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Dyakonov Surface Waves at the Boundary of Anisotropic Biaxial Crystals

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A general approach to analysis of Dyakonov surface waves at the interfaces of anisotropic biaxial crystals is proposed, taking into account arbitrary spatial orientation of the media tensors principal axes. This approach is based on the operator representation of macroscopic Maxwell equations corresponding to the quantum-mechanical equations for photon states in an inhomogeneous anisotropic media. Surface wave dispersion law is investigated in the most general case. It is established that the interface eigenmode dispersion is closely related to the dispersion of bulk waves in the partnering media, which is a specific feature of Dyakonov waves. The electromagnetic field spatial distribution is investigated in the direction orthogonal to the boundary plane. The surface wave angular existence domain is determined. It's dependencies on the rotation angles of the media optical axes are studied as well.

Keywords: electromagnetic surface waves, interface photon states, anisotropic media, biaxial materials.

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Introduction

Surface electromagnetic waves are a special type of electromagnetic fields, the energy of which is localized near the boundaries of media with different permittivity or permeability. A separate class of surface waves includes waves whose existence is caused by a jump in the anisotropic properties of materials at the interface. The first theoretical predictions of the possibility of the existence of electromagnetic waves propagating along the interfaces of anisotropic crystals were made in the works of F.M. Marchevsky [1] and M.I. Dyakonov [2]. In the future, surface waves of this type were called Dyakonov waves and for a long time were the object of only theoretical studies. However, after their experimental detection [3–6], this type of surface waves has gained some prospects in terms of the possibility of their use in various photonics and integrated optics devices [7,8].

Theoretical studies [1,2] initially considered surface waves arising on the heterogeneous boundary of an isotropic medium and an anisotropic uniaxial crystal, whose optical axis lies in the plane of the interface. It was shown that excitation of surface waves in such structures is possible only in a small angular range in the interface plane. The directional diagram and its angular distribution are determined by the values of the components of the permittivity tensor of an anisotropic material and the orientation of its principal axes relative to the interface plane. In the following, the problem of propagation of Dyakonov surface waves along the interfaces of isotropic and anisotropic biaxial crystals was solved [9–13]. The literature has also considered more complex structures formed by identical uniaxial [14] and biaxial [15] materials. Only some particular cases of biaxial crystal interfaces with relatively simple spatial orientations of their optical axes were analyzed. In addition, other varieties of Dyakonov waves, the existence of which is possible at the interfaces of other types of substances, such as hyperbolic, chiral and bianisotropic materials [16–19], as well as arising in limited media [20–23] have been studied in the literature.

This paper proposes the most general approach to the analysis of Dyakonov surface waves at the interfaces of anisotropic biaxial crystals with arbitrary orientation of the principal axes of their dielectric and magnetic permeabilities. The developed theoretical approach is based on the operator representation of Maxwell equations [24], which allows us to formulate the problem of determining the interface eigenmodes of the electrodynamic system under study as the problem of finding the eigennumbers and eigenvectors of the Hermitian operator in the one-photon Hilbert space. With the help of this method, the law of dispersion of Dyakonov surface waves is calculated, the angular range of their existence and its dependence on the angle of rotation of the optical axes of the media relative to each other are studied, and the spatial distribution of the electromagnetic field in the structures in question is determined.

1. Surface electromagnetic modes at the interface of anisotropic media

Consider a heterogeneous boundary between two arbitrarily oriented anisotropic media. Let the plane xy of the Cartesian coordinate system lie in the plane of the interface (Fig. 1). Let's assume that the medium 1 is located in the area $z < 0$, and the medium 2 — in the area $z > 0$. The corresponding tensors of permittivity or permeability are denoted as $\boldsymbol{\varepsilon}_1$, $\boldsymbol{\varepsilon}_2$ and $\boldsymbol{\mu}_1$, $\boldsymbol{\mu}_2$. The wave vector of the

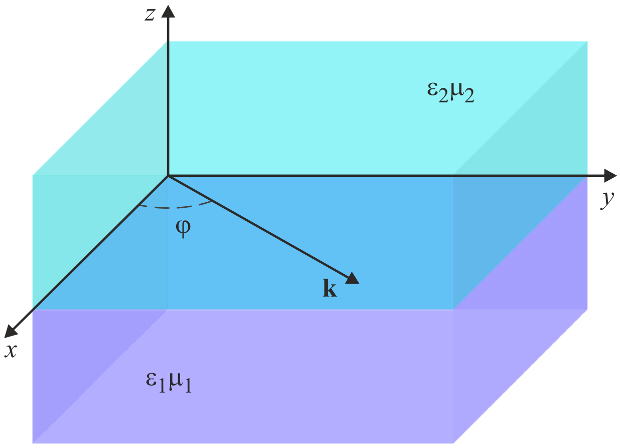

Figure 1. Partition boundary and entered coordinate system.

electromagnetic wave $\mathbf{k}$ is directed at an angle φ to the axis x in the interface plane.

The stationary Maxwell equations for the complex amplitudes of the electromagnetic field in the absence of sources have the following form:

$$\nabla \times \mathbf{H} = -i\,\frac{\omega}{c}\,\boldsymbol{\varepsilon}\mathbf{E},$$

$$\nabla \times \mathbf{E} = i\,\frac{\omega}{c}\,\boldsymbol{\mu}\mathbf{H}. \quad (1)$$

In the general case of anisotropic media, $\boldsymbol{\varepsilon}$ and $\boldsymbol{\mu}$ must be understood as tensors of dielectric permittivity and magnetic permeability.

As was shown in [24], equations (1) are one of possible representations of the following operator equations:

$$ic(\hat{\mathbf{s}}\cdot\hat{\mathbf{k}})|H\rangle = \omega\hat{\varepsilon}|E\rangle,$$

$$-ic(\hat{\mathbf{s}}\cdot\hat{\mathbf{k}})|E\rangle = \omega\hat{\mu}|H\rangle. \quad (2)$$

Here $\hat{\mathbf{s}}, \hat{\mathbf{k}}$ — Hermitian operators of the spin momentum $s = 1$ and wave vector, respectively. The media parameters are described by Hermitian operators of permittivity and permeability $\hat{\varepsilon}$ and $\hat{\mu}$. Two photon state vectors $|E\rangle$ and $|H\rangle$ in the complex one-particle Hilbert space are corresponded to the electromagnetic field strengths.

Using auxiliary operators and state vectors

$$\hat{\Omega} = ic\hat{\varepsilon}^{-1/2}(\hat{\mathbf{s}}\cdot\hat{\mathbf{k}})\hat{\mu}^{-1/2},$$

$$\hat{\Omega}^{+} = -ic\hat{\mu}^{-1/2}(\hat{\mathbf{s}}\cdot\hat{\mathbf{k}})\hat{\varepsilon}^{-1/2},$$

$$|\tilde{E}\rangle = \hat{\varepsilon}^{1/2}|E\rangle,$$

$$|\tilde{H}\rangle = \hat{\mu}^{1/2}|H\rangle$$

equations (2) can be reduced to two equations to find the eigennumbers ω_v^2 and eigenvectors $|\tilde{E}_v\rangle$ and $\tilde{H}_v\rangle$ of Hermitian operators

$$\hat{\Omega}\hat{\Omega}^{+}|\tilde{E}_v\rangle = \omega_v^2|\tilde{E}_v\rangle,$$

$$\hat{\Omega}^{+}\hat{\Omega}|\tilde{H}_v\rangle = \omega_v^2|\tilde{H}_v\rangle. \quad (3)$$

The eigenvectors defined in this way are orthogonal and can be normalized to unity

$$\langle\tilde{E}_v|\tilde{E}_{v'}\rangle = \delta_{vv'},$$

$$\langle\tilde{H}_v|\tilde{H}_{v'}\rangle = \delta_{vv'}.$$

These states of the photon in a certain basis will describe its energy-normalized electromagnetic eigenmodes, including the surface ones.

As a basis, consider photon states with a certain coordinate $|\mathbf{x}\rangle$ and a certain linear polarization along the axes of the Cartesian coordinate system $|i\rangle$, where $i = 1, 2, 3$ or $i = x, y, z$. We define it as the direct product of these vectors $|\mathbf{x}, i\rangle = |\mathbf{x}\rangle \otimes |i\rangle$. The resulting set of states satisfies the following conditions of orthonormality and completeness:

$$\langle\mathbf{x}, i|\mathbf{x}'j\rangle = \delta(\mathbf{x}-\mathbf{x}')\delta_{ij},$$

$$\sum_i \int d\mathbf{x}|\mathbf{x}, i\rangle\langle\mathbf{x}, i| = 1.$$

Later we will use this representation to determine the spatial distribution of the components of the electromagnetic field strengths.

Surface waves are localized solutions of field equations near the interface (3). This allows us to introduce a spatial constraint of the system in question along the axis z perpendicular to the plane of the interface, and to consider two dielectric layers of finite thickness approximately. Next, we carry out a periodic continuation of the system in question along the axis z. This greatly simplifies the numerical solution of Maxwell's equations, since in this case there is no need to solve the corresponding differential equations, and the problem itself is reduced to the search for eigennumbers and eigencolumns of the Hermitian matrix. Interface eigenmodes and corresponding eigenfrequencies arise in this approach naturally as stationary solutions of the original problem satisfying the necessary boundary conditions. Within one period of the system in question, the solution of Maxwell's equations, corresponding to surface waves, approximates the solution of the problem for two semi-infinite spaces. In this case, the choice of a sufficiently large thickness of dielectric layers allows one to achieve the required approximation accuracy.

In accordance with the described transition to a periodic structure similar to a photonic crystal, it is natural to introduce direct and reciprocal lattices. Arbitrary translation vectors of the direct $\mathbf{a}$ and reciprocal $\mathbf{b}$ lattices of a three-dimensional photonic crystal are defined as follows:

$$\mathbf{a} = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3,$$

$$\mathbf{b} = m_1\mathbf{b}_1 + m_2\mathbf{b}_2 + m_3\mathbf{b}_3,$$

where $\mathbf{a}_{1,2,3}$ and $\mathbf{b}_{1,2,3}$ — the main vectors of translations, $n_i, m_i = 0, \pm1, \pm2, \ldots$. It is assumed that all the previously considered operators have translational symmetry.

As a basis for the representation of the operator equations (3), we will use the photon states with a certain value of the wave vector, which in the translationally invariant system is conveniently represented as a sum of $\mathbf{b}+\mathbf{k}$, where $\mathbf{k}$ —the wave vector in the Brillouin zone of the photonic crystal.

Similar to the coordinate representation, we define a basis with a certain value of the wave vector and a certain linear polarization $|\mathbf{b}+\mathbf{k}, i\rangle = |\mathbf{b}+\mathbf{k}\rangle \otimes |i\rangle$. This set of states is also orthonormal and complete, i. e. satisfies the relations

$$\langle \mathbf{b}+\mathbf{k}, i|\mathbf{b}'+\mathbf{k}', j\rangle = \delta_{\mathbf{bb}'}\delta_{\mathbf{kk}'}\delta_{ij},$$

$$\sum_{\mathbf{b},\mathbf{k},i} |\mathbf{b}+\mathbf{k}, i\rangle\langle \mathbf{b}+\mathbf{k}, i| = 1.$$

The relation between vectors $|\mathbf{x}, i\rangle$ and $|\mathbf{b}+\mathbf{k}, i\rangle$ is determined by the following unitary transformation:

$$|\mathbf{b}+\mathbf{k}, i\rangle = \sum_j \int_V d\mathbf{x}|\mathbf{x}, j\rangle\langle \mathbf{x}, j|\mathbf{b}+\mathbf{k}, i\rangle,$$

$$\langle \mathbf{x}, j|\mathbf{b}+\mathbf{k}, i\rangle = \frac{1}{\sqrt{V}} \exp[i(\mathbf{b}+\mathbf{k})\mathbf{x}]\delta_{ji},$$

where $V = NV_0$ — the total volume of the photonic crystal, N —the number of its unite-cells, V_0 —the volume of the unite-cell. In the case of one-dimensional periodic continuation, which we introduced to analyze surface modes, the three-dimensional volume quantities V_0 and V are reduced to lengths L_0 and L, respectively.

Using a basis with a certain value of the wave vector and a certain polarization, we can obtain a system of matrix equations similar to (3). It turns out that all operators and eigenvectors in the basis $|\mathbf{b}+\mathbf{k}, i\rangle$ are diagonal with respect to $\mathbf{k}$ and $\mathbf{k}'$ indices, i.e. they look like block-diagonal matrices. This reduces the problem to finding eigennumbers and eigencolumns of matrices parametrically dependent on the vector $\mathbf{k}$:

$$\Omega(\mathbf{k})\Omega^{+}(\mathbf{k})\tilde{\mathbf{E}}_{\upsilon}(\mathbf{k}) = \omega_{\upsilon}^{2}(\mathbf{k})\tilde{\mathbf{E}}_{\upsilon}(\mathbf{k}),$$

$$\Omega^{+}(\mathbf{k})\Omega(\mathbf{k})\tilde{\mathbf{H}}_{\upsilon}(\mathbf{k}) = \omega_{\upsilon}^{2}(\mathbf{k})\tilde{\mathbf{H}}_{\upsilon}(\mathbf{k}). \qquad (4)$$

Then, using auxiliary eigenvectors, the initial state vectors of the photon corresponding to the υ-th mode are determined. In the considered representation, the initial (true) field strengths corresponding to the υ-th mode are determined from the relations

$$\mathbf{H}_{\upsilon}(\mathbf{k}) = \boldsymbol{\mu}^{-1/2}\tilde{\mathbf{H}}_{\upsilon}(\mathbf{k}),$$

$$\mathbf{E}_{\upsilon}(\mathbf{k}) = \boldsymbol{\varepsilon}^{-1/2}\tilde{\mathbf{E}}_{\upsilon}(\mathbf{k}).$$

Their components $E_{\mathbf{b}i,\upsilon}(\mathbf{k})$ and $H_{\mathbf{b}i,\upsilon}(\mathbf{k})$ allow to calculate the spatial distribution of the components of the electromagnetic field strength vectors

$$E_{i,\upsilon\mathbf{k}}(\mathbf{x}) = \frac{1}{\sqrt{V}} \sum_{\mathbf{b}} E_{\mathbf{b}i,\upsilon}(\mathbf{k}) \exp[i(\mathbf{b}+\mathbf{k})\mathbf{x}],$$

$$H_{i,\upsilon\mathbf{k}}(\mathbf{x}) = \frac{1}{\sqrt{V}} \sum_{\mathbf{b}} H_{\mathbf{b}i,\upsilon}(\mathbf{k}) \exp[i(\mathbf{b}+\mathbf{k})\mathbf{x}]. \qquad (5)$$

Thus, using the periodic continuation of the system in question and solving the problem in the basis of photon states with a certain value of the wave vector and polarization, we have made the transition from continuous coordinates to discrete variables, and reduced the system of Maxwell differential equations (1) to a system of linear algebraic equations (4). By solving this system, we can determine the dispersion law $\omega(\mathbf{k})$ and the spatial distribution of the eigenmode field in the structure under study.

2. Results of numerical modelling

In Section 2, we will apply the previously described method to analyze the surface eigenmodes at the interface of two anisotropic biaxial materials. For this purpose, let us introduce two functions $f_1(z)$ and $f_2(z)$, determining the coordinate dependence of the tensors of permittivity and permeability $\boldsymbol{\varepsilon}(z)$, $\boldsymbol{\mu}(z)$ in each medium. Let the functions $f_1(z)$ and $f_2(z)$ be equal to one in the areas $-d < z < 0$ and $0 < z < d$ occupied by the first and second media, respectively, and equal to zero at other values of coordinate z. Then, for the components of the permittivity and permeability tensors, we obtain

$$\varepsilon_{ij}(z) = \varepsilon_{ij}^{1} f_1(z) + \varepsilon_{ij}^{2} f_2(z),$$

$$\mu_{ij}(z) = \mu_{ij}^{1} f_1(z) + \mu_{ij}^{2} f_2(z),$$

where $\varepsilon_{ij}^{1,2}$, $\mu_{ij}^{1,2}$ — tensor components in the areas occupied by each material.

Let us first consider the simplest case of the spatial orientation of anisotropic crystals forming an interface in which the principle axes of their permittivities coincide with the axes of the chosen coordinate system. Set the values of the components as follows:

$$\boldsymbol{\varepsilon}^1 = \begin{pmatrix} 11 & 0 & 0 \\ 0 & 12 & 0 \\ 0 & 0 & 6 \end{pmatrix}, \quad \boldsymbol{\varepsilon}^2 = \begin{pmatrix} 15 & 0 & 0 \\ 0 & 10 & 0 \\ 0 & 0 & 5 \end{pmatrix},$$

$$\boldsymbol{\mu}^1 = \boldsymbol{\mu}^2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

Next, we will also analyze the question of the existence of surface waves when the mutual spatial orientation of the dielectric tensors changes. To this end, rotate the crystal 1 with respect to the axes z and y, defining the corresponding rotation angles as ξ and η. The rotation matrices $\mathbf{R}_z(\xi)$ and $\mathbf{R}_y(\eta)$ can be represented as

$$\mathbf{R}_z(\xi) = \begin{pmatrix} \cos\xi & -\sin\xi & 0 \\ \sin\xi & \cos\xi & 0 \\ 0 & 0 & 1 \end{pmatrix},$$

$$\mathbf{R}_y(\eta) = \begin{pmatrix} \cos\eta & 0 & \sin\eta \\ 0 & 1 & 0 \\ -\sin\eta & 0 & \cos\eta \end{pmatrix}.$$

The new values of the components of the permittivity tensor $\boldsymbol{\varepsilon}^1$ after rotation can be calculated from the components of the original tensor $\boldsymbol{\varepsilon}_o^1$ by the formula

$$\boldsymbol{\varepsilon}^1 = \mathbf{R}(\xi, \eta)\boldsymbol{\varepsilon}_o^1\mathbf{R}^T(\xi, \eta), \ \ \mathbf{R}(\xi, \eta) = \mathbf{R}_z(\xi)\mathbf{R}_y(\eta).$$

As a unit of length, we choose the period of the system — the linear size of the lattice unite-cell L_0. Then, the thickness of the dielectric layers $d = 0.5L_0$, and the units of the wave vector and frequency are defined as $k_0 = 1/L_0$ and $\omega_0 = ck_0$, respectively. We take the modulus of the wave vector to be $k = 200k_0$. The reciprocal lattice vector directed along the axis z is defined as $b_n = 2\pi n/L_0$, where $n = -N_b \dots 0 \dots N_b$, the number $N_b = 75$, with the dimension of matrix $\Omega(\mathbf{k})$ equal to 453×453. Note, that for a given value of the vector modulus $\mathbf{k}$, the ratio of electromagnetic wave length to system period does not exceed the value $\lambda/L_0 \cong 1/(kL_0) = 0.005$.

Setting the structure parameters and determining the eigennumbers of the matrices in equations (4), we obtain the law of dispersion of eigenmodes $\omega(\mathbf{k})$, which we will further represent as a dependence of the refraction index on the wave vector $n(\mathbf{k})$. Fig. 2 shows the calculated dependences $n_1(\mathbf{k})$ and $n_2(\mathbf{k})$, corresponding to the bulk waves propagating in one of the interface-forming materials. At certain values of the components of the media permittivity tensors, the laws of dispersion of bulk waves overlap each other. This means that in the direction of the wave vector corresponding to the intersection axis, it is possible to excite electromagnetic waves in both media at the same frequency. In this case, it turns out that in a small range of $\Delta\varphi$ directions, another dispersion branch is possible, which corresponds to its interface eigenmodes.

In the case we consider, the curves $n_1(\mathbf{k})$ and $n_2(\mathbf{k})$ are symmetric ellipses. Therefore, it is sufficient to consider one of the angular intervals $\Delta\varphi$ located in the first quadrant of the plane xy. The result of calculating the surface wave dispersion law $n_o(\mathbf{k})$ near the intersection axis is shown in Fig. 3. The dependence n_o on the wave vector $\mathbf{k}$ appears only in a small range of angles, defining the angular existence domain of Dyakonov waves. The boundaries of the existence domain are designated as φ', φ'', with the axis of intersection of the laws of dispersion of volume waves located at an angle of φ_o. In the propagation directions φ' and φ'', the law of dispersion of surface waves is completely transformed into the law of dispersion of bulk waves in one of the media.

When using the method based on the periodic continuation of the system and the application of the Fourier decomposition, there is a question about the convergence of the calculation results. Consider, how the dispersion law of surface waves $n_o(\mathbf{k}, N)$ changes as the number of harmonics $N = 2N_b + 1$ increases. For this purpose, we fix the vector $\mathbf{k}$ in the direction of the angle φ_o and determine the relative change in the refraction index as the number N increases:

$$\delta n_o(N) = \frac{n_o(N) - n_o(N+1)}{n_o(N)}.$$

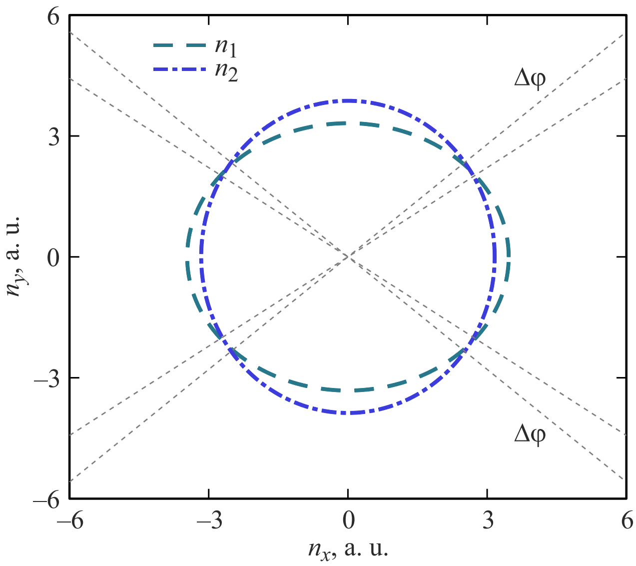

Figure 2. Sections of the dispersion surfaces $n_1(\mathbf{k})$ and $n_2(\mathbf{k})$ of bulk waves in the xy plane in media 1 and 2.

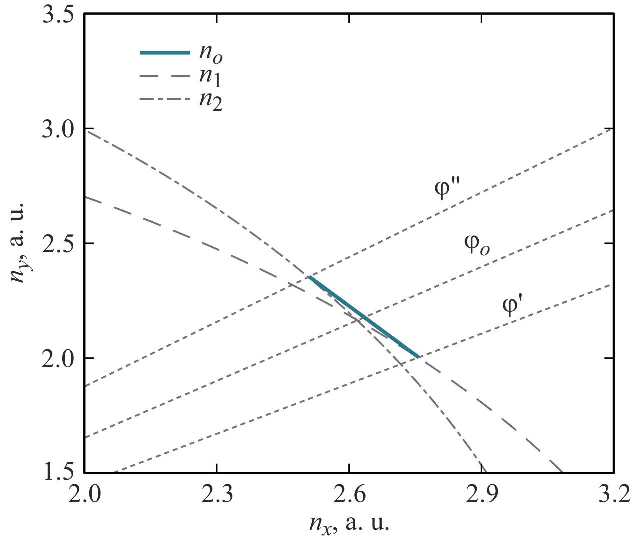

Figure 3. The law of dispersion of surface waves $n_o(\mathbf{k})$.

Figure 4 shows the result of calculating the dependence $\delta n_o(N)$. Note, that for small values of N the structure of dielectric layers with a sharp jump in permittivity cannot be approximated satisfactorily. However, with a larger number of harmonics, the dependence $\delta n_o(N)$ tends monotonically to zero, and the dispersion law of the interface eigenmodes practically ceases to depend on the number of Fourier components.

Let us fix the direction of the vector $\mathbf{k}$ along the intersection axis φ_o and determine the spatial distribution of the vectors of electromagnetic field strengths by restoring them using the relations (5). The result is shown in Fig. 5, 6. The obtained dependencies confirm that the calculated dispersion law $n_o(\mathbf{k})$ corresponds to the electromagnetic

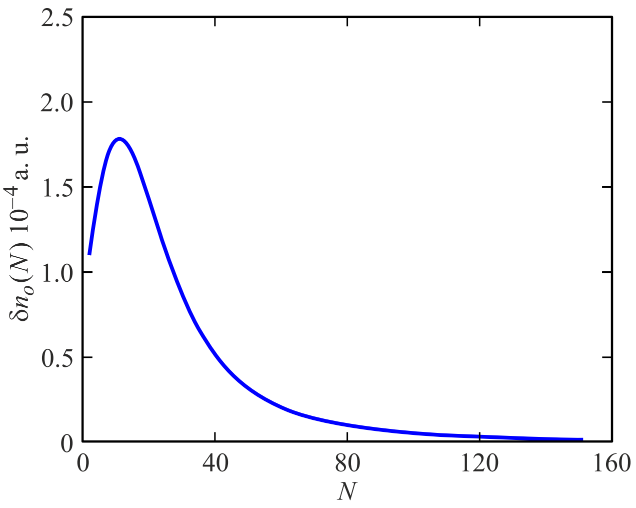

Figure 4. Dependence of the relative change in the refraction index of the surface wave on the number of Fourier harmonics used.

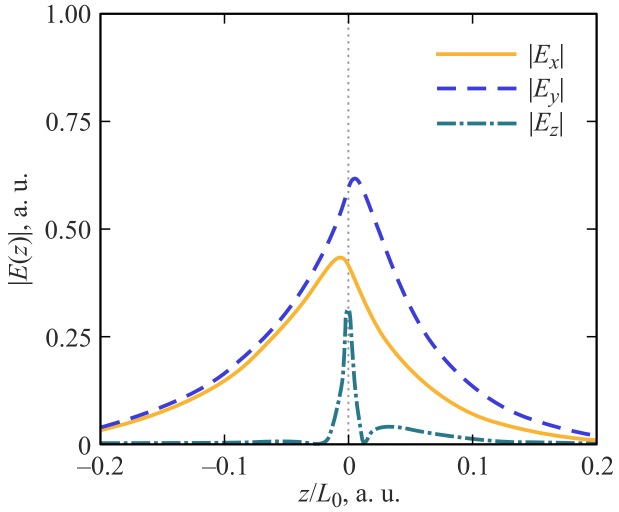

Figure 5. Spatial distribution of the moduli components of the electric field strength vector $\mathbf{E}(z)$.

waves damped in each of the materials as they move away from the interface plane and allow us to estimate the degree of their localization.

Let us analyze the change in the angular existence domain of Dyakonov surface waves when changing the spatial orientation of anisotropic media relative to each other. Consider the rotation of crystal 1 with respect to the axis perpendicular to the interface. The result of calculating the dependence of the angular range of the existence of surface waves on the rotation angle ξ of the medium 1 relative to the axis z is shown in Fig. 7 for the I and IV quadrants of the plane xy. As the orientation of the axes of the permittivity tensor of one of the media changes, the symmetrical arrangement of the angular domains of existence is broken. In this case, surface waves can propagate at any angle ξ, but the angular ranges lying in different quadrants of the interface plane are of different magnitude.

Next, consider a similar rotation of crystal 1 at an angle η with respect to one of the axes lying in the plane of the boundary (axis y). The value of the angle ξ is assumed to be zero. The result of calculating the dependence of the angular existence domain of surface waves on η is shown in Fig. 8. In this case, the angular ranges from the different quadrants of the interface plane change symmetrically. The greatest width of the angular range of existence is observed at $\eta = 0$. In this case, there are critical values of the rotation angle, at which the angular existence domain of Dyakonov surface waves disappears completely.

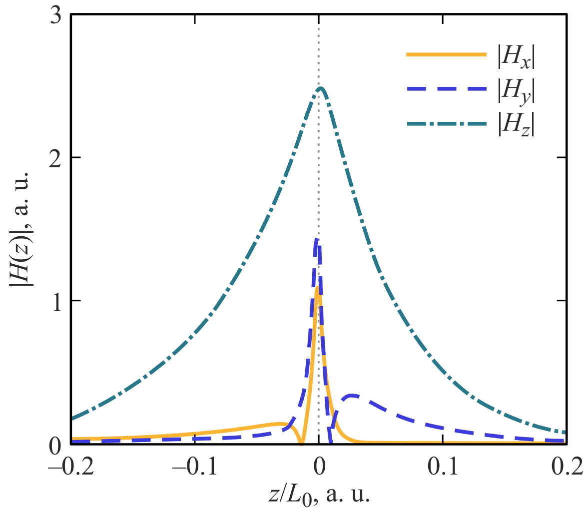

Figure 6. Spatial distribution of the moduli of the magnetic field vector components $\mathbf{H}(z)$.

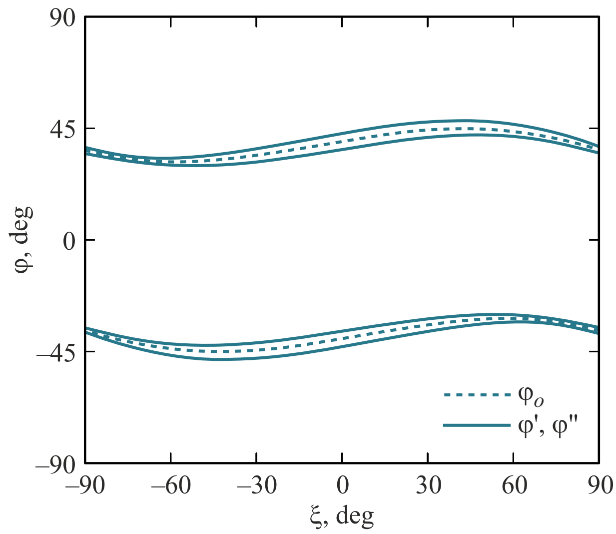

Figure 7. Dependence of the angular range of existence of surface waves on the rotation angle ξ of the medium 1 with respect to the axis z.

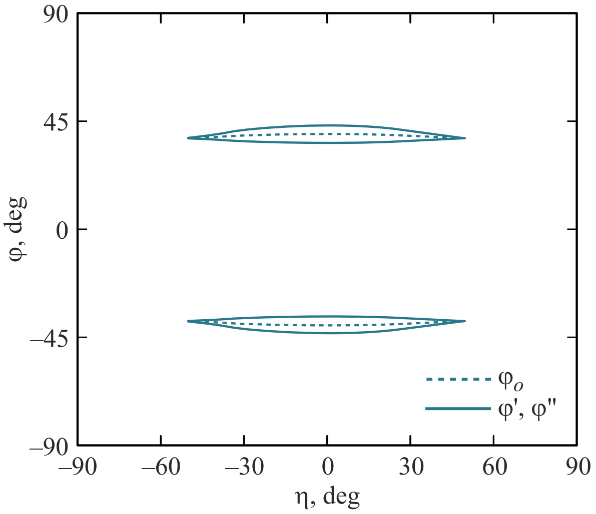

Figure 8. Dependence of the angular range of existence of surface waves on the angle of rotation η of the medium 1 with respect to the axis y.

Conclusion

This paper proposes a general approach to the analysis of Dyakonov surface waves propagating along interfaces formed by arbitrarily oriented anisotropic biaxial crystals. It is assumed that the anisotropic properties of these crystals, described by the tensors of permittivity and permeability, are generally different. The developed theoretical apparatus is based on the use of the operator representation of Maxwell's equations, which allows us to formulate the problem of determining the surface eigenmodes of the interface as a problem for finding eigennumbers and vectors of Hermitian operators. Within the framework of this method, the law of dispersion of Dyakonov surface waves in the form of the dependence of the refraction index on the wave vector is defined. The relations between the law of dispersion of bulk electromagnetic waves propagating in each of the boundary media and the dispersion of Dyakonov surface waves has been established. Essential in this case is the presence of the intersection of surfaces of the refraction indices of bulk waves in these media in the plane of the boundary. The section of the dispersion surface corresponding to the interface eigenmodes appears near the specified intersection. The dependences of the angular existence domain of the Dyakonov waves on the angles of relative rotation of the media were investigated in the work. The calculated dependencies made it possible to determine, at which spatial orientations of anisotropic crystals the surface electromagnetic waves can propagate, and in which cases the maximum value of the angular domain of their existence is achieved.

Conflict of interest

The authors declare that they have no conflict of interest.

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