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Surface polaritons in symmetry planes of biaxial crystals

A N Furs, V M Galynsky and L M Barkovsky

Department of Theoretical Physics, Belarussian State University, Fr. Skarina Ave. 4, Minsk 220050, Belarus

E-mail: Barkovsky@bsu.by

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Abstract

The problem of the surface polariton existence in symmetry planes of nonmagnetic biaxial crystals is studied theoretically. The plane interface of such a crystal and a semi-infinite isotropic medium is considered. With the use of the integral formalism formulated in our earlier work, the dispersion equation is derived for the polaritons under consideration. The existence conditions for the dispersion equation solutions are obtained in the form of algebraic inequalities for principal values of inverse dielectric permittivity tensors. If these conditions are satisfied, then excitation of surface waves is possible along the allowed propagation directions, which constitute sectors in the interface plane. Exact expressions are obtained that determine location of these sectors with respect to the symmetry axes of the crystal.

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1. Introduction

Recently, research has focused closely on polariton states in condensed matter including surface polaritons. Such states may be characterized by a term 'half light, half matter' [1], inasmuch as for polariton excitations the properties of light and matter are intertwined in a remarkable manner.

Surface polaritons, being the electromagnetic excitations localized near the interface at a distance of the order of wavelength, can be tentatively divided into two classes. The first of them represents well-studied surface waves at the interface of isotropic media with opposite signs of dielectric permittivities and strong frequency dispersion [2]. Surface plasmon polaritons are among them. Not long ago, a second class of surface polaritons was theoretically predicted [3, 4], which appear owing to anisotropy of contacting materials and are called singular surface electromagnetic waves. Unlike surface electromagnetic waves of the first class, singular surface polaritons can be excited in bianisotropic materials with positive definite

dielectric permittivity and magnetic permeability tensors ε and μ when dispersion is little. In particular, such surface polaritons appear in anisotropic dielectric and magnetic media, as well as gyrotropic and Faraday media [5, 6]. The allowed propagation directions of polaritons form sectors in the interface plane. The greater the anisotropy of one or two contacting media, the greater the angular width of these sectors. Optical anisotropy manifests itself to a considerable extent for singular surface polaritons when the interface is formed by different cuts of the same uniaxial crystal [7–9]. Such an interface can be formed if the uniaxial crystal is divided in half by a plane passing through its optical axis and then parts of the crystal are turned around each other. As a result, their optical axes are made crosswise in the interface plane.

Surface electromagnetic waves at the interface of a uniaxial crystal and an isotropic medium were studied in [3, 4, 10]. The more complicated case of surface waves in the symmetry planes of biaxial crystals was considered in [11]. There, the dispersion relation was found for such waves in the form of a system of algebraic equations. But in view of the complexity of the obtained equations, the authors restricted themselves to solving the system only for the case of weakly anisotropic crystals using expansions in terms of small anisotropy parameters. Approximate formulae were found which determine position of the sectors of the allowed propagation directions for polaritons. Meanwhile, singular surface polaritons typically reveal themselves just in strongly anisotropic crystals.

The aim of the present work is a more thorough study of surface polaritons in the symmetry planes of biaxial crystals with arbitrary degree of anisotropy without the use of any approximations. In the process, we apply the general integral approach worked out originally in the theory of surface elastic waves (see [12] and references therein) and then extended by us to surface polaritons [13–15]. The essence of this approach is in a representation of Maxwell's equations by a system of matrix equations with six-dimensional vectors involved in it. These vectors are composed of tangential components of electric and magnetic strength vectors at the interface. As a result, the dispersion equation for surface waves is expressed in terms of the surface impedance tensors, which in turn are calculated as a product of the special tensors in the integral representation (see section 2).

Advantages of the integral approach are the following. The dispersion equations are derived uniformly regardless of complexity of the constitutive equations for contacting linear media [15]. Moreover, for arbitrary cuts of anisotropic and bianisotropic media, the dispersion equations can in principle be derived analytically with the use of modern systems of computer algebra. They are presented in a general form F(v) = 0, where $v = \omega/(ck)$ is a reduced frequency of a surface wave. As a rule, F(v) is monotonic function of v. It allows comparatively simple analysis of existence of the dispersion equations.

While existence conditions for surface electromagnetic waves are being established, it is important to find the so-called limiting frequencies of these waves [15]. Calculation of these for biaxial crystals is based on study of the refraction surface sections (sections 3 and 4). Further, in sections 5 and 6, the surface impedance tensors are found and necessary existence conditions are established for surface polaritons in the symmetry planes of biaxial crystals. Derivation of the dispersion equation and analysis of existence of its solutions for arbitrary relations involving the material parameters of the contacting biaxial crystal and isotropic medium are given in section 7. Proceeding to the limit of surface waves in uniaxial crystals is discussed in section 8.

Here, we study surface polaritons only in non-magnetic, non-chiral transparent biaxial crystals with real symmetric dielectric permittivity tensors. Consideration of chiral or absorbing biaxial crystals is possible in principle with the use of general approach developed in [15] but it is more complicated. This is a topic of further publications. Note that simple

introduction of chirality for isotropic media (Faraday media) when the dielectric tensor is Hermitian leads to fundamentally new physical effects with respect to surface polaritons. In particular, one of them is unidirectional propagation of surface polaritons—if the surface wave can propagate in some direction b along the interface, then it cannot propagate in the opposite direction -b (see [5, 6] for details).

In this paper, we use the following notation of operations with three-dimensional scalars, vectors and tensors. The scalar (internal) product of vectors u and v is marked as uv, the vector (external) product as $u \times v$ and the tensor product as $u \otimes v$. The scalar product of a tensor β and a vector u is a vector $w = \beta u$ with components $w_i = \beta_{ij}u_j$ (summation is implied over repeating indices). A dual antisymmetric pseudotensor of the second rank u^{\times} can be associated with vector u in accordance with formula $(u^{\times})_{ik} = e_{ijk}u_j$, where e_{ijk} is the Levi-Civita pseudotensor and u_j are Cartesian components of vector u. For such tensors, the relations $u^{\times}v = u \times v$, $vu^{\times} = v \times u$ take place, i.e. vector product of vectors u and v is replaced by scalar product of dual tensor u^{\times} and vector v.

2. General case of surface electromagnetic wave propagation at the interface of anisotropic dielectric media

Consider first a general case of surface electromagnetic waves at the interface of anisotropic dielectric media.

Let q be a unit normal to the interface of anisotropic media directed from the medium with permittivity tensor $\varepsilon = \varepsilon(\omega)$ to the medium with tensor $\varepsilon' = \varepsilon'(\omega)$, where ε and ε' are real symmetric tensors and ω is the frequency of the surface wave. The Cartesian axis z is directed along q, coordinate plane z = 0 aligning with the interface. Field distribution in both media can be presented by a superposition of the two inhomogeneous partial waves. For instance, in the medium z < 0 characterized by tensor ε , we have

$$H(\mathbf{r},t) = \sum_{s=1}^{2} C_s H_s^0 \exp[ik(\mathbf{b} + \eta_s \mathbf{q})\mathbf{r} - i\omega t] = \sum_{s=1}^{2} C_s H_s^0 \exp\left[i\omega\left(\frac{1}{c}\mathbf{m}_s \mathbf{r} - t\right)\right],$$

$$E(\mathbf{r},t) = \sum_{s=1}^{2} C_s E_s^0 \exp[ik(\mathbf{b} + \eta_s \mathbf{q})\mathbf{r} - i\omega t] = \sum_{s=1}^{2} C_s E_s^0 \exp\left[i\omega\left(\frac{1}{c}\mathbf{m}_s \mathbf{r} - t\right)\right],$$
(1)

where a unit vector **b** determines the propagation direction of the wave along the interface plane, k is the projection of the wave vector to **b**, H_s^0 and E_s^0 are vector amplitudes of the partial waves and C_s are weight factors (s = 1, 2). Complex coefficients η_s (Im $\eta_s < 0$) characterize decay of the surface wave when moving away from the interface. They are included in the complex refraction vectors

$$\boldsymbol{m}_s = \frac{1}{\nu} (\boldsymbol{b} + \eta_s \boldsymbol{q}), \qquad s = 1, 2,$$

where reduced frequency $v = \omega/(ck)$ represents the phase velocity of the surface wave in units of *c* (velocity of light in vacuum). Fields H'(r, t), E'(r, t) in the second medium (z > 0) are also described by equations of type (1) with the change of symbols H_s^0 , E_s^0 , C_s , η_s , m_s to those with a prime. But here the decay coefficients η'_s are subject to the condition Im $\eta'_s > 0$.

Boundary conditions for the waves (1) take the form

$$\boldsymbol{H}_{\tau}^{0} = \boldsymbol{H}_{\tau}^{\prime 0}, \qquad \boldsymbol{q} \times \boldsymbol{E}^{0} = \boldsymbol{q} \times \boldsymbol{E}^{\prime 0}, \tag{2}$$

where

$$\boldsymbol{H}_{\tau}^{0} = \sum_{s=1}^{2} C_{s} \boldsymbol{H}_{s\tau}^{0}, \qquad \boldsymbol{q} \times \boldsymbol{E}^{0} = \sum_{s=1}^{2} C_{s} \boldsymbol{q} \times \boldsymbol{E}_{s}^{0},$$

$$H_{\tau}^{\prime 0} = \sum_{s=1}^{2} C_{s}^{\prime} H_{s\tau}^{\prime 0}, \qquad q \times E^{\prime 0} = \sum_{s=1}^{2} C_{s}^{\prime} q \times E_{s}^{\prime 0}$$

and subscript τ denotes tangential components of the vector fields (projection of the field vectors to the interface plane).

Resulting values of the electric and magnetic strengths at the interface $q \times E^0$ and H^0_{τ} ($q \times E'^0$ and H'^0_{τ}) connect between themselves linearly through a planar surface impedance tensor γ (γ') [16]:

$$\boldsymbol{q} \times \boldsymbol{E}^{0} = \boldsymbol{\gamma} \boldsymbol{H}_{\tau}^{0}, \qquad \boldsymbol{q} \times \boldsymbol{E}^{\prime 0} = \boldsymbol{\gamma}^{\prime} \boldsymbol{H}^{\prime 0}_{\tau}. \tag{3}$$

Eliminating vector variables from (2) and (3), we obtain a dispersion equation for the surface polaritons

$$(\overline{\gamma - \gamma'})_t = 0, \tag{4}$$

where $(\overline{\gamma - \gamma'})_t$ is a trace of the tensor adjoined to $\gamma - \gamma'$.¹

In [13–15], it was shown that anti-Hermitian surface impedance tensors can be calculated by formulae²

$$\gamma = \frac{1}{\nu}Q^{-}(-iI - S), \qquad \gamma' = \frac{1}{\nu}Q'^{-}(iI - S').$$
 (5)

Tensors Q and S have an integral representation

$$Q = -\frac{1}{\pi} \int_0^{\pi} (e_2 e_2)^- d\phi, \qquad S = -\frac{1}{\pi} \int_0^{\pi} (e_2 e_2)^- (e_2 e_1) d\phi.$$
(6)

Integrals in equations (6) include tensorial bilinear forms of arbitrary vector arguments u and v defined by

$$(\boldsymbol{u}\boldsymbol{v})_{kn} = c_{klmn}\boldsymbol{u}_l\boldsymbol{v}_m,\tag{7}$$

where the fourth rank tensor c_{klmn} is introduced

$$c_{klmn} = -\frac{(\varepsilon^{-1})_{lm}a_ka_n + \nu^2 I_{kr}e_{rli}\varepsilon_{ij}^{-1}e_{jmp}I_{pn}}{a\varepsilon^{-1}a - \nu^2} + \nu^2 b_l b_m I_{kn}$$

and $a = b \times q$. Vectors e_1 and e_2 in (6) are expressed in terms of the vectors b and q

$$e_1 = b\cos\phi + q\sin\phi, \qquad e_2 = -b\sin\phi + q\cos\phi.$$
 (8)

Tensors Q' and S' can also be calculated by formulae (6) and (7) with the replacement of ε with ε' in (7).

The left-hand side of dispersion equation (4) is a function of the reduced frequency ν . Its solution $\nu = \nu_S$ describes a surface electromagnetic wave localized close to the interface if $0 < \nu_S < \hat{\nu}_L$, where $\hat{\nu}_L = \min(\nu_L, \nu'_L)$ and ν_L, ν'_L are the so-called *limiting frequencies* of surface electromagnetic waves in each contacting medium. These frequencies have a great importance for determining existence conditions of surface polaritons and can be found geometrically using the refraction surface sections by a plane passing through vectors **b** and **q** (see [14, 15] and next section). Furthermore, tensors Q and S (6) exist only if $\nu \in [0, \nu_L)$, and Q' and S' exist only if $\nu \in [0, \nu'_L)$. For an isotropic medium with permittivity ε' , the limiting frequency is $\nu'_L = 1/\sqrt{\varepsilon'}$. If anisotropic dielectric with permittivity tensor ε contacts with

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¹ By definition, the adjoined tensor is $\overline{\beta}_{ij} = \frac{1}{2} e_{klj} e_{mni} \beta_{km} \beta_{ln}$ [17]. The trace $\overline{\beta}_t$ of the tensor adjoined to planar tensor β ($\beta q = q\beta = 0$) is equal to the determinant of the matrix representing β in a subspace orthogonal to q.

² Symbol ⁻ denotes pseudoinversion operation of the planar tensors, i.e. inversion in a subspace orthogonal to q. By definition, $QQ^- = Q^-Q = I$, where $I = -q^{\times 2} = 1 - q \otimes q$ is a projective operator to the boundary plane [18, 19].

an isotropic medium, then the necessary existence condition can be expressed as follows (see [14]):

$$-i\lim_{\nu\to\nu_1}a\gamma a>0.$$
(9)

Under condition (9), it is possible to select a value of permittivity ε' of the isotropic medium in order to allow propagation of a surface electromagnetic wave along a given direction *b*.

3. Refraction surface sections of biaxial crystals

We apply the results of the previous section to the surface electromagnetic waves at the interface of biaxial crystal with permittivity tensor

$$\varepsilon = a_1^{-1} c_1 \otimes c_1 + a_2^{-1} c_2 \otimes c_2 + a_3^{-1} c_3 \otimes c_3$$
(10)

and isotropic medium with permittivity ε' . In formula (10), unit vectors c_1, c_2, c_3 are directed along the principal axes of the tensor ε , and $a_1^{-1} = \varepsilon_1, a_2^{-1} = \varepsilon_2, a_3^{-1} = \varepsilon_3$ are the principal values of ε at the wave frequency ω . To denote inverse permittivity of the isotropic medium, we use the symbol $a' = 1/\varepsilon'$. All material parameters a_1, a_2, a_3, a' are supposed to be real and positive.

Let a plane crystal cut be perpendicular to one of the principal axes of the tensor ε , i.e. it coincides with one of the crystallographic symmetry planes of the crystal. Hereinafter when using the term 'biaxial crystal' with respect to surface electromagnetic waves, we presume that the cut plane is oriented in such a manner. Without loss of generality, we can get an axis directed along c_2 as a normal to the cut plane and assume that vectors c_1 , c_2 , c_3 produce a right-hand triple and, in addition, $a_1 > a_3$.

Surface electromagnetic wave propagation direction is specified by an angle α measured from the vector c_1 : $b = c_1 \cos \alpha + c_3 \sin \alpha$. Vectors b and $a = b \times q$ lie in the cut plane, so

$$c_1 = b \cos \alpha - a \sin \alpha, \qquad c_2 = q, \qquad c_3 = b \sin \alpha + a \cos \alpha.$$
 (11)

To determine the dependence of limiting frequencies v_L for surface electromagnetic waves in a biaxial crystal on angle α , we need to study the refraction surface of this crystal and its section by a *reference plane* (plane passing through vectors **b** and **q**). The refraction vector of the body electromagnetic wave with phase normal n ($n^2 = 1$) is determined by the equation m = nn, where *n* is a wave refractive index. Refraction surface constitutes a locus of extreme points of the refraction vectors, whose beginnings are aligned in the reference point *O*. Vectors m satisfy an equation det($m^{\times} \varepsilon^{-1} m^{\times} + 1$) = 0 or in the expanded form (see [17])

$$m^2 m \varepsilon m + m (\overline{\varepsilon} - \overline{\varepsilon}_t) m + \det \varepsilon = 0.$$
⁽¹²⁾

Taking into account vector m decomposition $m = m_1c_1 + m_2c_2 + m_3c_3$ and relations

$$\overline{\varepsilon} = a_2^{-1} a_3^{-1} c_1 \otimes c_1 + a_1^{-1} a_3^{-1} c_2 \otimes c_2 + a_1^{-1} a_2^{-1} c_3 \otimes c_3,$$

$$\overline{\varepsilon}_t = a_2^{-1} a_3^{-1} + a_1^{-1} a_3^{-1} + a_1^{-1} a_2^{-1}, \qquad \det \varepsilon = a_1^{-1} a_2^{-1} a_3^{-1},$$

equation (12) takes the form

$$(m_1^2 + m_2^2 + m_3^2) (a_2 a_3 m_1^2 + a_1 a_3 m_2^2 + a_1 a_2 m_3^2) - (a_2 + a_3) m_1^2 - (a_1 + a_3) m_2^2 - (a_1 + a_2) m_3^2 + 1 = 0.$$
 (13)

Equation (13) determines the relation between refraction vector components m_1, m_2, m_3 and is an equation for the refraction surface of body electromagnetic waves in biaxial crystals. This surface is closed and consists of two sheets, inasmuch as two waves can propagate along a given direction n with two different phase velocities. Vector components m_1, m_2, m_3 enter



Figure 1. Refraction surface sections of the biaxial crystals with the reference planes: (a) $a_1 = 0.7, a_2 = 0.9, a_3 = 0.1, \alpha = 50^\circ$; (b) $a_1 = 0.9, a_2 = 0.7, a_3 = 0.1, \alpha = 50^\circ$; (c) $a_1 = 0.9, a_2 = 0.7, a_3 = 0.1, \alpha = \alpha_0 = 60^\circ$.

into (13) in even powers so the refraction surface is centrosymmetrical, and coordinate planes passing through basis vectors c_1 and c_2 , c_2 and c_3 , c_3 and c_1 are symmetry planes of the refraction surface.

The reference plane with unit normal *a* forms an angle α with vector c_1 . In view of the surface refraction symmetry, it is enough to study its reference plane section only at angle range $0 \le \alpha \le \pi/2$.

Now we find equations of the section curves. The left- and right-hand sides of equations (11) scalarly multiplied by the vector m take the form

$$m_1 = m_b \cos \alpha - m_a \sin \alpha, \qquad m_2 = m_q, \qquad m_3 = m_b \sin \alpha + m_a \cos \alpha,$$
 (14)

where m_b , m_q , m_a are components of m in (b, q, a) basis. For any vector in the reference plane, its component along a equals zero: $m_a = 0$. If we substitute (14) into (13) and suppose $m_a = 0$, we obtain the following curve equation:

$$\left(m_b^2 + m_q^2\right) \left(a_2 dm_b^2 + a_1 a_3 m_q^2\right) - (a_2 + d)m_b^2 - (a_1 + a_3)m_q^2 + 1 = 0,$$
(15)

where

$$d = a_1 \sin^2 \alpha + a_3 \cos^2 \alpha. \tag{16}$$

Note that $a_3 \leq d \leq a_1$. The section consists of inner S_1 and outer S_2 curves. If the reference plane passes through an optical axis (direction along which two eigenwaves propagate with the same phase velocity), then they have common points. Since equation (15) is a fourth-order equation with respect to m_b and m_q , then any straight line in the section plane may cross the curves at not more than four points. This implies that inner curve must be convex, while outer curve may be either convex or concave (see figure 1).

Let refraction vector m in section plane be directed at angle θ to vector b. Then, its components equal

$$m_b = |\mathbf{m}|\cos\theta, \qquad m_q = |\mathbf{m}|\sin\theta,$$
 (17)

where $|m| = \sqrt{m^2} = \sqrt{m_b^2 + m_q^2}$ is a modulus of vector *m*. Now we substitute (17) into (15) and write equation (15) in the polar coordinates |m| and θ :

$$m^{4}(a_{2}d\cos^{2}\theta + a_{1}a_{3}\sin^{2}\theta) - m^{2}[(a_{2}+d)\cos^{2}\theta + (a_{1}+a_{3})\sin^{2}\theta] + 1 = 0.$$
 (18)

From (18), we find equations of the curves in the reference plane:

$$m^{2} = n^{2} = \frac{1}{2}(a_{2}d\cos^{2}\theta + a_{1}a_{3}\sin^{2}\theta)^{-1}\{(a_{2}+d)\cos^{2}\theta + (a_{1}+a_{3})\sin^{2}\theta \\ \pm [[(a_{2}+d)\cos^{2}\theta + (a_{1}+a_{3})\sin^{2}\theta]^{2} - 4(a_{2}d\cos^{2}\theta + a_{1}a_{3}\sin^{2}\theta)]^{\frac{1}{2}}\},$$
(19)

where plus sign corresponds to the outer curve S_2 and minus sign corresponds to the inner curve S_1 . Then, we return in equations (19) to the variables m_b and m_q considering (17) and introducing notation $\kappa = m_a^2/m_b^2 = \tan^2 \theta$:

$$2m_b^2(1+\kappa)(a_2d+a_1a_3\kappa)\{a_2+d+(a_1+a_3)\kappa\}$$

$$\pm \left[\left[a_2 + d + (a_1 + a_3)\kappa \right]^2 - 4(1 + \kappa)(a_2d + a_1a_3\kappa) \right]^{\frac{1}{2}} \right\}^{-1} = 1.$$
(20)

It is obvious (see (20)) that curves S_1 and S_2 are symmetrical relative to the coordinate axes directed along vectors b and q.

Limiting frequencies v_L of the surface waves can be found geometrically by the following way. Let *L* be a straight line parallel to vector *q* and originally located at infinity, which moves towards -b until the first contact with the section curve S_2 of the outer sheet of the refraction surface (figure 1). Then, the limiting frequency v_L is reciprocal of the distance from the point *O* to the line *L*, passing through one or several points of tangency. When $v = v_L$, at least one of the coefficients η_1 , η_2 in (1) becomes real and now corresponds to the body partial wave. In order to establish location of the contact by the straight line *L*, it is important to investigate parts of the section curve S_2 close to the coordinate axis m_b , i.e. when κ is small. We choose in equation (20) the upper sign corresponding to curve S_2 and retain only terms with first order of κ , so at $a_2 > d$, we have

$$dm_b^2 + \frac{a_1a_3 - d(a_1 + a_3 - a_2)}{a_2 - d}m_q^2 = 1$$
(21)

and at $a_2 < d$,

$$a_2 m_b^2 + \frac{a_1 a_3 - a_2 (a_1 + a_3 - d)}{d - a_2} m_q^2 = 1.$$
 (22)

Thus, parts of the section curve close to the *b*-direction approximately seem as a second-order curve with a general equation $h_b m_b^2 + h_q m_q^2 = 1$. This curve crosses m_b -axis at point *A* at the distance $OA = 1/\sqrt{h_b}$. Depending on the sign of the coefficient h_q of m_q^2 , equations (21) and (22) correspond either to an ellipse ($h_q > 0$) or to a hyperbola ($h_q < 0$). In the first case, the section curve S_2 is a convex curve at small values of m_q and in the second case, the curve is concave.

Consider the following cases of relations involving parameters a_1 , a_2 and a_3 contained in tensor ε (10):

(i)
$$a_2 \ge a_1 > a_3$$
, (ii) $a_1 > a_2 > a_3$, (iii) $a_1 > a_3 \ge a_2$.

If relation (i) is satisfied, then $a_2 > d$ at $\alpha \neq \frac{\pi}{2}$ and we analyse equation (21). It is easy to show that the coefficient of m_q^2 will be positive:

$$a_1a_3 - d(a_1 + a_3 - a_2) > a_1a_3 - a_1(a_1 + a_3 - a_2) = a_1(a_2 - a_1) \ge 0;$$

therefore, outer section curve is convex at small m_q . Distance *OA* equals $1/\sqrt{d}$ and depends on α (i.e. depends on the position of the reference plane). Similarly, if relation (iii) is satisfied, then $a_2 < d$ at $\alpha \neq 0$, so equation (22) causes the curve S_2 to be convex at small m_q too and to cross the coordinate axis at distance $OA = 1/\sqrt{a_2}$ which does not depend on α . Finally, for the relation (ii), we have $a_2 \ge d$. Let angle α_0 be determined by equation $a_2 = d$ (see also (16))

$$\sin \alpha_0 = \sqrt{\frac{a_2 - a_3}{a_1 - a_3}}$$
(23)

and angles α_1 and α_2 be determined by the equations $a_1a_3 - d(a_1 + a_3 - a_2) = 0$ and $a_1a_3 - a_2(a_1 + a_3 - d) = 0$, respectively,

$$\sin \alpha_1 = \sqrt{\frac{a_3(a_2 - a_3)}{(a_1 + a_3 - a_2)(a_1 - a_3)}}, \qquad \sin \alpha_2 = \sqrt{\frac{a_1(a_2 - a_3)}{a_2(a_1 - a_3)}}, \qquad (24)$$

resulting in vanishing of coefficient h_q of m_q^2 in equations (21) and (22). Then, in the case (ii), an inequality $\alpha_1 < \alpha_0 < \alpha_2$ is satisfied, and at $0 \le \alpha < \alpha_1$ or $\alpha_2 < \alpha \le \frac{\pi}{2}$, a part of the curve S_2 close to the point A is convex, but at $\alpha_1 < \alpha < \alpha_2$ it is concave. If $\alpha < \alpha_0$, then $OA = 1/\sqrt{d}$, otherwise $OA = 1/\sqrt{a_2}$.

Thus, when relation (ii) is satisfied and while angle α is increased from 0 to $\frac{\pi}{2}$, at $\alpha = \alpha_1$, convexity of the curve part S_2 near point A changes to concavity, but at $\alpha = \alpha_2$ it is vice versa. Intermediate angle α_0 (23) corresponds to the contact of the inner and outer section curves at point A (see figure 1(c)). In that case, the section reference plane passes through the optical axis of the biaxial crystal whose direction is given by the unit vector $\mathbf{c}' = \mathbf{c}_1 \cos \alpha_0 + \mathbf{c}_3 \sin \alpha_0$. Owing to symmetry of the refraction surface, a vector \mathbf{c}'' (vector of other optical axis) is obtained by replacement of α_0 with $-\alpha_0$ in the last equation: $\mathbf{c}'' = \mathbf{c}_1 \cos \alpha_0 - \mathbf{c}_3 \sin \alpha_0$. Note that vectors \mathbf{c}' and \mathbf{c}'' are included in the Fedorov axial representation of the permittivity tensor for biaxial crystal [17]

$$\varepsilon^{-1} = a_2 + \frac{a_1 - a_3}{2} (\mathbf{c}' \otimes \mathbf{c}'' + \mathbf{c}'' \otimes \mathbf{c}').$$

4. Limiting frequencies of surface electromagnetic waves in biaxial crystals

It is easy to calculate limiting frequency v_L of a surface electromagnetic wave in the case when the outer section curve S_2 is a convex curve near the point A (see figure 1(a)). Then, the straight line L contacts curve S_2 at the point A and limiting frequency v_L equals reciprocal of length of the line segment OA. Particularly, as is set forth in previous section, $v_L = \sqrt{d}$ at any α when relations (i) are satisfied, or in case (ii) with conditions $0 \le \alpha \le \alpha_1$ satisfied. Next, $v_L = \sqrt{a_2}$ at any α when relations (iii) are satisfied, or in case (ii) with satisfied conditions $\alpha_2 \le \alpha \le \frac{\pi}{2}$.

If curve S_2 is concave close to the point A and line L contacts this curve at two points (conditions (ii) with $\alpha_1 < \alpha < \alpha_2$), then limiting frequencies need to be calculated individually. We differentiate equation (15) with respect to m_q and take into account that for a contact point $dm_b/dm_q = 0$. As a result, we have

$$m_q^2 = \frac{a_1 + a_3}{2a_1 a_3} - \frac{a_2 d + a_1 a_3}{2a_1 a_3} m_b^2,$$
(25)

with the assumption that $m_q \neq 0$. After substitution of (25) in equation (15) for the section curves and taking into consideration that the limiting frequency v_L is calculated by means of coordinate m_b as $v_L = 1/m_b$, we get

$$(a_1 - a_3)^2 v_{\rm L}^4 - 2[(a_1 + a_3)(a_2d + a_1a_3) - 2a_1a_3(a_2 + d)]v_{\rm L}^2 + (a_2d - a_1a_3)^2 = 0.$$
(26)

C	Relations				
Case	between a_1, a_2, a_3	Angle α	Limiting frequency $v_{\rm L}$		
(i)	$a_2 \geqslant a_1 > a_3$	$0 \leq \alpha < \frac{\pi}{2}$	$v_{\rm L} = \sqrt{d}$		
(ii(a))	$a_1 > a_2 > a_3$	$0 \leq \alpha < \alpha_1$	$v_{\rm L} = \sqrt{d}$		
(ii(b))	$a_1 > a_2 > a_3$	$\alpha_1 \leqslant lpha \leqslant lpha_2$	$v_{\rm L} = \widetilde{v}_{\rm L} \ (27)$		
(ii(c))	$a_1 > a_2 > a_3$	$\alpha_2 < \alpha \leq \frac{\pi}{2}$	$v_{\rm L} = \sqrt{a_2}$		
(iii)	$a_1 > a_3 \geqslant a_2$	$0 < \alpha \leq \frac{\pi}{2}$	$v_{\rm L} = \sqrt{a_2}$		

Table 1. Limiting frequencies v_L of surface electromagnetic waves in biaxial crystals.

We denote solutions of biquadratic equation (26) as $\tilde{\nu}_L$ and finally obtain an expression for the limiting frequency

$$\widetilde{\nu}_{\rm L}^2 = \frac{1}{(a_1 - a_3)^2} [(a_1 + a_3)(a_2d + a_1a_3) - 2a_1a_3(a_2 + d) + 2\sqrt{a_1a_3(a_1 - a_2)(a_2 - a_3)(a_1 - d)(d - a_3)}].$$
(27)

Note that selection of the positive sign of the radical in (27) is determined by the requirement of continuity of limiting frequency v_L at points $\alpha = \alpha_1$ and $\alpha = \alpha_2$ (24). Indeed, when $\alpha = \alpha_1$ (i.e. $a_2 = a_1 + a_3 - a_1 a_3/d$), limiting frequency has to be equal to $v_L = \sqrt{d}$, but when $\alpha = \alpha_2$ ($d = a_1 + a_3 - a_1 a_3/a_2$), it has to be equal to $v_L = \sqrt{a_2}$. It is true only if in solution (27) of biquadratic equation (26), the positive sign of the radical is selected.

The obtained values of limiting frequencies v_L are charted in table 1, used later for establishing existence conditions of surface waves at the interface of a biaxial crystal and an isotropic medium. From the obtained equations for v_L , it is evident that function $v_L = v_L(\alpha)$ is non-decreasing on the interval $\left[0, \frac{\pi}{2}\right]$ and has a limit

$$\nu_{\rm L} \leqslant \min(\sqrt{a_2}, \sqrt{d}). \tag{28}$$

Strict inequality in (28) is achieved only in the case (ii) at $\alpha_1 < \alpha < \alpha_2$ and equality is achieved in other cases.

5. Derivation of the surface impedance tensors γ and γ'

The dispersion equation for surface electromagnetic waves at the interface of a biaxial crystal and an isotropic medium will be obtained by substitution of the surface impedance tensors γ and γ' of the contacting media to formula (4). To find these tensors, we first need to calculate bilinear tensorial forms (e_2e_2) and (e_2e_1) related to a biaxial crystal, then tensors $(e_2e_2)^-$ and $(e_2e_2)^-(e_2e_1)$, and finally Q and S (6). Tensors Q' and S' in formula (5) for γ' are calculated analogously as Q and S with replacement $a_1, a_2, a_3 \rightarrow a'$ (going from the biaxial crystal to the isotropic medium).

According to (7), general expressions for the bilinear tensorial forms (e_2e_2) and (e_2e_1) take the coordinate-free form

$$(e_2e_j) = -(a\varepsilon^{-1}a - \nu^2)^{-1} \Big[e_2\overline{\varepsilon^{-1}}e_j(a\otimes a) + \nu^2 I e_2^{\times}\varepsilon^{-1}e_j^{\times}I \Big] + e_2b\otimes be_j\nu^2 I,$$
(29)

where j = 1, 2 and $e_2 b \otimes b e_j$ is the dyad $b \otimes b$ multiplied by vector e_2 from the left and by vector e_j from the right. Tensors ε^{-1} and $\overline{\varepsilon^{-1}}$ in (29) are given by formulae

$$\varepsilon^{-1} = \sum_{k=1}^{3} a_k c_k \otimes c_k, \qquad \overline{\varepsilon^{-1}} = a_1 a_2 a_3 \sum_{k=1}^{3} a_k^{-1} c_k \otimes c_k.$$

Therefore,

$$e_{2}\overline{\varepsilon^{-1}}e_{j} = a_{1}a_{2}a_{3}\sum_{k=1}^{3}a_{k}^{-1}e_{2}c_{k}\otimes c_{k}e_{j},$$

$$Ie_{2}^{\times}\varepsilon^{-1}e_{j}^{\times}I = -\sum_{k=1}^{3}a_{k}I(c_{k}\times e_{2})\otimes (c_{k}\times e_{j})I.$$
(30)

Since $I = b \otimes b + a \otimes a$, then

$$(\mathbf{c}_k \times \mathbf{e}_j)\mathbf{I} = \mathbf{I}(\mathbf{c}_k \times \mathbf{e}_j) = [(\mathbf{c}_k \times \mathbf{e}_j)\mathbf{b}]\mathbf{b} + [(\mathbf{c}_k \times \mathbf{e}_j)\mathbf{a}]\mathbf{a}.$$
(31)

By substituting vectors c_1 , c_2 , c_3 (11) and e_1 , e_2 (8) into equations (30) and (31), and then by substituting these equations in (29), we obtain decomposition of the forms (e_2e_2) and (e_2e_1) in the tensor basis $b \otimes b$, $b \otimes a$, $a \otimes b$, $a \otimes a$:

$$(e_{2}e_{2}) = (d - v^{2})^{-1} \{v^{2}[(d - v^{2})\sin^{2}\phi + d\cos^{2}\phi]b \otimes b \\ + v^{2}(a_{1} - a_{3})\sin\alpha\cos\alpha\cos^{2}\phi(b\otimes a + a\otimes b) \\ - [(a_{2} - v^{2})(d - v^{2})\sin^{2}\phi + (a_{1}a_{3} - v^{2}(a_{1} + a_{3} - d))\cos^{2}\phi]a \otimes a\}, \quad (32)$$
$$(e_{2}e_{1}) = \sin\phi\cos\phi(d - v^{2})^{-1} \{v^{4}b\otimes b + v^{2}(a_{1} - a_{3})\sin\alpha\cos\alpha(b\otimes a + a\otimes b)\}$$

$$-[a_1a_3 - (a_2 - \nu^2)(d - \nu^2) - \nu^2(a_1 + a_3 - d)]a \otimes a\}.$$
(33)

In the subspace orthogonal to vector q (in the interface plane), bilinear tensorial forms (e_2e_2) and (e_2e_1) can be represented by 2×2 matrices with elements equal to the coefficients of the decomposition of these forms in the tensor basis. Therefore, the determinant of (e_2e_2) which equals the trace of the adjoined tensor (e_2e_2) is

$$\overline{(e_2e_2)}_t = [b(e_2e_2)b][a(e_2e_2)a] - [b(e_2e_2)a][a(e_2e_2)b]$$

= $-\nu^2(d-\nu^2)^{-1}(A\cos^4\phi + B\sin^2\phi\cos^2\phi + C\sin^4\phi),$

where terms in brackets are matrix elements of the form (e_2e_2) and

$$A = a_1 a_3, \qquad B = a_1 a_3 + a_2 d - v^2 (a_1 + a_3), \qquad C = (a_2 - v^2)(d - v^2).$$
(34)
The tensor pseudoinverse to $(e_2 e_2)$ equals

$$(e_{2}e_{2})^{-} = (A\cos^{4}\phi + B\sin^{2}\phi\cos^{2}\phi + C\sin^{4}\phi)^{-1} \left\{ \frac{1}{\nu^{2}} [(a_{2} - \nu^{2})(d - \nu^{2})\sin^{2}\phi + (a_{1}a_{3} - \nu^{2}(a_{1} + a_{3} - d))\cos^{2}\phi]b \otimes b + (a_{1} - a_{3})\sin\alpha\cos\alpha\cos^{2}\phi + (b \otimes a + a \otimes b) - [(d - \nu^{2})\sin^{2}\phi + d\cos^{2}\phi]a \otimes a \right\}.$$
(35)

Multiplying $(e_2e_2)^-$ (35) by (e_2e_1) (33), we obtain

$$(e_{2}e_{2})^{-}(e_{2}e_{1}) = \sin\phi\cos\phi(A\cos^{4}\phi + B\sin^{2}\phi\cos^{2}\phi + C\sin^{4}\phi)^{-1} \\ \times \{\nu^{2}[(a_{2} - \nu^{2})\sin^{2}\phi + (a_{1} + a_{3} - d)\cos^{2}\phi]b\otimes b \\ + (a_{1} - a_{3})(a_{2} - \nu^{2})\sin\alpha\cos\alpha b\otimes a - \nu^{2}(a_{1} - a_{3})\sin\alpha\cos\alpha a\otimes b \\ + [(a_{1}a_{3} - (a_{2} - \nu^{2})(d - \nu^{2}) - \nu^{2}(a_{1} + a_{3} - d))\sin^{2}\phi \\ + (a_{1}a_{3} - d(a_{2} - \nu^{2}))\cos^{2}\phi]a\otimes a\}.$$
(36)

According to (6), tensors Q and S can be found by averaging over angle ϕ of expressions (35) and (36). Inasmuch as expression (36) is proportional to products of only odd powers of $\sin \phi$ and $\cos \phi$, then S = 0. At the same time,

$$Q = -\frac{1}{\nu^2} \{ (a_2 - \nu^2)(d - \nu^2) J_{02} + [a_1 a_3 - \nu^2 (a_1 + a_3 - d)] J_{20} \} \mathbf{b} \otimes \mathbf{b}$$

- $(a_1 - a_3) \sin \alpha \cos \alpha J_{20} (\mathbf{b} \otimes \mathbf{a} + \mathbf{a} \otimes \mathbf{b}) + [(d - \nu^2) J_{02} + d J_{20}] \mathbf{a} \otimes \mathbf{a}, \quad (37)$

where

$$(J_{02}; J_{20}) = \frac{1}{\pi} \int_0^{\pi} \frac{(\sin^2 \phi; \cos^2 \phi) \, \mathrm{d}\phi}{A \cos^4 \phi + B \sin^2 \phi \cos^2 \phi + C \sin^4 \phi} = \frac{1}{\pi} \int_{-\infty}^{+\infty} \frac{(1; x^2) \, \mathrm{d}x}{A x^4 + B x^2 + C}.$$

Calculating the integrals, we obtain

$$J_{02} = \frac{1}{\sqrt{C(B + 2\sqrt{AC})}}, \qquad J_{20} = \frac{1}{\sqrt{A(B + 2\sqrt{AC})}}.$$
 (38)

Substituting values A, B, C (34) into (38) and then (38) into (37), we find the final expression for the tensor Q

$$Q = \frac{1}{\sqrt{\Delta(\nu)}} \left\{ -\frac{1}{\nu^2} \left[\sqrt{(a_2 - \nu^2)(d - \nu^2)} + \frac{1}{\sqrt{a_1 a_3}} [a_1 a_3 - \nu^2 (a_1 + a_3 - d)] \right] \mathbf{b} \otimes \mathbf{b} - \frac{1}{\sqrt{a_1 a_3}} (a_1 - a_3) \sin \alpha \cos \alpha (\mathbf{b} \otimes \mathbf{a} + \mathbf{a} \otimes \mathbf{b}) + \left(\sqrt{\frac{d - \nu^2}{a_2 - \nu^2}} + \frac{d}{\sqrt{a_1 a_3}} \right) \mathbf{a} \otimes \mathbf{a} \right\},$$
(39)

where

 $\Delta(\nu) = B + 2\sqrt{AC} = a_1a_3 + a_2d - \nu^2(a_1 + a_3) + 2\sqrt{a_1a_3(a_2 - \nu^2)(d - \nu^2)}.$ (40) Then, determinant of tensor Q is

$$\overline{Q}_t = -\frac{1}{\nu^2 \sqrt{a_1 a_3}} \sqrt{\frac{d-\nu^2}{a_2-\nu^2}},$$

whereupon it is easy to obtain the pseudoinverse tensor Q^- and the surface impedance tensor γ for the biaxial crystal with the cut plane coinciding with its symmetry plane

$$\gamma = -\frac{i}{\nu}Q^{-} = \frac{i}{\nu\sqrt{\Delta(\nu)}} \left\{ \nu^{2} \left(d\sqrt{\frac{a_{2} - \nu^{2}}{d - \nu^{2}}} + \sqrt{a_{1}a_{3}} \right) \mathbf{b} \otimes \mathbf{b} + \nu^{2}(a_{1} - a_{3})\sqrt{\frac{a_{2} - \nu^{2}}{d - \nu^{2}}} \sin\alpha\cos\alpha(\mathbf{b}\otimes\mathbf{a} + \mathbf{a}\otimes\mathbf{b}) - \left[\sqrt{a_{1}a_{3}}(a_{2} - \nu^{2}) + \sqrt{\frac{a_{2} - \nu^{2}}{d - \nu^{2}}} [a_{1}a_{3} - \nu^{2}(a_{1} + a_{3} - d)] \right] \mathbf{a}\otimes\mathbf{a} \right\}.$$
 (41)

For the isotropic medium contacting with the biaxial crystal, tensor S' is zero and Q' is obtained from Q by changing in (39) values a_1, a_2, a_3, d to the inverse permittivity $a' = \varepsilon'^{-1}$

$$Q' = -\frac{1}{\nu^2} \sqrt{\frac{a'-\nu^2}{a'}} \mathbf{b} \otimes \mathbf{b} + \frac{1}{\sqrt{a'(a'-\nu^2)}} \mathbf{a} \otimes \mathbf{a}.$$

Then, according to the second formula of (5), the surface impedance tensor of the isotropic medium equals

$$\gamma' = \frac{\mathbf{i}}{\nu} Q'^{-} = -\mathbf{i}\nu \sqrt{\frac{a'}{a' - \nu^2}} \mathbf{b} \otimes \mathbf{b} + \frac{\mathbf{i}}{\nu} \sqrt{a'(a' - \nu^2)} \mathbf{a} \otimes \mathbf{a}.$$
 (42)

In the next section, we examine the tensor γ at $\nu \rightarrow \nu_L$ in order to establish the necessary existence conditions for surface polaritons at the interface of biaxial crystals and isotopic media according to (9).

6. Surface impedance tensor γ at $\nu \rightarrow \nu_{\rm L}$

Now we consider function $\Delta(\nu)$ (40) contained in expression (41) for the tensor γ . It is evident that it is a decreasing function on the interval $[0, \nu_L]$, and that $\Delta(0) > 0$. As was established in section 4, the value of the limiting frequency ν_L depends on the relations between material parameters a_1, a_2, a_3 (see table 1). If $\nu_L = \sqrt{d}$ or $\nu_L = \sqrt{a_2}$, then the value $\Delta(\nu_L)$ is proportional with a coefficient $|a_2 - d|^{-1}$ to the multiplier near m_q^2 in equation (21) or (22) of the part of the outer curve of the refraction surface section. But as is shown in section 3, this multiplier is positive in all cases listed in table 1, except (ii(b)). Therefore, $\Delta(\nu_L) > 0$ for the indicated values of ν_L .

If the relations (ii(b)) are satisfied, then $v_L = \tilde{v}_L$ (see formula (27)). We prove by contradiction that $\Delta(\tilde{v}_L) = 0$. Suppose $\Delta(\tilde{v}_L) = B + 2\sqrt{AC} \neq 0$, then $B^2 - 4AC \neq 0$. But the quantity $B^2 - 4AC$ at $v = \tilde{v}_L$ coincides with the left-hand side of (26) for \tilde{v}_L , so we come to a contradiction. Thus, in this case, tensor γ diverges at $v = v_L$.

From equation $\Delta(\tilde{\nu}_L) = 0$, it follows that

$$\sqrt{a_1 a_3 (a_2 - \widetilde{\nu}_{\rm L}^2) (d - \widetilde{\nu}_{\rm L}^2)} = -\frac{1}{2} [a_1 a_3 + a_2 d - \widetilde{\nu}_{\rm L}^2 (a_1 + a_3)]. \tag{43}$$

Now we apply necessary condition (9) of surface polariton existence at the interface of crystal and isotropic medium. The left-hand side of relation (9) is determined by the coefficient of dyad $a \otimes a$ in (41). So,

$$\lim_{\nu \to \nu_{\rm L}} g(\nu) \sqrt{\frac{a_2 - \nu^2}{d - \nu^2}} < 0, \tag{44}$$

where

$$g(\nu) = a_1 a_3 - \nu^2 (a_1 + a_3 - d) + \sqrt{a_1 a_3 (a_2 - \nu^2)(d - \nu^2)}$$
(45)

is a decreasing function on the interval $[0, v_L]$. Next, we examine for which kind of relations listed in table 1 the inequality (44) is satisfied.

Relations (i) and (ii(a)), $v_{\rm L} = \sqrt{d}$. It is necessary to investigate the sign of the function g(v) which is multiplied in (44) by the diverging coefficient $(d - v^2)^{-\frac{1}{2}}$. If $\alpha \neq 0$, we have

$$g(\nu_{\rm L}) = g(\sqrt{d}) = -(a_1 - d)(d - a_3) < 0.$$

Consequently, inequality (44) is satisfied.

Relation (ii(b)), $v_L = \tilde{v}_L$. Supposing that $\alpha \neq \alpha_2$, we take into account inequality (28) and equation (43):

$$\begin{split} g(\widetilde{v}_{\rm L}) &= a_1 a_3 - \widetilde{v}_{\rm L}^2 (a_1 + a_3 - d) - \frac{1}{2} (a_1 a_3 + a_2 d) + \frac{1}{2} \widetilde{v}_{\rm L}^2 (a_1 + a_3) \\ &= a_1 a_3 + \widetilde{v}_{\rm L}^2 d - \frac{1}{2} (a_1 a_3 + a_2 d) - \frac{1}{2} \widetilde{v}_{\rm L}^2 (a_1 + a_3) \\ &< \frac{1}{2} (a_1 a_3 + a_2 d) - \frac{1}{2} \widetilde{v}_{\rm L}^2 (a_1 + a_3) = -\sqrt{a_1 a_3 (a_2 - \widetilde{v}_{\rm L}^2) (d - \widetilde{v}_{\rm L}^2)} \leqslant 0. \end{split}$$

Thus, in this case, inequality (44) is satisfied for $\alpha \in [\alpha_1, \alpha_2)$.

Relations (ii(c)) and (iii), $v_L = \sqrt{a_2}$. Inequality (44) is not satisfied because its left-hand side vanishes. This means that in case (ii(c)) or (iii) excitation of the surface polaritons is impossible. Specifically, a surface wave cannot propagate along a cut plane of the *negative uniaxial crystal* ($a_1 > a_3 = a_2$) with optical axis situated in this plane. This fact was first established in [3, 4].

Thus, condition (9) is in essence a prohibitive condition and it allows one, without preliminary solving the dispersion equation, to establish relations of material parameters of an anisotropic medium, so as to forbid surface waves. For surface waves in symmetry planes of

a biaxial crystal, inequality (9) leads to the following necessary (but not sufficient) condition of wave existence. The inverse permittivity a_2 referring to the crystallographic axis along the interface normal q should be greater than the other inverse permittivities a_1 and a_3 for axes in the symmetry plane.

7. Analysis of the dispersion equation solutions

The dispersion equation for the surface polaritons at the interface of a biaxial crystal and an isotropic medium is obtained by substituting expressions (41) and (42) for γ and γ' in equation (4). It takes the form

$$F(v) = 0, \tag{46}$$

where

$$F(\nu) = a' + \sqrt{a_1 a_3} \sqrt{\frac{a_2 - \nu^2}{d - \nu^2}} + \frac{1}{\sqrt{\Delta(\nu)}} \left[g(\nu) \sqrt{\frac{a_2 - \nu^2}{d - \nu^2}} \sqrt{\frac{a'}{a' - \nu^2}} + \left(d\sqrt{\frac{a_2 - \nu^2}{d - \nu^2}} + \sqrt{a_1 a_3} \right) \sqrt{a'(a' - \nu^2)} \right]$$
(47)

and functions $\Delta(v)$ and g(v) are defined by (40) and (45), respectively. The dispersion equation describes surface polaritons for any cut planes of the biaxial crystal parallel to the symmetry planes provided that a_1, a_2, a_3, a' are positive.

It is obvious that F(0) > 0. Equation (46) has a unique solution $\nu = \nu_S$ only if the function $F(\nu)$ changes its sign on the interval $(0, \hat{\nu}_L)$, i.e. if

$$\lim_{\nu \to \hat{\nu}_{\rm L}} F(\nu) < 0,\tag{48}$$

where $\hat{v}_L = \min(v_L, v'_L)$, $v'_L = \sqrt{a'}$ is a limiting frequency of surface waves in the isotropic medium. Thus, condition (48) is a necessary and sufficient existence condition for surface electromagnetic waves. If it is satisfied, then at a given frequency ω , the wave vector projection $k_S = \omega/(cv_S)$ to the *b*-direction can be found with the use of solution $\nu = \nu_S$ of (46) and (47).

According to the relations between material parameters a_1 , a_2 , a_3 , a', the limiting frequency \hat{v}_L can take one of the following values: $\sqrt{a'}$, \sqrt{d} or \tilde{v}_L (the case $\hat{v}_L = \sqrt{a_2}$ is eliminated from consideration in view of previous section's results). Now we establish further restrictions of material parameters arising from condition (48).

Let $\hat{v}_{\rm L} = \sqrt{a'}$. Then, at the limit $\nu \to \hat{v}_{\rm L}$, function $F(\nu)$ diverges owing to coefficient $\sqrt{a'/(a'-\nu^2)}$ of $g(\nu)$ (see (47)), so inequality (48) is identical to $g(\sqrt{a'}) < 0$ or

$$a_1a_3 - a'(a_1 + a_3 - d) + \sqrt{a_1a_3(a_2 - a')(d - a')} < 0.$$
⁽⁴⁹⁾

If $a' \leq a_3$, then inequality (49) is not satisfied:

$$g(\sqrt{a'}) \ge g(\sqrt{a_3}) = a_3(d-a_3) + \sqrt{a_1a_3(a_2-a_3)(d-a_3)} \ge 0.$$

Let $\hat{v}_{\rm L} = \sqrt{d}$. The function F(v) at $v \to \hat{v}_{\rm L}$ diverges owing to the coefficients $\sqrt{(a_2 - v^2)/(d - v^2)}$. Then, condition (48) is equivalent to $\sqrt{a_1a_3} + [\Delta(\sqrt{d})]^{-\frac{1}{2}}[g(\sqrt{d})\sqrt{a'/(a'-d)} + d\sqrt{a'(a'-d)}] < 0$ or

$$-\sqrt{a'}[a_1a_3 - d(a_1 + a_3 - a')] > \sqrt{a_1a_3[a_1a_3 - d(a_1 + a_3 - a_2)](a' - d)}.$$
(50)

 Table 2. Relations between material parameters of the contacting media for which the dispersion equation does not have any solution.

Case	Relations between a_1, a_2, a_3	Angle α	Parameter a'	Reference to condition not satisfied
(i)	$a_2 \geqslant a_1 > a_3$		$a' \leqslant a_3$	(49)
			$a' \geqslant a_1$	(50)
(ii(a))	$a_1 > a_2 > a_3$	$0 \leqslant \alpha < \alpha_1$	$a' \leqslant a_3$	(49)
			$a' \geqslant a_2$	(50)
(ii(b))	$a_1 > a_2 > a_3$	$\alpha_1 \leqslant \alpha \leqslant \alpha_2$	$a' \leqslant a_3$	(49)
			$a' \geqslant a_2$	(51)
(ii(c))	$a_1 > a_2 > a_3$	$\alpha_2 < \alpha \leq \frac{\pi}{2}$	Any	(44)
(iii)	$a_1 > a_3 \geqslant a_2$	2	Any	(44)

In the case (i) (see table 1) and, in addition, $a' \ge a_1$, the relation (50) is not satisfied. Indeed, in this case, the left-hand side of (50) is non-positive:

$$-\sqrt{a'}[a_1a_3 - d(a_1 + a_3 - a')] \leqslant -\sqrt{a'}[a_1a_3 - d(a_1 + a_3 - a_1)] = -\sqrt{a'}(a_1 - d)a_3 \leqslant 0.$$

Inequality (50) is also not satisfied if the material parameters yield to relations (ii(a)) and $a' \ge a_2$:

$$-\sqrt{a'}[a_1a_3 - d(a_1 + a_3 - a')] \leqslant -\sqrt{a'}[a_1a_3 - d(a_1 + a_3 - a_2)] < 0.$$

Here, it is taken into account that $a_1a_3 - d(a_1 + a_3 - a_2) > 0$ at $0 \le \alpha < \alpha_1$ (section 3).

Finally, we examine the case $\hat{\nu}_L = \tilde{\nu}_L$. Function $F(\nu)$ diverges at $\nu \rightarrow \hat{\nu}_L$ owing to vanishing of the value $\Delta(\tilde{\nu}_L)$. Thus, a necessary and sufficient existence condition (48) is fulfilled only if expression in square brackets in (47) is negative for $\nu = \hat{\nu}_L$:

$$g(\widetilde{\nu}_{\rm L})\sqrt{\frac{a_2-\widetilde{\nu}_{\rm L}^2}{d-\widetilde{\nu}_{\rm L}^2}}\sqrt{\frac{a'}{a'-\widetilde{\nu}_{\rm L}^2}} + \left(d\sqrt{\frac{a_2-\widetilde{\nu}_{\rm L}^2}{d-\widetilde{\nu}_{\rm L}^2}} + \sqrt{a_1a_3}\right)\sqrt{a'(a'-\widetilde{\nu}_{\rm L}^2)} < 0.$$
(51)

Inequality (51) is greatly reduced owing to equations (26) and (43). Multiplying both parts of (51) by $(d - \tilde{v}_L^2) \sqrt{a_1 a_3 (a' - \tilde{v}_L^2) / a'}$, we obtain

$$a_{1}a_{3}(d-\widetilde{\nu}_{L}^{2})(a_{2}+a'-2\widetilde{\nu}_{L}^{2})+[a_{1}a_{3}+a'd-\widetilde{\nu}_{L}^{2}(a_{1}+a_{3})]\sqrt{a_{1}a_{3}(a_{2}-\widetilde{\nu}_{L}^{2})(d-\widetilde{\nu}_{L}^{2})}<0.$$

After equation (43) is substituted, we have

$$(a_1 - a_3)^2 \widetilde{\nu}_{\rm L}^4 - [(a_1 + a_3)(2a_1a_3 + a_2d + a'd) - 2a_1a_3(a_2 + a') - 4a_1a_3d]\widetilde{\nu}_{\rm L}^2 + (a_1a_3 + a_2d)(a_1a_3 + a'd) - 2a_1a_3d(a_2 + a') > 0.$$
(52)

In the end, using (26) and eliminating $\tilde{\nu}_L^4$ from (52), we obtain

$$(a_2 - a') \{ (a_1 a_3 - a_2 d) d - \widetilde{\nu}_L^2 [2a_1 a_3 - d(a_1 + a_3)] \} > 0.$$
(53)

The multiplier in curly braces is positive owing to inequalities (28) and $a_1a_3 - d(a_1+a_3-a_2) < 0$ for angles α in the range (α_1, α_2) (case (ii(b)))

$$(a_1a_3 - a_2d)d - \tilde{\nu}_{\mathsf{L}}^2[2a_1a_3 - d(a_1 + a_3)] > (a_1a_3 - a_2d)d - d[2a_1a_3 - d(a_1 + a_3)] > 0.$$

Thus, condition (51) comes to a simple inequality $a' < a_2$. One can show that we also obtain the same result from (48) if $\alpha = \alpha_1$.



Figure 2. Sectors of allowed propagation directions b of surface polaritons.

To summarize our analysis, we present table 2. We indicate relations involving a_1, a_2, a_3, a' , when the dispersion equation (46) does not have any solution and hence propagation of the surface wave is impossible. Evidently, the table does not include the relations

(I)
$$a_2 \ge a_1 > a' > a_3$$
, (II) $a_1 \ge a_2 > a' > a_3$. (54)

Only these relations for material parameters can satisfy the necessary and sufficient existence condition (48). However, it is possible not for all angles α (i.e., not for arbitrary propagation directions of surface polaritons) but only for

$$\alpha_{\min} < \alpha < \alpha_{\max},$$

where

$$\sin^{2} \alpha_{\min} = \frac{a_{3}(a'-a_{3})[a_{1}(a_{2}-a_{3})-a'(a'-a_{3})]}{(a_{1}-a_{3})[a'^{3}-2(a_{1}+a_{3})a'^{2}+(a_{1}+a_{3})^{2}a'-a_{1}a_{3}(a_{1}-a_{2}+a_{3})]},$$

$$\sin^{2} \alpha_{\max} = \frac{1}{2(a_{1}-a_{3})a'^{2}} \left\{ a_{1}[a_{2}a_{3}-a'(3a_{3}-2a')] -\sqrt{a_{1}a_{3}(a_{2}-a')[a_{1}a_{2}a_{3}-5a_{1}a_{3}a'+4(a_{1}+a_{3})a'^{2}-4a'^{3}]} \right\}.$$
(55)

Expressions (55) and (56) for limiting angles α_{\min} and α_{\max} are obtained by changing inequalities (50) and (49) to equalities and taking into account (16). As for condition (51), as stated above, it does not lead to any restriction of α . It is reduced to inequality $a' < a_2$ which is satisfied when (54) takes place.

Dispersion equation (46) does not change its form when α is replaced by $-\alpha$ or $\pi - \alpha$. Thus, the boundary plane of a biaxial crystal and an isotropic medium contains four sectors of allowed propagation directions **b** of surface polaritons (figure 2). They are determined by angles α in intervals ($\alpha_{\min}, \alpha_{\max}$), ($\pi - \alpha_{\max}, \pi - \alpha_{\min}$), ($\alpha_{\min} - \pi, \alpha_{\max} - \pi$), ($-\alpha_{\max}, -\alpha_{\min}$).

Now we investigate dependence of limiting angles α_{\min} and α_{\max} on the inverse permittivity a' of isotropic medium when parameters a_1, a_2, a_3 of biaxial crystal are fixed. It is easy to see that

$$\lim_{a' \to a_3} \alpha_{\min} = \lim_{a' \to a_3} \alpha_{\max} = 0, \tag{57}$$



Figure 3. Dependence of limiting angles α_{\min} and α_{\max} on the inverse permittivity a' of isotropic medium: (a) $a_1 = 0.7$, $a_2 = 0.9$, $a_3 = 0.1$; (b) $a_1 = 0.9$, $a_2 = 0.7$, $a_3 = 0.1$.

i.e., when $a' \rightarrow a_3$, existence sectors are situated close to the crystal axis given by the unit vector c_1 and their angular width is vanishingly small.

Assume that relations (I) for the parameters (see (54)) occur. Then, parameter a' cannot exceed a_1 and

$$\lim_{a'\to a_1}\alpha_{\min}=\lim_{a'\to a_1}\alpha_{\max}=\frac{\pi}{2}.$$

Here, at $a' \rightarrow a_1$, angular width of the sectors also becomes small, and they are situated close to the crystal axis given by the unit vector c_3 . Typical plots of dependence of angles α_{\min} and α_{\max} versus a' for that case are shown in figure 3(a).

The case of material parameter relations (II) when optical axes of the biaxial crystal are situated in the interface plane is of more interest. Here, a' is arranged between a_3 and a_2 , and when $a' \rightarrow a_3$ equations (57) are satisfied as before. However, it is easy to establish that

$$\lim_{a'\to a_2}\alpha_{\min}=\alpha_1,\qquad \lim_{a'\to a_2}\alpha_{\max}=\alpha_2$$

and in doing so $\alpha_{\min} < \alpha_1, \alpha_{\max} < \alpha_2$, where the angles α_1 and α_2 are determined by formulae (24). If value a' is just a little smaller than a_2 , then the existence interval practically coincides with (α_1, α_2) . Note that the optical axis of the crystal with position characterized by angle α_0 (23) lies in the corresponding sector of the allowed propagation directions since $\alpha_1 < \alpha_0 < \alpha_2$. As soon as a' becomes equal to or exceeds parameter a_2 , existence intervals having finite angular widths at $a' \leq a_2$ disappear totally and surface wave cannot propagate in any direction in the interface plane. The reason is that for all $\alpha \in (\alpha_1, \alpha_2)$, condition (53) now fails to operate. This case is illustrated by figure 3(*b*). When $a' = a_2$, a wave in biaxial crystal fails to be localized close to the interface for entire range of $\alpha \in (\alpha_1, \alpha_2)$ (coefficients η_1 and η_2 in (1) become real and $\eta_1 = -\eta_2$; that corresponds to the total internal reflection of the body wave in the biaxial crystal from the boundary of the isotropic medium).

Let us recall that relations (54) and expressions (55) and (56) are obtained with the assumption that the normal q to the interface plane coincides with c_2 , and $a_1 > a_3$ (see section 3). Thus, as follows from (54), it is necessary and sufficient for existence of the



Figure 4. Solid line shows $v_s^2 = v_s^2(\alpha)$ when $a_1 = 0.9$, $a_2 = 0.7$, $a_3 = 0.1$, a' = 0.6; dashed and doted lines show $d = d(\alpha) = a_1 \sin^2 \alpha + a_3 \cos^2 \alpha$ and $\tilde{v}_L^2 = \tilde{v}_L^2(\alpha)$, respectively. Angles $\alpha_0, \alpha_1, \alpha_2, \alpha'$ are calculated by formulae (23), (24) and (62), and $\alpha_{\min}, \alpha_{\max}$ by formulae (55) and (56).

surface electromagnetic waves that parameter a_3 be the smallest among a_1, a_2, a_3, a' , and next ascending parameter be a'.

It is clear that surface polaritons can be excited only in two symmetry planes of the same biaxial crystal. One of these planes includes optical axes of the crystal, and relations (54(II)) are satisfied. The other plane is perpendicular to the tensor ε^{-1} principal axis which corresponds to the greatest among the inverse permittivities a_1, a_2, a_3 . When coming from the first plane to the second plane, one needs to change $a_1 \leftrightarrow a_2$ in all equations. Inequalities (II) in doing so are changed by (I).

Thus, conditions (54) establish existence of solutions of dispersion equation (46) and (47). These solutions can be found numerically. In figure 4, we show the plot of v_s^2 as a function of the propagation direction angle α at fixed values of inverse permittivities in case of relations (II). Plots $d = d(\alpha)$ and $\tilde{v}_L^2 = \tilde{v}_L^2(\alpha)$ (27) are also given which are used for finding the square of the limiting frequency of the surface waves.

Now we define the anisotropy parameters of the crystal $\chi_1 = (a_1 - a_3)/a_3$, $\chi_2 = (a_2 - a_3)/a_3$ and the parameter for the isotropic medium $\chi' = (a' - a_3)/a_3$. Then, conditions (54) take the form

(I)
$$\chi_2 \ge \chi_1 > \chi' > 0$$
, (II) $\chi_1 \ge \chi_2 > \chi' > 0$ (58)

and formulae (55) and (56) are written as

$$\sin^2 \alpha_{\min} = \frac{\chi'}{\chi_1} \left[1 + \frac{\chi'(\chi_1 - \chi')^2}{(1 + \chi_1)(\chi_2 - \chi') + \chi'(\chi_1 - \chi')} \right]^{-1},$$
(59)

$$\sin^{2} \alpha_{\max} = \frac{\chi'}{\chi_{1}} + \frac{1}{2\chi_{1}(1+\chi')^{2}} \Big\{ (1+\chi_{1})(\chi_{2}-\chi') + 2\chi'(1+\chi')(\chi_{1}-\chi') \\ -\sqrt{(1+\chi_{1})(\chi_{2}-\chi')[(1+\chi_{1})(\chi_{2}-\chi') + 4\chi'(1+\chi')(\chi_{1}-\chi')]} \Big\}.$$
(60)

We dwell on a case of small parameters χ_1 and χ_2 which is important for practical purposes when natural or artificial anisotropic materials (for example, photoelastic ones [20, 21]) are considered. Then, expressions (59) and (60) can be expanded to the first approximation by χ_1, χ_2 and χ' to have the form

$$\sin^2 \alpha_{\min,\max} \approx \frac{\chi'}{\chi_1} \left[1 \mp \frac{\chi'(\chi_1 - \chi')^2}{(1 + \chi_1)(\chi_2 - \chi') + \chi'(\chi_1 - \chi')} \right].$$
(61)

The fraction denominator in square brackets in (61) can be presented as a sum of terms $\chi_2 - \chi'$ which is linear with respect to small anisotropy parameters and other quadratic terms $\chi_1(\chi_2 - \chi') + \chi'(\chi_1 - \chi')$. These quadratic terms become essential when parameter χ' is near to χ_2 ($\chi' \leq \chi_2$ or $a' \leq a_2$). Note that in [11] when approximate formulae for angles α_{\min} and α_{\max} were derived, only the linear term $\chi_2 - \chi'$ was obtained.

It is clear from (61) that the greater the crystal anisotropy, the greater the angular width $\alpha_{max} - \alpha_{min}$ of existence sectors turns out to be (the situation is typical for singular surface polaritons in anisotropic media). The position of existence sectors in the interface plane is described by a central angle α'

$$\sin \alpha' = \sqrt{\frac{\chi'}{\chi_1}} = \sqrt{\frac{a' - a_3}{a_1 - a_3}}.$$
(62)

In figure 4, this angle corresponds to the point of crossing the plot $d = d(\alpha)$ and horizontal line with ordinate a'.

8. Interface of uniaxial crystal and isotropic medium

If one of the inverse permittivities a_1 or a_3 coincides with a_2 , then we come to study the surface electromagnetic waves at the interface of the isotropic medium and the uniaxial crystal with the optical axis in the interface plane. This event was first analysed in [3, 4]. As was noted above, surface waves are impossible at the cuts of negative crystals when $a_1 > a_3 = a_2$. At the same time, for positive crystals, relations (54) take the form $a_2 = a_1 > a' > a_3$. From formula (23), it follows that for such crystals $\alpha_0 = \frac{\pi}{2}$, i.e. the optical axis is directed along vector c_3 (see figure 2). So, for describing propagation of surface waves, it is convenient to use angle $\varphi = \frac{\pi}{2} - \alpha$ formed by vectors b and c_3 . As a result, from (55) and (56), the following expressions for limiting angles are obtained:

$$\sin^2 \varphi_{\min} = 1 - \sin^2 \alpha_{\max} = \frac{\xi}{2} \Big[1 - \chi \xi + \sqrt{(1 - \chi \xi)^2 + 4\chi} \Big], \tag{63}$$

$$\sin^2 \varphi_{\max} = 1 - \sin^2 \alpha_{\min} = \frac{(1+\chi)^3 \xi}{(1+\chi)^2 (1+\chi\xi) - \chi^2 (1-\xi)^2},$$
(64)

where $\chi = (\varepsilon_e - \varepsilon_o)/\varepsilon_o$ is the anisotropy parameter of the uniaxial crystal and $\xi = (\varepsilon' - \varepsilon_o)/(\varepsilon_e - \varepsilon_o)$ is the parameter for the isotropic medium; ε_o and ε_e are the permittivities referring to ordinary and extraordinary waves, respectively. Expressions (63) and (64) were first obtained in [4].

9. Conclusion

The main result obtained above is in establishing the existence conditions (54) for singular surface polaritons, which propagate along the symmetry plane of the biaxial crystal contacting with the isotropic medium. The exact expressions (55) and (56) are obtained for limiting angles of the sectors of the allowed propagation directions. Surface polaritons can propagate only if relations (54(I)) or (54(II)) of 12 possible relations involving material parameters a_1 , a_2 , a_3 , a' ($a_1 > a_3$) take place. When inequalities (II) are satisfied and the inverse permittivity of

the isotropic medium a' continuously changes from a_3 to a_2 , then the angular width of the existence sectors increases. As soon as a' exceeds a_2 , these sectors vanish abruptly and entirely (figure 3(*b*)). This fact may be used for constructing optical shutters based on surface electromagnetic waves.

With use of the methods developed in [14, 15], surface polaritons can analogously be studied for other plane cuts of biaxial crystal, for example, for those that contain only one of the symmetry axes. To derive the polariton dispersion equation for cut planes without any symmetry elements of the crystal, it is advisable to use systems of computer algebra.

The results obtained are also applicable when anisotropy is induced externally in one of the contacting media. For example, electro-optical cubic crystals of 23 and $\overline{43m}$ symmetry classes are optically isotropic when an external electric field is absent. If the external field is applied, they become biaxial (Pockel's effect). Changing the electric intensity, one can dynamically vary the position of the surface polariton existence sectors at the interface of such a crystal and non-electro-optical isotropic medium.

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