + \tilde{\xi}_{ijkl} e_{ij}$$

(2)

with

$$\sigma_{ij}^M = c_{ijkl}^* e_{kl} + \frac{\partial u}{\partial x_k} \sigma_{ij}^0$$

$$\varepsilon_{ij}^* = \varepsilon_{ijkl}^* e_{kl}$$

(4)

$\sigma_{ij}$ is the stress tensor, $\varepsilon_{ijkl}^*$ is the stiffness tensor, $\tilde{\xi}_{ijkl}$ is the piezolectric stress tensor, $\varepsilon_{ij}^*$ is the dielectrical permittivity tensor, $E$ is the electric field vector, $D$ is the dielectric displacement vector and $e_{ij}$ is the strain tensor. A superscript ‘0’ denotes initial (bias) conditions.
Due to the presence of a bias stress or even a bias electric field, the coefficients are stress dependent and are related to the stress free constants as follows
\[
\varepsilon_{ijkl}^* = \varepsilon_{ijkl} + \varepsilon_{ijkl}^0 E_m
\]
(5)
\[
\varepsilon_{kij}^* = \varepsilon_{kij} + \varepsilon_{kij}^0 + \varepsilon_{kij}^0 E_n
\]
(6)
\[
\varepsilon_{knij}^* = \varepsilon_{knij} + \varepsilon_{knij}^0 + \varepsilon_{knij}^0 E_n
\]
(7)

For the frequencies we are interested in, the system is quasi static, whence the electrical field can be written as
\[
\mathbf{E} = -\nabla \varphi
\]
(8)

Then, the equation of motion becomes
\[
\frac{\partial \sigma_{ij}}{\partial r_j} = \rho^* \frac{\partial^2 u_i}{\partial t^2}
\]
(9)
with \(\rho^*\) the density of the initially stressed crystal, while the electrical wave equation becomes
\[
\nabla \cdot \frac{\partial^2}{\partial t^2} \left( -\varepsilon_{ij} \frac{\partial \varphi}{\partial r_i} + \varepsilon_{kij}^* \frac{\partial u_j}{\partial r_j} \right) = 0
\]
(10)

Then we express the wave field in terms of its mechanical and electrical components. Hence the displacement field \(\mathbf{u}\) is written as
\[
\mathbf{u} = \mathbf{AP} \exp \left( k_{x}^{inc} x + k_{y}^{inc} y + k_{z} z - \omega t \right)
\]
(11)
whereas the electric potential becomes
\[
\varphi = \mathbf{B} \exp \left( k_{x}^{inc} x + k_{y}^{inc} y + k_{z} z - \omega t \right)
\]
(12)

It can be shown relatively easy that
\[
\mathbf{B} = \frac{k_{x} k_{y} k_{z}^{*} \mathbf{AP}_{q}}{\varepsilon_{mn}^* k_{m}^{*} k_{n}^{*}}
\]
(13)

Therefore whenever \(\mathbf{AP}_{q}\) is known for given wave vector \(\mathbf{k}\), \(\mathbf{B}\) is known as well. The equations (9-10) can be combined as
\[
M_{pq} P_q = 0
\]
(14)

This linear equation is a generalization of the classical Christoffel’s equation for anisotropic materials, with

\[
M_{pq} = k_e \left\{ \varepsilon_{mn}^* k_{m}^{*} \left( \varepsilon_{pq} + \delta_{pq} \varepsilon_{mn}^* k_{n}^{*} - \left( \varepsilon_{pq} \right) \rho^* \delta_{pq} \right) \right\}
\]
(15)

Requirement of nontrivial solutions involves
\[
\det M = 0
\]
(16)

This can be transformed into a polynomial of degree 8 in \(k_3\) for given \(k_1\) and \(k_2\) (obtained from Snell’s law).
\[
\sum_{x=0}^{8} a_x k_3^x = 0
\]
(17)

Hence it is possible to solve this polynomial equation for each given wave vector component along the interface. The result is 8 different modes. It can be shown that for symmetries higher than or equal to monoclinic symmetry, the results always appear in pairs with opposite propagation sense.

### 3. Slowness curves

In what follows the slowness curves are shown for Lithium Niobate crystals in unstressed state. During the presentation, results will also be shown for the stressed state.

Figure 1: Three dimensional representation of first type of quasi acoustic slowness curve

We limit the examples to the quasi acoustic modes. The results correspond perfectly to the cross sections as
presented by Auld [2-3]. It is seen that the slowness curves are different from orthotropic materials (for example fiber reinforce composites).

One peculiarity for example is the fact that for a given type of mode, sound propagating upwards has a different velocity than sound propagating downwards. Contrary to [7], Degtyar and Rokhlin [5-6] state that in the constitutive equations (4) there must be that displacement gradient. That is because also plastic deformation effects would be incorporated, which can be present in the case of very high initial stress. As can be seen in (4), we have taken that into account as well for reasons of generality.

4. Continuity conditions

Before expressing the continuity conditions, it is necessary to emphasize that for each bulk mode, its phase must be related to its origin. Finding this origin is not just a matter of taking a look at the sign of the \( k \) vector, but one should consider the energy propagation direction [2-3].

\[
F_i = -\sigma_{ij} \frac{\partial u_j^*}{\partial x} + \frac{\varphi (i \omega D)^*}{2} \tag{18}
\]

which becomes for the stressed piezoelectric case and after time averaging

\[
\langle F \rangle = \left( \begin{array}{c} (\varepsilon_{wi}^* + \sigma_{wi}^* \delta_{ij})[A^*]^T \begin{bmatrix} k \end{bmatrix} P_i^* \\
+ \sigma_{ri}^* k \begin{bmatrix} k \end{bmatrix} P_i^* A P_i^* \\
\end{array} \right) \\
\times \omega \left( \delta_{\omega e} + (1 - \delta_{\omega e}) \text{sign}(1 \omega) \right) \\
\times \exp \left( -2 \text{Im} (k_i x + k_j y + k_z) \right) \tag{19}
\]

Hence for each propagation mode, a propagation sense can be attributed by means of (19) and therefore also an origin. For each layer of the considered system the present modes are therefore given their physical origin correctly. Since (19) is a consequence of the complex energy flux description, it can also be used for inhomogeneous modes if necessary. Inhomogeneous waves are waves having a complex wave vector and are generally accompanied by an exponentially growing or decaying amplitude along their wave front. They have been studied mostly in relation to surface waves and plate waves. It is expected that in the future they will also be applied for piezo-electric materials as well.

As in the case of standard anisotropic materials one requires continuity of normal stress and normal displacement for liquid/solid interfaces and normal stress and total displacement for solid/solid interfaces. However this only leads to solving a system having 6 modes per layer. The additional 2 modes are found by also requiring continuity of the electric potential. Besides, it has also been shown before by Degtyar and Rokhlin [5] that continuity is required not just for the

Figure 2: Three dimensional representation of second type of quasi acoustic slowness curve.

That is of course because Lithium Niobate has 3m symmetry (trigonal).

Figure 3: Three dimensional representation of third type of quasi acoustic slowness curve.
acoustic stress, but also for the complete stress. If not, then important errors would occur in the vicinity of critical angles of incidence. We have incorporated this fact in our model as well. At the moment we are simulating the interaction of sound with stressed and unstressed piezoelectric layered systems. The results will be presented extensively during the meeting.

5. Concluding Remarks

The theoretical background has been presented behind the description of the interaction of ultrasound with layered piezoelectric materials. Numerical examples will be shown extensively during the presentation. The understanding of the interaction of sound with pre-stressed piezoelectric materials is not only of interest for science, but also possibly for creating new technologies in the future based on the application of a bias field in piezoelectric materials. Sometimes, for example in underwater acoustics, transducers are subjected to high pressure. The present report is a first step in a deeper understanding of such phenomena. Contrary to a paper that already exists on the phenomenon of BG waves in piezoelectric crystals, we have included plastic deformations as well and we have incorporated continuity of total stress in our equations as to agree with the scientific findings of Degtyar and Rokhlin for non-piezoelectric materials.

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7. References