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Reflection and refraction of bulk acoustic waves in piezoelectric crystals under the action of bias electric field and uniaxial pressure

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***Abstract*—Main theory results concerned with bulk elastic wave reflection/refraction on the boundary between two piezoelectric crystals subjected to the action of bias electric field or mechanical stress have presented. Some calculations for $LiNbO_3$ and $Bi_{12}GeO_{20}$ crystals have made.**

Keywords - reflection, refraction; bulk elastic wave, bias electric field, mechanical stress, piezoelectric crystal

I. INTRODUCTION

There are many aspects of interest to processes of acoustic wave's reflection/refraction on the boundary of two hard contacting mediums: ultrasonic wave propagation problems, acoustoelectronics devices, acoustic microscopy etc. Basic equations of such processes were obtained in 50th of 20 century [1].

Now we have developed above mentioned approach involving the influence of bias external fields. First the theory of reflection and refraction of bulk acoustic waves (BAW) on a boundary of two crystalline piezoelectric solids has obtained. We have taken into account early results concerning with BAW propagation in the infinite homogeneous piezoelectric single crystals subjected to the action of constant electric field **E** or uniaxial mechanical pressure **P** [2].

II. THEORY

Using main results obtained early [2] we have received basic equations describing any BAW reflection/refraction processes on the boundary of two hard contacting piezoelectric solids under the bias electric field **E** or uniaxial mechanical pressure **P**. Wave equation and electrostatics equation referred to the natural (undeformed) state have a form:

$$\rho_0 \ddot{\tilde{U}}_A = \tilde{\tau}_{AB,B} + \tilde{U}_{A,FB}\bar{\tau}_{FB}, \qquad (1)$$
$$\tilde{D}_{M,M} = 0.$$

In (1) ρ_0 is the crystal density taken in undeformed state, $\tilde{U}_A$ – vector of dynamical elastic displacement, τ_{AB} – tensor of thermodynamic stresses, D_M – electric displacement vector, $\bar{\tau}_{FB} = -\bar{\tau}P_F P_B$ – static tensor of uniaxial mechanical stress (minus sign indicates the compression), P_B – unit vector of compression force. Sign "~" here and further is marked all the time depending variables. Comma after the lower index signifies the space derivative. Latin coordinate lower indexes vary up 1 to 3, and sum rule on twice repeating index is implied.

If we taken into account **E** or **P** action, state equations for dynamical components of thermodynamic stresses and electric displacement would be written as:

$$\tilde{\tau}_{AB} = C^*_{ABCD}\tilde{\eta}_{CD} - e^*_{NAB}\tilde{E}_N, \qquad (2)$$
$$\tilde{D}_N = e^*_{NAB}\tilde{\eta}_{AB} + \varepsilon^*_{NM}\tilde{E}_M,$$

where η_{AB} – deformation tensor. Effective elastic, piezoelectric and dielectric constants are determined by formulas

$$\begin{aligned} C^*_{ABKL} &= C^E_{ABKL} + \left(C^E_{ABKLQR}d_{NQR} - e_{NABKL}\right)EM_N - \\ &- C^E_{ABKLQR}S^E_{QRMN}P_M P_N\bar{\tau}, \\ e^*_{NAB} &= e_{NAB} + \left(e_{NABKL}d_{MKL} + H_{NMAB}\right)EM_P - \\ &- e_{NABKL}S^E_{KLMD}P_M P_D\bar{\tau}, \\ \varepsilon^*_{NM} &= \varepsilon^\eta_{NM} + \left(H_{NMAB}d_{PAB} + \varepsilon^\eta_{NMP}\right)EM_P - \\ &- H_{NMAB}S^E_{ABKL}P_K P_L\bar{\tau}. \end{aligned} \qquad (3)$$

In (3) $\bar{\tau}$ is the value of static mechanical stress, E is absolute value of static electric field, S^E_{ABKL} is elastic compliances tensor, C^E_{ABKLQR}, e_{NABKL}, H_{NMAB} are nonlinear elastic, piezoelectric and electrostriction material tensors respectively.

The rectangular coordinate system in which X'_3 axis directs along the normal to the boundary of two contacting solids and X'_1 - along the boundary, has used. Let's bulk elastic wave falls on the boundary out of the crystal occupied half-space X'_3<0. For example Fig. 1 represents the configuration of incident, reflected and refracred waves. Solutions of wave

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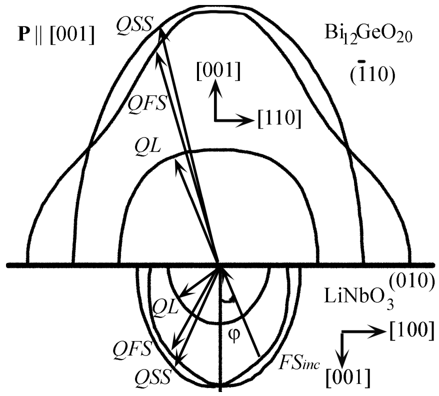

Figure 1. Section of refraction surfaces for two hard contacticg crystals.

equations are proposed in the form of plane waves, and it is convenient to write the formulas for plane elastic wave and electric potential wave using refraction vector $\mathbf{m} = \mathbf{N}/v$ ($\mathbf{N}$ is unit vector of the wave normal and v is the phase velocity of bulk wave):

$$\begin{aligned} U_C &= \alpha_C \exp[i\omega(t - m_j x_j)], \\ \varphi &= \alpha_4 \exp[i\omega(t - m_j x_j)], \end{aligned} \tag{4}$$

where α_C, α_4 are amplitudes of elastic wave and electric potential wave.

Inserting (4) into (1) and taken into account the terms having linear degree on $\mathbf{E}$ or $\mathbf{P}$ only the system of four homogeneous equations has been obtained:

$$[\Gamma_{BC} - \delta_{BC}\rho_0]\tilde{U}_B = 0, \tag{5}$$

where components of modified Green-Christoffel tensor Γ_{BC} have the form:

$$\begin{aligned} \Gamma_{BC} &= [C^*_{ABCD} + (2C^E_{MBFN}S^E_{ADCF} + \delta_{BC}\delta_{AM}\delta_{DN})P_M P_N \bar{\tau} + \\ &+ 2C^E_{ABFD} d_{JFC} M_J E] m_A m_D, \\ \Gamma_{B4} &= e^*_{IAB} m_I m_A, \\ \Gamma_{4B} &= \Gamma_{B4} + 2e_{AFD} S^E_{MNCF} P_M P_N m_A m_D \bar{\tau} + \\ &+ 2e_{PFD} d_{JDC} m_P m_F M_J E, \\ \Gamma_{44} &= -\varepsilon^*_{MI} m_M m_I. \end{aligned} \tag{6}$$

Calculation of $\mathbf{m}$ vectors gives a possibility to obtain values of reflection and refraction angles and phase velocities of bulk waves. Important parameters are the amplitude coefficients of reflected and refracted bulk waves.

It is necessary to formulate boundary conditions for the two hard contacting piezoelectric crystals. So the system of linear equations for eight amplitude coefficients of reflected (a_n) and refracted (b_n) bulk waves has the form:

$$\begin{aligned} &\sum_{n=1}^{4} (b_n G_B^{(n)[I]} - a_n G_B^{(n)[II]}) = \hat{G}_B^{(n)[II]}, \\ &\sum_{n=1}^{4} (U_B^{(n)[I]} b_n - U_B^{(n)[II]} a_n) = \hat{U}_B^{(n)[II]}, \\ &\sum_{n=1}^{4} (b_n D_3^{(n)[I]} - a_n D_3^{(n)[II]} = \hat{D}_3^{(n)[II]}. \end{aligned} \tag{7}$$

Incident wave values marked by the «∧» sign. Upper index «I» corresponds to the crystal occupying the $X'_3>0$ half-space, index «II» – to the $X'_3<0$ half-space, and such designations are introduced:

$$\begin{aligned} G_B^{(n)[I,II]} &= (C^{*[I,II]}_{B3KL}\delta_{KP} + 2d^{(I,II)}_{AKF}C^{(I,II)E}_{3IFL}M_A E - \\ &- 2S^{[I,II]}_{KPMN}C^{[I,II]}_{3BKL}P_M P_N \bar{\tau}) m_L^{(n)}\alpha_P^{(n)} - e^{*[I,II]}_{P3B} m_P^{(n)}\alpha_4^{(n)} + m_P^{(n)}\alpha_B^{(n)} P_3 P_P \bar{\tau}, \\ D_3^{(n)[I,II]} &= (e^{*[I,II]}_{3AB} + 2d^{(I,II)}_{JKP}e^{(I,II)}_{3PL}M_J E + 2S^{[I,II]}_{ABKP}e^{[I,II]}_{3AB}P_F P_P \bar{\tau}) m_B^{(n)}\alpha_A^{(n)} - \\ &- \varepsilon^{*[I,II]}_{3K} m_K^{(n)}\alpha_4^{(n)}. \end{aligned} \tag{8}$$

In (7), (8) and further indexes n = 1,…,3 are marked longitudinal (1) or shear (2, 3) reflected and refracted elastic waves. Index n = 4 corresponds to electric potential wave.

III. Results and Discussion

Let's consider the influence of static homogeneous electric field on the bulk wave's reflection from the free boundary of piezoelectric crystal belonging to 23 point symmetry group. Wave propagates in (010) plane (sagittal plane). The normal to the boundary crystal plane coincides with [001] direction. Dispersion equation for reflected wave (E=0) under the fall of longitudinal (L) or fast shear (FS) waves has the form [3]:

$$\begin{aligned} &\left(C^E_{11}m_1^2 + C^E_{44}m_3^2 - \rho_0\right)\left(C^E_{44}m_1^2 + C^E_{11}m_1^2 - \rho_0\right) - \\ &- \left(C^E_{12} + C^E_{44}\right)^2 m_1^2 m_3^2 = 0. \end{aligned} \tag{9}$$

If we consider the incidence of piezoactive slow shear wave (SS) with polarization along [010] (orthogonal to the incident plane), dispersion equation can be present as

$$[C^E_{44}\left(m_1^2 + m_3^2\right) - \rho_0]\varepsilon^{\eta}_{11}\left(m_1^2 + m_3^2\right) - 4e_{14}^2 m_1^2 m_3^2 = 0. \tag{10}$$

Consequently there are reflected longitudinal (the quasi-longitudinal one (QL)) and fast shear (fast quasi-shear one (QFS)) waves only. If slow quasi-shear wave falls QSS-wave is reflected only and its amplitude coefficient A_R is close to the unity. Owing to the piezo-activity of given wave there exists a wave of the electrical potential.

The influence of the electric field along [001]-direction according to Curie principle lowers the initial 23 point symmetry of crystal to monoclinic one, point group 2 where two-hold symmetry axis is directed also along [001] –direction. So new efficient material constants which were equal zero in absence of the field are induced: C_{16}, C_{36}, C_{45}, e_{15}, e_{33}, e_{31}. Thereby dispersion equations become the polynomials of eighth degree with respect to m_3 component of reflected waves.

Fig. 2 represents amplitude coefficients A_R of reflected waves in $Bi_{12}GeO_{20}$ crystal free surface at the E||[001] in (010)-plane of the incidence in cases of incident QL, QFS and QSS-waves. When QL-wave falls under 60^0 degrees from the normal to free surface there exist the reflected wave transformation - now QFS-wave is reflecting only (Fig. 2, c). When QFS-wave falls, the phenomena of the internal reflectance for reflected QL-wave appears starting with 38^0 incident angle (the refraction vector becomes complex one) (Fig. 2, d). The E-action decreasing crystal symmetry has a result the appearance of reflected QSS-wave particularly in the QSS-wave incidence (Fig. 2, e). If E = 0 the acoustic axis of the tangent type exists along the normal to free surface. The application E||[001] causes the removal of degeneration for shear waves propagating along [001]-direction. Herewith the initial acoustic axis is split on two cone type one lying in (110)-plane. So even normal incidence of QSS-wave brings to the appearance of reflected shear waves of both types with values of the real parts of amplitude coefficients equal to factor 0.78 and 0.71 for fast and slow shear waves accordingly. Note that for all variants of the incident waves when E ≠ 0, values of amplitude reflection coefficients are always complex ones.

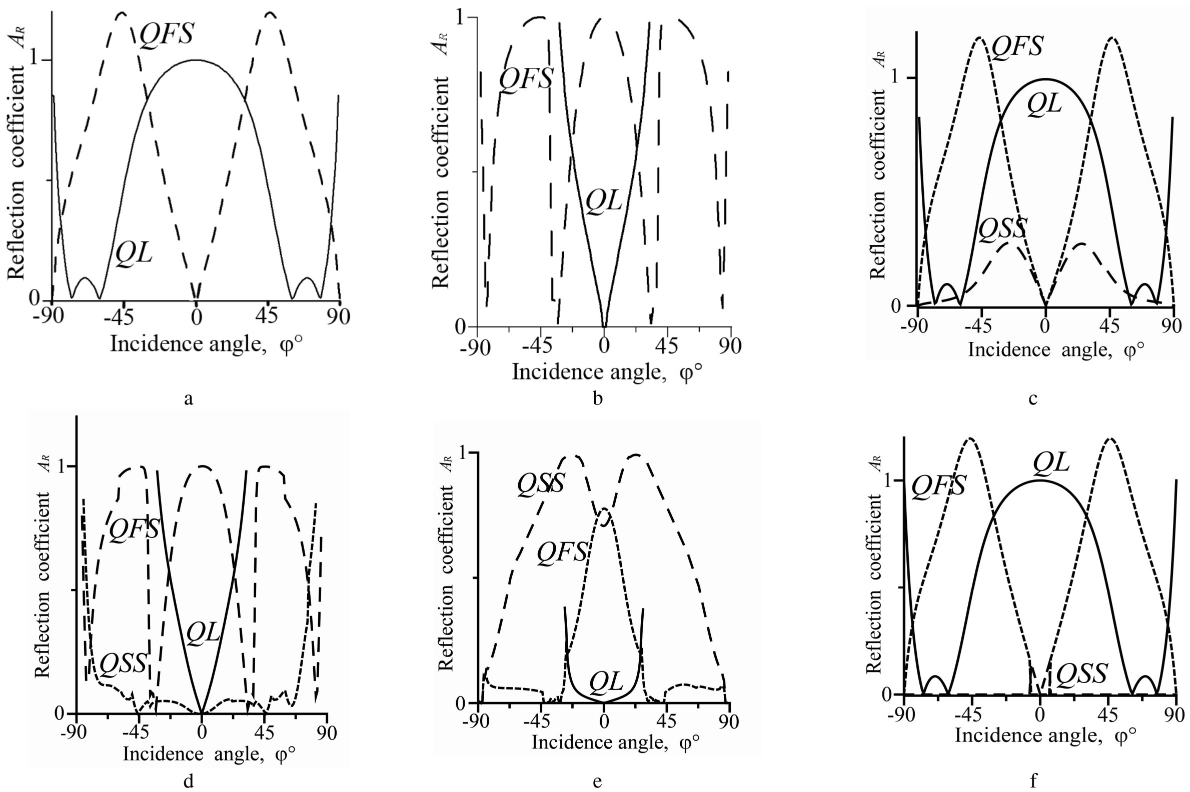

Figure 2. Reflection (A_R) amplitude coefficients for waves reflected on the free boundary of $Bi_{12}GeO_{20}$ crystal under E- or P-application. Waves falls in (010) plane. a, b, - E, P = 0; c, d, e – E||[001]; f – P||[001]; a, c, f – incident L-wave; b, d – incident FS-wave; e – incident SS-wave.

Application of external uniaxial mechanical stress (∞/mm point symmetry) along [100]-direction reduces the symmetry of the crystal to rhombic one, class 222, as distinct from E-application which causes the symmetry decreasing to monoclinic class 2. In consequence the modification of some existing material constants occurs only. Thereby the influence of uniaxial mechanical stress reduces to quantitative changes of reflection amplitude coefficients. However application of uniaxial mechanical stress along [100]-direction causes the removal of degeneration for shear waves propagating along [001]-direction which was the acoustic axis of the tangent type in undisturbed state. Acoustic axis is split on two cone types lying in (010)-plane as distinct from E-application in which the acoustic axis splitting occurs in (110)-plane. As a result if longitudinal wave falls in interval between two induced acoustic axes the slow shear wave is reflected (Fig. 2, f).

Fig. 3 represents reflection and refraction amplitude coefficients for waves on the boundary plane between $LiNbO_3$ (LN) and $Bi_{12}GeO_{20}$ (BGO) crystals under E- or P-application. Let's electric field acts along [001]-direction (orthogonal to boundary plane) for incidence variants of all three types of waves to be used (Fig. 3, d, e). At E||[001] in BGO crystal the removal of shear waves degeneration occurs while for NL crystal given variant of E||[001], i.e. along three-hold axis of the symmetry, does not change the symmetry of the crystal. But in this case shear waves degeneration vanishes too. If QL-wave falls there are all three types reflected and refracted waves, but amplitude reflection coefficient of QL-wave has the largest value. This fact is explained by big difference between phase velocities of investigated crystals. The E-influence produces minimal changes of reflection and refraction amplitude coefficients. However if it considered shear wave incidence reflection amplitude coefficients change effectively in consequence of the degeneration removal while values of refracted amplitude coefficients are relatively small. Under the QFS-wave incidence at E||[001] the transformation of the type of reflected shear waves occurs while in "linear" case (E = 0) reflected shear waves have of great importance. The E-influence particularly reveals itself at QSS-wave incidence (Fig. 3, f). In this instance under E = 0 slow shear wave is reflected only and values of amplitude coefficients for other reflected and refracted waves have a negligible quantity. Due to the fact that acoustic axis along [001]-direction has split at E||[001], QSS-wave in BGO crystal will not be a "pure" mode. As a result reflected shear wave occurs.

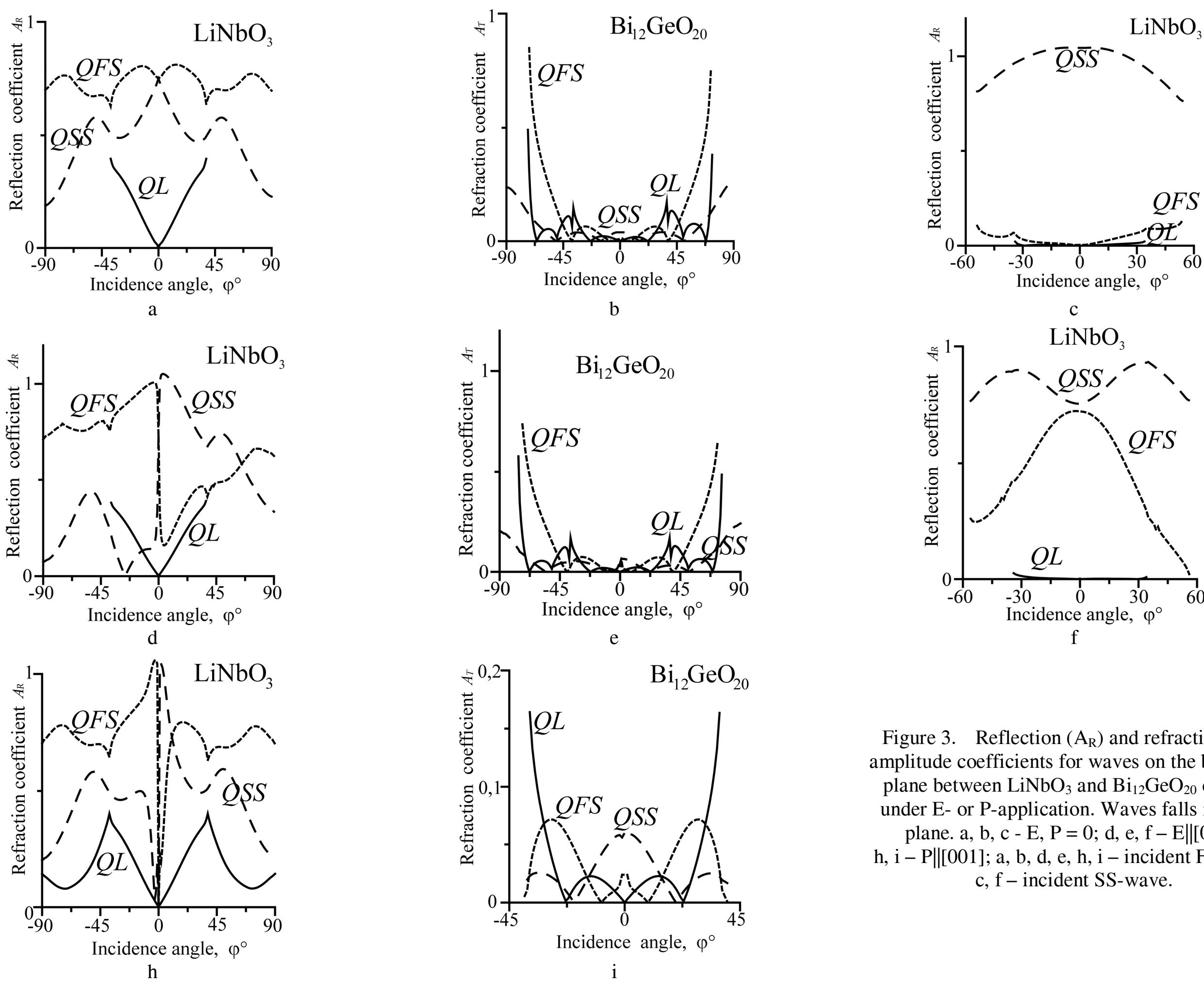

Figure 3. Reflection (A_R) and refraction (A_T) amplitude coefficients for waves on the boundary plane between $LiNbO_3$ and $Bi_{12}GeO_{20}$ crystals under E- or P-application. Waves falls in (010) plane. a, b, c - E, P = 0; d, e, f – E||[001]; h, i – P||[001]; a, b, d, e, h, i – incident FS-wave; c, f – incident SS-wave.

Fig. 3 (h, i) represents reflection and refraction amplitude coefficients for waves on the boundary plane between LN ((010)-plane) and BGO ($(\bar{1}10)$ -plane) crystals under P-application along [001]-direction, i.e. orthogonal to the contact plane of crystals. If QL-wave falls there are presented all three types of reflected and refracted waves, but reflected QL-wave has a dominant position that is explained by the big difference between phase velocities of these crystals. P-application changes values of reflection and refraction amplitude coefficients, particularly it apply to reflected QSS-waves. It is significant that in this case the transformation of the refracted waves occurs. Under normal incidence of the longitudinal wave also longitudinal one is refracted, but when QL-wave falls under the $\pm 40^0$ angle to the normal, refracted QS-waves exist only. However if shear waves fall, in consequence of the shear wave degeneration removal in BGO crystal amplitude coefficients of reflected waves change effectively while values of the refracted amplitude coefficients waves change slightly. In the case of QFS-wave incidence and P-action along [001] the transformation of the type of reflected shear waves occurs. While influence is absent, reflected shear waves are dominant (Fig. 3, h). Under the ±38° incidence angle the phenomena of the internal reflectance of the longitudinal wave is observed.

IV. Conclusion

Thus using given theory it is possible in details to analyze the character of reflection and refraction of acoustic waves on the hard boundary of piezoelectric solids under the application of bias fields. The data obtained can be useful for searching of practically important combinations of crystals for acoustoelectronics devices and sensors.

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