Crystallography Reports, Vol. 50, No. 6, 2005, pp. 986–993. Translated from Kristallografiya, Vol. 50, No. 6, 2005, pp. 1065–1072.
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PHYSICAL PROPERTIES OF CRYSTALS

Theory and Computer Simulation of the Reflection and Refraction of Bulk Acoustic Waves in Piezoelectrics under the Action of an External Electric Field

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Received August 7, 2003; in final form, May 30, 2005

Abstract—The basic equations describing the conditions for reflection and refraction of bulk acoustic wave at the interface between acentric crystals subjected to the action of a uniform external electric field are reported. Numerical analysis of the effect of this field on the reflection and refraction anisotropy of bulk acoustic waves at the crystal/vacuum and piezoelectric/elastic-isotropic-medium interfaces is performed. © *2005 Pleiades Publishing, Inc.*

INTRODUCTION

The theory of reflection and refraction of bulk acoustic waves (BAWs) at an interface between two nonpiezoelectric crystals was reported in [1, 2]. This theory was used, for example, to design polygonal ultrasonic delay lines. Further development of this theory is related to the consideration of the specific features of wave propagation in piezoelectrics [3]. The theory of propagation of bulk acoustic waves in piezoelectric crystals subjected to the action of a external electric field and stress was described in detail in [4, 5]. The effect of a uniform external electric field E on the propagation of surface acoustic waves (SAWs) in piezoelectric crystals was considered in [6]. In the first-order perturbation theory, the effect of $\mathbf{E}$ is determined by changes in the conditions for BAW and SAW propagation, which are related to the nonlinearity of elastic, piezoelectric, and dielectric properties and the electrostriction. Therefore, the effect of $\mathbf{E}$ can be calculated if the material constants of the nonlinear electromechanical properties are known. By date, complete sets of the coefficients of the nonlinear electromechanical properties have been investigated for some piezoelectric crystals (lithium niobate, crystals with sillenite structure, and langasite) [5, 7, 8].

REFLECTION AND REFRACTION OF ELASTIC WAVES AT THE INTERFACE BETWEEN PIEZOELECTRIC CRYSTALS UNDER THE ACTION OF A DC ELECTRIC FIELD

Using the results of [5], we will derive necessary equations describing the effect of $\mathbf{E}$ on the conditions for the BAW reflection and refraction at an interface between two media. In the initial coordinate system, the wave equations for waves with small amplitudes in homogeneously deformed acentric media and the equation of electrostatics have the form [5]

$$\rho_0 \ddot{\tilde{\mathbf{U}}}_A = \tilde{\tau}_{AB,\,B}, \qquad \tilde{\mathbf{D}}_{M,\,M} = 0, \tag{1}$$

where ρ_0 is the density of a unstrained crystal (initial state), $\tilde{\mathbf{U}}_A$ is the vector of dynamic elastic displacements (hereinafter, the sign ~ denotes the time-dependent quantities), τ_{AB} is the tensor of thermodynamic stresses, and $\mathbf{D}_M$ is the electric-displacement vector. A comma after an index denotes a spatial derivative and two periods above a variable denote the second derivative with respect to time. Latin coordinate indices run from 1 to 3. In what follows, summation over double indices is implied.

When the effect of $\mathbf{E}$ is taken into account, the state equation for the dynamic components of thermodynamic stresses and the electric displacement have the form

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

where η_{CD} is the strain tensor and the effective elastic, piezoelectric, and dielectric constants are determined by the relations

$$\begin{aligned} C^*_{ABKL} &= C^E_{ABKL} + (C^E_{ABKLQR} d_{NQR} - e_{NABKL}) E\mathbf{M}_N, \\ e^*_{NAB} &= e_{NAB} + (e_{NABKL} d_{PKL} + H_{NPAB}) E\mathbf{M}_P, \\ \varepsilon^*_{NM} &= \varepsilon^\eta_{NM} + (H_{NMAB} d_{PAB} + \varepsilon^\eta_{NMP}) E\mathbf{M}_P. \end{aligned} \quad (3)$$

Here, d_{NQR} is the tensor of "linear" piezoelectric coefficients; C^E_{ABKLQR}, e_{NABKL}, ε^η_{NMP}, and H_{NPAB} are the nonlinear elastic, piezoelectric, dielectric, and electrostriction material tensors, respectively; $\mathbf{M}_N$ is the unit vector of the external electric field, and E is the magnitude of the external electric field.

To consider the problem of the BAW reflection and refraction at an interface of two acentric media, let us choose the orthogonal coordinate system with the X'_3 axis directed normally to the interface and the X'_1 axis lying in the interface plane. It is assumed that an elastic wave is incident on the interface from the crystal occupying the half-space $X'_3 < 0$. Solutions to the wave equation will be sought for in the form of plane waves. It is convenient to consider the conditions for the wave reflection and refraction using the expressions for a plane elastic harmonic wave and a wave of electrical potential, written in terms of the refraction vectors $\mathbf{m} = \mathbf{N}/v$ ($\mathbf{N}$ is the unit vector of the wave normal, and v is the phase velocity of a BAW):

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

where α_C and α_4 are the amplitudes of the elastic displacement and electrical potential, respectively.

Substituting expressions (4) into (1) and leaving only the terms linear in E, we obtain the system of four homogeneous equations [6]:

$$\begin{pmatrix} \Gamma_{11} - \rho_0 & \Gamma_{12} & \Gamma_{13} & \Gamma_{14} \\ \Gamma_{21} & \Gamma_{22} - \rho_0 & \Gamma_{23} & \Gamma_{24} \\ \Gamma_{31} & \Gamma_{32} & \Gamma_{33} - \rho_0 & \Gamma_{34} \\ \Gamma_{41} & \Gamma_{42} & \Gamma_{43} & \Gamma_{44} \end{pmatrix} \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \alpha_3 \\ \alpha_4 \end{pmatrix} = 0, \quad (5)$$

where the components of the modified Green–Christoffel tensor have the form

$$\begin{aligned} \Gamma_{BC} &= (C^*_{ABCD} + 2C^E_{ABFD} d_{JFC} M_J E) m_A m_D, \\ \Gamma_{B4} &= e^*_{IAB} m_I m_A, \\ \Gamma_{4B} &= \Gamma_{B4} + 2e_{PFD} d_{JDC} m_P m_F M_J E, \\ \Gamma_{44} &= -\varepsilon^\eta_{KL} m_K m_L. \end{aligned} \quad (6)$$

The determinant of system (5) is a polynomial of power 8 with respect to the component m_3 of the refraction vectors of the reflected and refracted BAWs at a given direction of an incident elastic wave. Generally, the values of m_3 may be complex due to the effect of total internal reflection [2]. In this case, the values of m_3 should have a negative imaginary part for the crystal occupying the lower half-space $X'_3 < 0$ (reflected waves), and a positive imaginary part for the crystal in the upper half-space $X'_3 > 0$ (refracted waves). As a result, the condition for the decay of reflected and refracted waves in the bulk of the corresponding crystals will be satisfied.

Determination of the refraction vectors $\mathbf{m}$ makes it possible to obtain the values of the angles of reflection and refraction of BAWs and the corresponding phase velocities. However, the most important energy characteristics of reflection and refraction are the amplitude coefficients of the reflected and refracted waves, which characterize the distribution of the incident-wave energy between the reflected and refracted waves. To determine these coefficients, the boundary conditions should be formulated. In the case of a rigid acoustic contact between two crystals, the boundary conditions for the thermodynamic-stress tensor are reduced to the requirement for the continuity of the normal components of the stress tensors of reflected and refracted waves and the continuity of the elastic-displacement vectors [2]:

$$\begin{aligned} \tau^{(1)}_{IJ} n_J &= \tau^{(2)}_{IJ} n_J, \\ \mathbf{U}^{(1)} &= \mathbf{U}^{(2)}, \end{aligned} \quad (7)$$

where n_J is the normal unit vector on the interface. Taking into account the piezoelectric properties of the crystals, we have to formulate the boundary conditions for the electric-field characteristics. The conditions for the continuity of the tangential components of the electric field vector at the interface and the continuity of the normal components of the electric-displacement vector in the quasi-static limit can be written as

$$\begin{aligned} \varphi^{(1)} &= \varphi^{(2)}, \\ (\mathbf{D}^{(1)}, \mathbf{n}) &= (\mathbf{D}^{(2)}, \mathbf{n}). \end{aligned} \quad (8)$$

Substituting solutions (4) into Eqs. (7) and (8) and leaving only the terms linear in E, we obtain finally a system of linear equations with respect to the eight amplitude coefficients of the reflected and refracted waves:

$$\begin{aligned} \sum_{\mu=1}^{4} (b_\mu G^{(1)}_{\mu B} - a_\mu G^{(2)}_{\mu B}) &= G^{(2)}_{0B}, \\ \sum_{\mu=1}^{4} (\tilde{U}^{(\mu)}_B b_\mu - \tilde{U}^{(\mu)}_B a_\mu) &= \tilde{U}^0_B, \\ \sum_{\mu=1}^{4} (b_\mu D^{(1)}_\mu - a_\mu D^{(2)}_\mu) &= D^{(2)}_0, \end{aligned} \quad (9)$$

where a_μ are the amplitude reflection coefficients and b_μ are the amplitudes of the refractive indices. In addition, the following designations are used:

$$G_{\mu B}^{(1,2)} = (C_{B3KL}^{(1,2)*} + 2d_{AKF}^{(1,2)} C_{3IFL}^{(1,2)E} M_A E) m_L^{(\mu)} \alpha_K^{(\mu)} + e_{P3B}^{(1,2)*} m_P^{(\mu)} \alpha_4^{(\mu)},$$

$$D_\mu^{(1,2)} = (e_{3KL}^{(1,2)*} + 2d_{JKP}^{(1,2)} e_{3PL}^{(1,2)} M_J E) m_L^{(\mu)} \alpha_K^{(\mu)} - \varepsilon_{3K}^{(1,2)*} m_K^{(\mu)} \alpha_4^{(\mu)}, \quad (10)$$

$$G_{0B}^{(2)} = (C_{B3KL}^{(2)*} + 2d_{AKF}^{(2)} C_{3IFL}^{(2)E} M_A E) m_L^0 \alpha_K^0 + e_{P3B}^{(2)*} m_P^0 \alpha_4^0,$$

$$D_0^{(2)} = (e_{3KL}^{(2)*} + 2d_{JKP}^{(2)} e_{3PL}^{(2)} M_J E) m_L^0 \alpha_K^0 - \varepsilon_{3K}^{(2)*} m_K^0 \alpha_4^0.$$

In (9) and (10), the superscript 1 corresponds to the crystal occupying the half-space $X_3' > 0$, the superscript 2 corresponds to the half-space $X_3' < 0$, the index 0 denotes the incident elastic wave, and the index μ denotes the types of the reflected and refracted elastic waves: a longitudinal (*L*) wave (1), a fast shear (*FS*) wave (2), and a slow shear (*SS*) wave (3).

When only the reflection of a wave from the crystal–vacuum interface is considered, it is necessary to change the boundary conditions. In this case, the stresses on the crystal surface should absent; i.e., $\sum_{J=1}^{3} \tau_{3J} = 0|_{X_3=0}$. The boundary conditions include also the requirement for continuity of the normal components of the electric displacement at the crystal–vacuum interface and the validity of the Laplace equation for the potential wave in a vacuum. The system of linear equations for the four amplitude coefficients can be written as

$$\sum_{\mu=1}^{3} \{-a_\mu (C_{3KPI}^{*} \alpha_P^{(\mu)} + 2d_{AKF} C_{3KFI}^{E} M_A E) m_K^{(\mu)} - a_4 e_{K3I}^{*} m_K^{(\mu)} \alpha_4^{(\mu)}\} = (C_{3KPI}^{*} \alpha_P^0 + 2d_{AKF} C_{3KFI}^{E} M_A E) m_K^0 - e_{K3I}^{*} m_K^0 \alpha_4^0, \quad (11)$$

$$\sum_{\mu=1}^{3} \{-a_\mu (e_{3KL}^{*} + 2d_{JKP} e_{3PL} M_J E) m_L^{(\mu)} \alpha_K^{(\mu)} - a_4 (\varepsilon_{3K}^{*} m_K^{(\mu)} - i\varepsilon_0) \alpha_4^{(\mu)}\} = (e_{3KL}^{*} + 2d_{JKP} e_{3PL} M_J E) m_L^0 \alpha_K^0 - \varepsilon_{K3}^{*} m_K^0 \alpha_4^0, \quad (12)$$

where ε_0 is the dielectric constant.

Note that these expressions for the boundary conditions are obtained for the case when a uniform external electric field is applied to the crystal and the edge effects are neglected. The equations obtained take into account all changes in the configuration of the anisotropic continuous medium related to its static strain and, in particular, the changes in the crystal shape: extensions and rotations of elementary lines parallel to the sample edges [5].

CALCULATION OF THE EFFECT OF A DC ELECTRIC FIELD ON THE REFLECTION OF BAWS FROM THE FREE BOUNDARY OF A PIEZOELECTRIC CRYSTAL

As an example, we will consider the effect of an uniform external electric field on the reflection of BAWs from a free boundary of a cubic piezoelectric with symmetry 23. Let a wave be incident in the (010) plane (the sagittal plane). The normal to the interface coincides with the [001] direction. The dispersion equation for reflected BAWs (at $E = 0$) in the case of incidence of an *L* wave or an *FS* wave on the interface can be written as [3]

$$(C_{11}^E m_1^2 + C_{44}^E m_3^2 - \rho_0)(C_{44}^E m_1^2 + C_{11}^E m_1^2 - \rho_0) - (C_{12}^E + C_{44}^E)^2 m_1^2 m_3^2 = 0. \quad (13)$$

When a slow shear (*SS*) wave is incident on the interface, which is piezoelectrically active in the given sagittal plane and has a polarization directed along the [010] axis, i.e., orthogonally to the plane of incidence, the dispersion equation has the form

$$(C_{44}^E(m_1^2 + m_3^2) - \rho_0)\varepsilon_{11}^{\eta}(m_1^2 + m_3^2) - 4e_{14}^2 m_1^2 m_3^2 = 0. \quad (14)$$

Therefore, in the case of the incidence of an *L* wave of a *FS* wave (polarized in the plane of incidence), only *L* (quasi-longitudinal (*QL*)) and *FS* (fast quasi-shear (*FQS*)) waves will be reflected. In the case of incidence of a slow quasi-shear (*SQS*) wave, only an *SQS* wave is reflected, whose amplitude coefficient is very close to unity. However, owing to the piezoelectric activity of this wave, along with the elastic *SQS* wave, there is also a potential wave. Therefore, taking into account that the refraction vector of the reflected *SQS* wave is real, the amplitude coefficient for this wave is complex and its imaginary part characterizes the phase shift between the incident and reflected waves [3].

Application of an electric field to a crystal in the [001] direction, according to the Curie principle, decreases the crystal symmetry to the monoclinic class 2, in which the twofold symmetry axis is also directed along the [001] axis. As a result, new effective material constants (equal to zero in the absence of a field) are

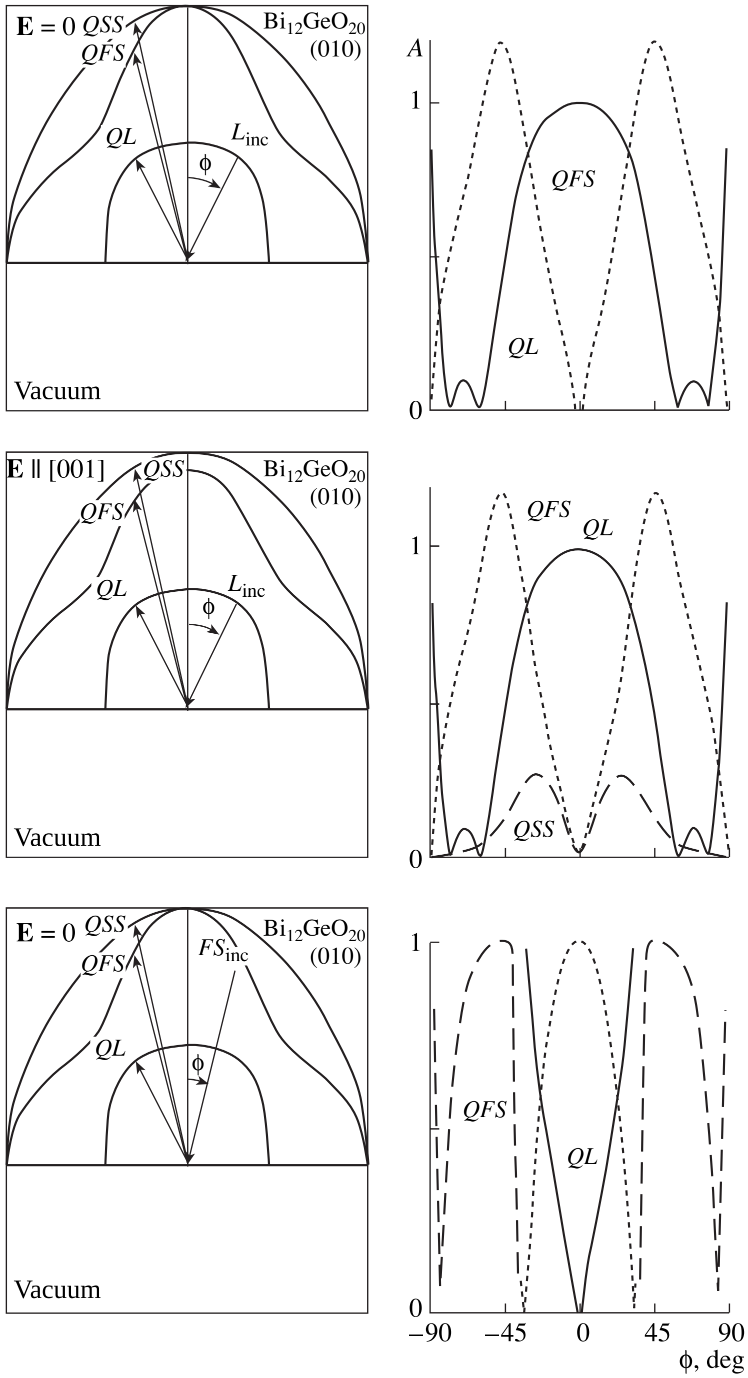

Fig. 1. Real parts of the amplitude reflection coefficients of BAWs reflecting from the germanosillenite-crystal/vacuum interface for the incidence in the plane (010).

induced:

$$\tilde{C}_{16} = (C_{166}d_{14} - e_{124})E,\ \tilde{C}_{36} = (C_{144}d_{14} - e_{114})E,$$
$$\tilde{C}_{45} = (C_{456}d_{14} - e_{154})E,\ \tilde{e}_{15} = (e_{156}d_{14} + H_{44})E, \quad (15)$$
$$\tilde{e}_{33} = (e_{114}d_{14} + H_{11})E,\ \tilde{e}_{31} = (e_{124}d_{14} + H_{12})E.$$

Thus, dispersion equations (13) and (14) become polynomials of power 8 with respect to the components m_3 of the reflected waves. Figure 1 shows the real part of the amplitude reflection coefficients of BAWs in a $Bi_{12}GeO_{20}$ crystal at **E** ∥ [001] in the plane of incidence (010) for BAWs of the *QL*, *FQS*, and *SQS* types. When a *QL* wave is incident at an angle of 60°, transformation of reflected elastic waves occurs and only the *FQS* wave is reflected. In the case of incidence of an *FQS*

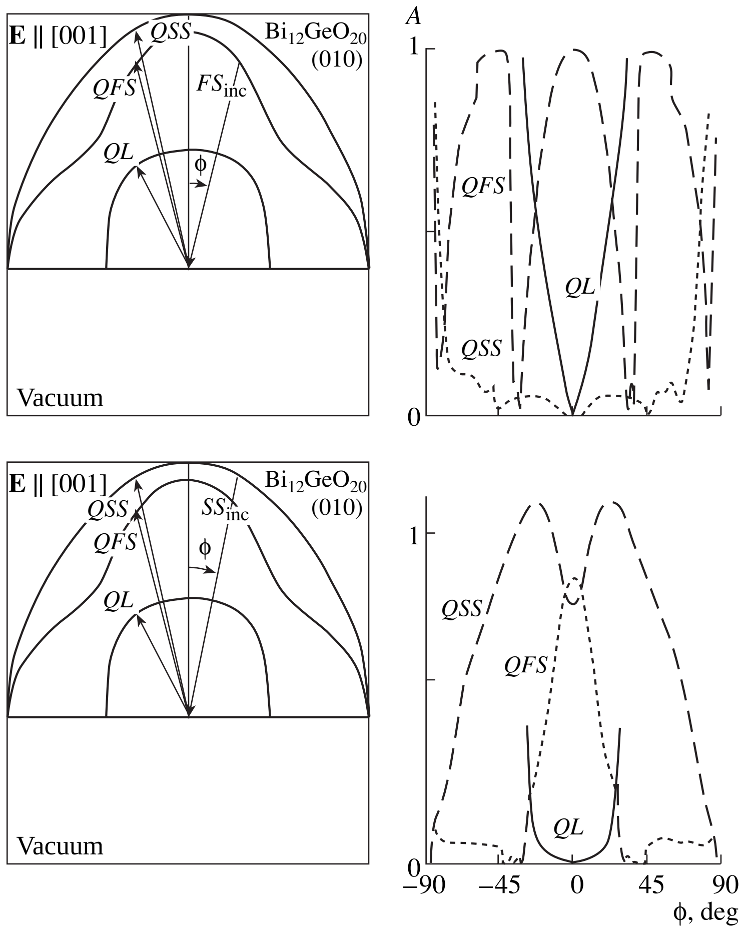

Fig. 1. (Contd.)

wave, for the reflected *QL* wave, beginning with an angle of incidence of 38°, the phenomenon of total internal reflection is observed. (The refraction vector of the elastic wave becomes complex.)

In the case of incidence of an *SQS* wave, application of an external electric field, which decreases the crystal symmetry, generates all three types of reflected waves. In the absence of a field directed along the normal to the free surface, there is an tangential acoustic axis [9]. Application of an electric field **E || **[001], as discussed previously [10, 11], removes the degeneracy of shear waves in the [001] direction. In this case, the initial acoustic axis is split into two conical axes lying in the (110) plane. Therefore, even normal incidence of an *SQS* wave leads to the generation of reflected shear waves of both types with real parts of the amplitude coefficients of 0.78 and 0.71 for the *FS* and *SS* waves, respectively. Note that, when an electric field is applied, the amplitude coefficients of reflected waves are always complex.

EFFECT OF A DC ELECTRIC FIELD ON THE REFLECTION AND REFRACTION OF BAWS AT THE INTERFACE BETWEEN AN ISOTROPIC ELASTIC MEDIUM AND A PIEZOELECTRIC CRYSTAL

Figure 2 shows the results of the calculation of the real parts of the amplitude reflection coefficients and amplitude refractive indices of BAWs in a system composed of fused quartz and germanosillenite $Bi_{12}GeO_{20}$ for the case when an external electric field is applied only to the $Bi_{12}GeO_{20}$ crystal along the twofold axis [001], i.e., normally to the interface between these media. The cases of incidence of *L* and shear waves polarized either in the plane of incidence or normally to it are investigated. When **E** = 0, for an incident *L* wave, there are only a reflected *L* wave and a shear wave (polarized in the plane of incidence) and a refracted *L* wave and an *FS* wave (polarized in the plane of incidence). A characteristic feature of this case is the transformation of the type of refracted waves since, at an angle of incidence of 58°, only the *FS* wave exists (from all refracted waves).

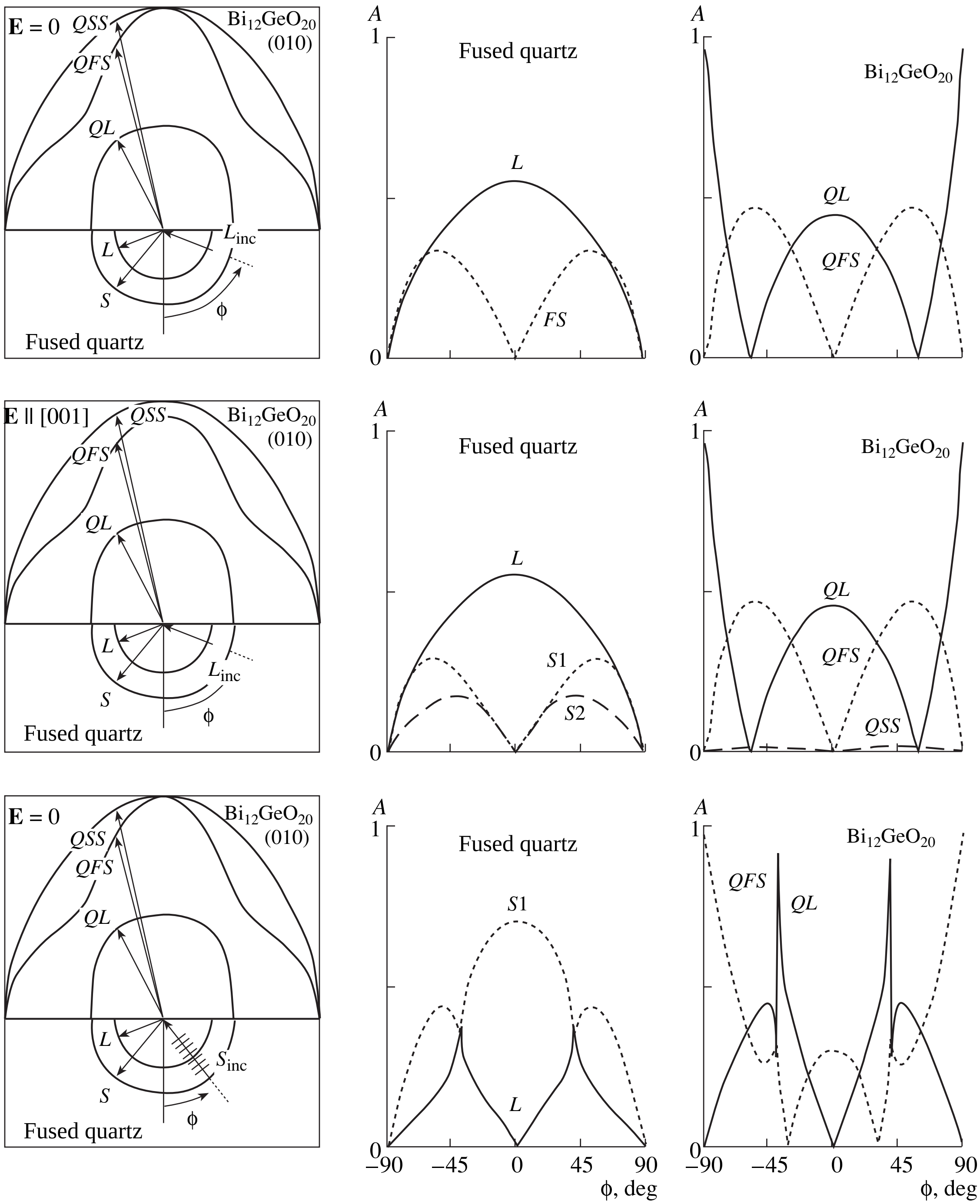

Fig. 2. Real parts of the amplitude reflection coefficients and amplitude refractive indices of BAWs incident on the fused-quartz/germanosillenite interface in the (010) plane. The case of incidence from the fused quartz.

A similar situation occurs when a shear wave polarized in the plane of incidence is incident on the interface. In this case, at an angle of incidence of 32°, there is only a refracted *L* wave. However, at an angle of incidence of 40°, the total internal reflection of this wave is observed.

When a shear wave polarized orthogonally to the plane of incidence is incident on the interface, the wave of the same type is reflected. However, concerning refracted waves, there is only an *SS* wave in germanosillenite, which has a longitudinal piezoelectric activity. The piezoelectric activity of the *SS* wave leads to the generation of an electrostatic potential wave at the piezoelectric-crystal/isotropic-medium interface. This wave is not related to elastic vibrations in the isotropic medium and decays exponentially with an

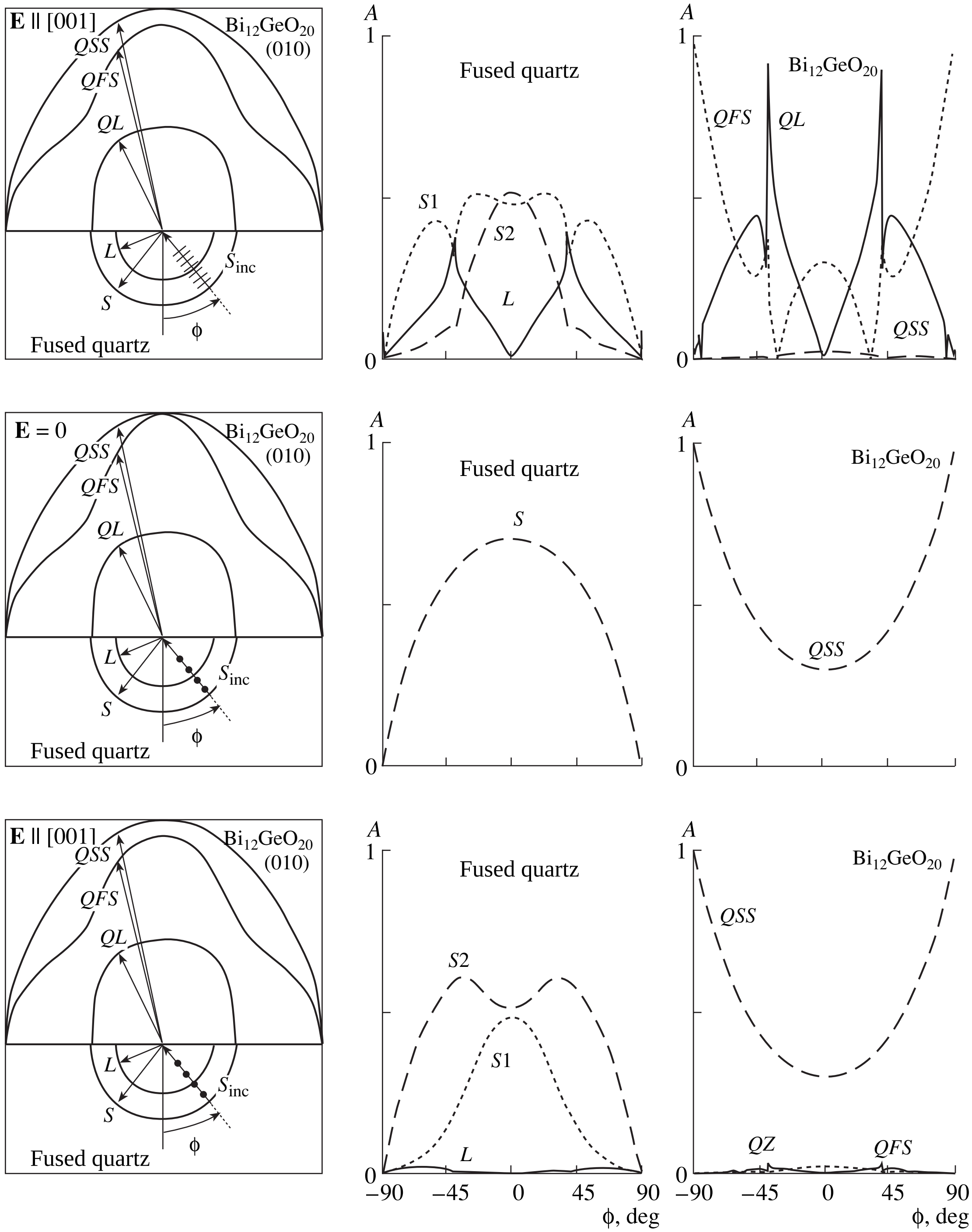

Fig. 2. (Contd.)

increase in the distance from the interface. As a result of the presence of a potential wave, the amplitude coefficient of the reflected elastic wave is a complex value and its refraction vector is real.

Application of an electric field **E** ∥ [001] to a $Bi_{12}GeO_{20}$ crystal, owing to the reduction in the crystal symmetry, leads to that the incidence of an elastic wave of any type from an isotropic medium generates all three types of refracted and reflected waves. An interesting example is the incidence of a shear wave polarized normally to the plane of incidence. In this case, it appears as two reflected shear waves arise in the isotropic medium, one of which is polarized in the plane of incidence and the other is polarized normally to it. Naturally, shear waves of only one type can exist in an isotropic medium. Nevertheless, the change in the boundary conditions caused by the application of an external electric field to a $Bi_{12}GeO_{20}$ crystal leads also to the change in the direction of the polarization vector of the incident *SQS* wave, which turns out to be directed at some angle to the plane of incidence. This circumstance allows for the existence of a reflected shear wave, also polarized at some angle to the plane of incidence.

CONCLUSIONS

The software package developed here makes it possible to investigate the processes of reflection and refraction of BAWs at interfaces between crystals of arbitrary symmetry and obtain results in the form of cross sections of refraction cavities. If the coefficients of the nonlinear electromechanical properties are known, this calculation can be supplemented by the consideration of the effect of an external electric field.

ACKNOWLEDGMENTS

This study was supported by the Federal Target Program “Integration,” project no. 67, and the President of the Russian Federation (the program “Leading Scientific Schools,” project no. NSh 939.2003.2).

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Translated by Yu. Sin’kov