Guided modes in a uniaxial multilayer

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An algorithm is presented for simulation of guided modes in a multilayer uniaxial structure with each layer characterized by its own ellipsoid of refractive indices and direction of optical axis. The proposed approach is based on presenting an electromagnetic field in each layer as a linear combination of ordinary and extraordinary waves coupled through the boundary conditions. The problem is reduced to two dimensions by considering the waves with a given projection of the wave vector on the plane of the waveguide. No a priori assumption about the guided-mode polarization is required in this method. Hybrid polarized modes appear naturally as solutions of a system of linear equations with respect to the amplitudes of the ordinary and extraordinary waves. The proposed approach covers a wide variety of important practical cases including isotropic waveguides, surface waves at the boundary between positive uniaxial crystal and isotropic medium, surface plasmons at metallic interfaces, uniaxial multilayers in a very general form, and leaky modes in such structures. © 2003 Optical Society of America


1. INTRODUCTION

Many electro-optical and nonlinear optical materials are uniaxial crystals. The most well-known example is lithium niobate (LiNbO3). A rather popular choice in recent years is barium borate (BaB2O4) (abbreviated as BBO). In a uniaxial crystal, light propagation is controlled by the direction of the optical axis and the refractive indices no and ne, where subscripts o and e refer to ordinary and extraordinary polarization, respectively. Guided modes in uniaxial crystals are well studied, especially for ion-diffused waveguides in LiNbO3. In contrast to the case of planar structures made of isotropic materials, the waveguide modes in uniaxial crystals have hybrid polarizations and their modal indices depend on the direction of propagation within the plane of the waveguide. When the optical axis has a certain orientation with respect to the waveguide plane and the propagation direction of the guided mode, e.g., when it is exactly normal to the waveguide plane or exactly parallel to the propagation direction, the symmetry of the structure allows for some simplification of the electrodynamic problem. Analytical solutions are possible in such simplified cases. Waveguide modeling in uniaxial materials has been a subject of many research papers published in recent decades. However, in the author’s opinion, the most general case has yet to be addressed. In this paper an algorithm is presented for simulation of the guided modes in a multilayer structure with each layer characterized by its own set of refractive indices and orientation of the optical axis. Similar to the approach of most models for light waves in multilayers, dimensionality of the problem is reduced by considering waves with a given projection of the wave vector on the waveguide plane. The general case that is discussed in this approach means complete freedom in choosing directions of optical axes and indices for each layer in the structure.

There are several important practical cases when such a model could be required. First, technological tolerances might result in, e.g., crystal axis orientation of an epitaxially grown film being slightly different from that of the substrate. Then the protecting layer, which is often made of amorphous materials such as silicon dioxide or nitride, becomes uniaxial because of thermal stress. Modeling of multilayer uniaxial structures with arbitrary orientation of the optical axis is required for adequate description of guided modes in such waveguides. Second, the phase matching in harmonic generation and optical parametric processes requires certain directions for the pumping beam. This is easily realized with bulk crystals by choosing a correct crystal cut and adjusting the input angle and polarization of the pump beam. It becomes, however, a problem when dealing with waveguides because the angular adjustment is not as easy as it is in the bulk case. A part of this problem is the absence of detailed information on angular dependence of modal indices. Instead of angular phase matching, periodical pooling is used to create a long-period grating compensating for the phase mismatch. On the other hand, similar to the case of a bulk crystal, no pooling will be required in a correctly designed and implemented waveguide structure. For example, one can imagine a weakly guiding channel waveguide oriented exactly along the phase-matching direction in a bulk crystal. The phase matching will certainly be preserved as long as the waveguide contribution to the modal index dispersion is small enough. When light is strongly confined to the guiding layer, waveguide dispersion cannot be neglected, but it can certainly be engineered to provide perfect phase matching. Consideration of phase matching in planar waveguides requires precise knowledge of a waveguide dispersion law, which could be obtained by using the algorithm described in Section 2. The subject of this paper is the simulation method itself, while the practical problems will be considered elsewhere.
2. ALGORITHM
Let us consider a multilayer structure in which all the layers as well as the substrate and the cladding are made of uniaxial materials (Fig. 1). We assign index \( i = 0 \) to the cladding, from 1 to \( N \) to the layers, and \( N + 1 \) to the substrate. We put the beginning of a Cartesian coordinate system at the top of the multilayer structure, and we orient the \( z \) axis normal to the layers and the \( y \) axis along the guided-mode propagation direction. Optical properties of all the layers including the cladding and the substrate are characterized by unit vectors of all the layers including the cladding and the sub-

...
vector along the layers. This means that the tangential components of all the wave vectors have to be identical. It also means that the normal wave-vector components must be, generally speaking, different for ordinary and extraordinary waves in each uniaxial layer, simply as a result of birefringence. This situation is, by its physical nature, close to that of light refraction at the interface with an anisotropic medium. In the general case, the incident wave generates two transmitted waves with different polarizations and different normal components of their wave vectors, while their tangential wave-vector components are identical and equal to that of the incident wave. This is why we would like to consider ordinary and extraordinary waves in each layer propagating in different directions. Maxwell’s equations, no doubt, allow for simultaneous propagation of waves with different polarizations in different directions. We will need only to make sure that the tangential components of the wave vectors are identical and adjust the wave amplitudes to satisfy the boundary conditions.

The electric flux density vectors then become

\[
D_o = D_o d_o(k_o), \quad D_e = D_e d_e(k_e) .
\]

We will refer to \(D_o\) and \(D_e\) as magnitudes of vectors \(D_o\) and \(D_e\), although in the general case they might be complex numbers, representing both amplitude and phase of a plane wave.

The strength of electric and magnetic fields in the ordinary and extraordinary waves, then, may be found by using the ordinary and extraordinary indices:

\[
E_o = D_o e_o(n_o, n_e, k_o, c), \quad e_o(n_o, n_e, k_o, c) = \frac{1}{n_o^2} \cdot d_o(k_o), \quad (7)
\]

\[
E_e = D_e e_e(n_o, n_e, k_e, c), \quad e_e(n_o, n_e, k_e, c) = \frac{1}{n_e^2} [d_e(k_e) \cdot e] e + \frac{1}{n_o^2} [d_e(k_e) - d_e(k_o) \cdot e] e , \quad (8)
\]

\[
H_o = D_o h_o(n_o, n_e, k_o, c), \quad h_o(n_o, n_e, k_o, c) = \frac{1}{\kappa} [k_o \times e_o(n_o, n_e, k_o, c)], \quad (9)
\]

\[
H_e = D_e h_e(n_o, n_e, k_e, c), \quad h_e(n_o, n_e, k_e, c) = \frac{1}{\kappa} [k_e \times e_o(n_o, n_e, k_e, c)]. \quad (10)
\]

In the above formulas, vectors \(e_o\), \(e_e\), \(h_o\), and \(h_e\) are unitless. For the sake of simplicity, we use the symmetric cgs system of units, so that electric and magnetic fields as well as electric and magnetic flux densities are expressed in the same units (gauss).

The dispersion law for the ordinary wave requires that

\[
k_{oz}^2 + k_{oy}^2 + k_{oz}^2 = \kappa^2 n_o^2 , \quad (11)
\]

and from the extraordinary one, we have

\[
k_{ez}^2 + k_{ey}^2 + k_{oz}^2 = \kappa^2 n_e^2 , \quad (11)
\]

\[
k_{ez}^2 + k_{ey}^2 + k_{oz}^2 = \kappa^2 n_e^2 .
\]

In each layer, including the cladding and the substrate, the electromagnetic field can be presented as a combination of plane waves satisfying conditions (3)–(10). To form a waveguide mode propagating along the \(y\) direction with modal index \(n^*\), we assume in Eqs. (11) and (12) that

\[
k_{ox} = k_{ex} = 0 , \quad (13)
\]

\[
k_{oy} = k_{ey} = \kappa n^* . \quad (14)
\]

This assumption reduces the dimensionality of the problem as long as all the fields no longer depend on \(x\). Such a supposition is often made in analysis of light propagation in multilayers. This approach, however, remains rather general because there is no restriction imposed on selection of the optical axis direction and the indices in each layer.

Assumptions (13) and (14) allow us to find the \(z\) components of the wave vectors by using Eqs. (11) and (12):

\[
k_{ez}^2 = \frac{\cos^2(\theta)}{n_o^2} + \frac{\sin^2(\theta)}{n_e^2} + k_{ez} kn^* \left[ \frac{1}{n_o^2} - \frac{1}{n_e^2} \right] \times \sin(2\theta) \sin(\phi) + (kn^*)^2 \left[ \frac{\sin^2(\theta) \sin^2(\phi)}{n_o^2} + 1 - \frac{\sin^2(\theta) \sin^2(\phi)}{n_e^2} - \frac{1}{n^*} \right] = 0 . \quad (19)
\]

Note that for an isotropic medium \((n_e = n_o)\), Eq. (19) clearly makes Eqs. (17) and (18) identical to Eqs. (15) and (16). The superscript \(\ast\) or \(-\) in the above formulas indicates waves propagating up or down along the \(z\) axis in the case of uniform waves (real \(k_z\) components) and shows direction of exponential decay in the case of nonuniform waves (imaginary \(k_z\) components).

Once the wave-vector components are identified, we can write an expression for the electromagnetic field in each layer. We take the electric flux density as a primary field and, for each layer \(i (1 \leq i \leq N)\), assign four amplitude vectors \(D_1^i, D_2^i, D_3^i, D_4^i\), and \(D_5^i\), corresponding to ordinary and extraordinary waves propagating (or decaying) up and down:

\[
D_1(y, z) = \exp(i n^* y) [D_1^+ \exp(i k_{oz}^+ z) + D_1^- \exp(i k_{oz}^- z)] + D_5^i \exp(i k_{ez}^+ z) + D_4^i \exp(i k_{ez}^- z) . \quad (20)
\]
The directions of these vectors are determined by Eqs. (3) and (4) together with Eqs. (13)–(18). Their magnitudes \( D \) are so far unknown. In the cladding \((i = 0)\) and the substrate \((i = N + 1)\), there are only waves decaying far from the multilayer structure:

\[
D_0(y, z) = \exp(in_yky)[D_0^+(z) + D_0^-(z)],
\]

\[
D_{N+1}(y, z) = \exp(in_yky)[D_{N+1}^-(z) + D_{N+1}^+(z)].
\]

The total number of unknown magnitudes \( D \) becomes \( 4N + 2 + 2 = 4(N + 1) \). They provide a full description of the electric flux density field and, through Eqs. (7)–(10), of all other field components. The electric and magnetic field vectors are determined through the vectors \( b_p \) and \( a_p \) \((p = \{o, e\})\) is the polarization index) appearing in Eqs. (7)–(10) and unambiguously determined by \( n_o, n_e \), optical axis direction \( c(\theta, \phi) \), and wave-vector components (13)–(18). For further purposes we will use a compact notation such as

\[
f_{pi} = f(n_{oi}, n_{ei}, k_{pi}, c(\theta_i, \phi_i)),
\]

where the field component \( f \) may be either \( e \) or \( h \), the superscript \( s \) is + or −, and the index \( i \) is running from 0 to \( N + 1 \).

Within each layer, by the very construction of formulas (20)–(22), the fields satisfy Maxwell’s equations. At the boundaries we require continuity of tangential components of electric \((E_x\) and \( E_y\)) and magnetic \((H_x\) and \( H_y\)) fields. Each interface therefore generates four boundary conditions. Each condition is based on Eqs. (7)–(10) with the electric flux density defined by Eqs. (20)–(22), so it becomes a linear expression with respect to magnitudes \( D \). There are \( N + 1 \) boundaries in a structure of \( N \) finite-thickness layers. This gives \( 4(N + 1) \) equations to find \( D \).

The four equations associated with the very first interface between the cladding and the multilayer structure are the following (two choices for the vector \( f \), that is, \( e \) or \( h \), and two choices for the tangential direction, \( \tau = x \) or \( \tau = y \)):

\[
D_{a0}^+(f_{a0})_\tau + D_{a0}^-(f_{a0})_\tau = D_{a1}^+(f_{a1})_\tau + D_{a1}^-(f_{a1})_\tau + D_{a1}^-(f_{a1})_\tau + D_{a1}^-(f_{a1})_\tau.
\]

(24)

Similar equations for the interface between layers with indices \( i \) and \( i + 1 \) are as follows:

\[
D_{ai}^+(f_{ai})_\theta + D_{ei}^+(f_{ei})_\theta = D_{ai}^+(f_{ai})_\theta + D_{ei}^+(f_{ai})_\theta + D_{ei}^+(f_{ai})_\theta + D_{ei}^+(f_{ai})_\theta,
\]

\[
D_{ai}^+(f_{ai})_\phi = D_{ai}^+(f_{ai})_\phi + D_{ai}^+(f_{ai})_\phi + D_{ai}^+(f_{ai})_\phi + D_{ai}^+(f_{ai})_\phi,
\]

(25)

where the phase terms \( \psi \) are

\[
\psi_{pi} = \exp(-ik_{pi}z_4).
\]

Finally, at the interface with the substrate, one gets

\[
D_{aN}^+(f_{aN})_\tau, \psi_{aN} + D_{aN}^+(f_{aN})_\tau, \psi_{aN} + D_{aN}^-(f_{aN})_\tau, \psi_{aN} + D_{aN}^-(f_{aN})_\tau, \psi_{aN} = D_{a(i+1)}^+(f_{a(i+1)})_\tau + D_{e(i+1)}^+(f_{e(i+1)})_\tau + D_{a(i+1)}^-(f_{a(i+1)})_\tau + D_{e(i+1)}^-(f_{e(i+1)})_\tau.
\]

(27)

Then we write Eqs. (24), (25), and (27) in a compact form:

\[
\hat{M}D = 0,
\]

(28)

where \( \hat{M} \) is a \( 4(N + 1) \times 4(N + 1) \) matrix and \( D \) is a \( 4(N + 1) \)-dimensional vector composed of magnitudes of vectors \( D_{a0}^+, D_{e0}^+, D_{ei}^+, \) and \( D_{ei}^- \). The matrix \( \hat{M} \) can be considered a function of a trial parameter \( n^* \), which appears in Eqs. (14)–(18) and determines the wave-vector components. A nontrivial solution of Eq. (28) exists if

\[
\det[\hat{M}(n^*)] = 0.
\]

(29)

We solve Eq. (29) numerically and find possible values of the modal index \( n^* \). Then the corresponding nontrivial vector \( D \) determines the electromagnetic field through Eqs. (7)–(10) and (20)–(22).

It should be emphasized once again: All the components of the matrix \( \hat{M} \) are \( x \) and \( y \) projections of vectors \( e_p \) [Eq. (7)], \( e_p \) [Eq. (8)], \( h_p \) [Eq. (9)], and \( h_p \) [Eq. (10)] on the plane of the waveguide multiplied by the phase terms (26). Thus each component of the matrix \( \hat{M} \) is directly calculated for a given multilayer structure and a given trial parameter \( n^* \). Deriving formulas for the components of the matrix \( \hat{M} \) is the essence of the proposed algorithm. No sophisticated numerical methods are involved in determination of the matrix \( \hat{M} \). Solving Eq. (29) for \( n^* \) and then finding \( D \) from Eq. (28) is a standard numerical procedure, so efficient numerical algorithms are available (see, e.g. Ref. 9). The fields \( \mathbf{E} \) and \( \mathbf{H} \) are then restored by using Eqs. (7)–(10).

3. NUMERICAL EXAMPLES

The following numerical examples confirm the validity of the proposed algorithm and demonstrate a variety of problems that could be solved by using this approach.

A. Isotropic Structure

In the proposed algorithm, there is no preliminary assumption on the polarization of the waveguide mode. In other words, by applying the proposed algorithm to isotropic multilayers, we get both transverse electric (TE) and transverse magnetic (TM) modal indices as a solution of Eq. (29) and modal profiles from Eq. (28). This becomes one of the possible simple cases, which we can use to test the proposed algorithm. Let us consider a waveguide formed by a \( t_1 = 1.0 \mu m \) thick amorphous silicon nitride \((n_1 = 2.2)\) layer on a fused silica \((n_2 = 1.45)\) substrate. The cladding is air \((n_o = 1.0)\). We assume a communication wavelength of \( \lambda = 1.55 \mu m \). In the proposed algorithm, isotropic materials are assigned identical ordinary and extraordinary indices, while directions of optical axes are arbitrary. The matrix \( \hat{M} \) itself, as well as the magnitudes \( D \) satisfying Eq. (28), is sensitive to the choice of directions \( c_0, c_1, \) and \( c_2 \) for the optical axis. However, the roots of Eq. (29) and the fields \( \mathbf{E} \) and \( \mathbf{H} \) do not depend on this choice. For the particular waveguide structure, the function \( \det[\hat{M}(n^*)] \) is shown in Fig. 2 for two choices of \( c_i \). The plot in Fig. 2(a) corresponds to
\( \theta_i = \phi_i = 0 \), and the plot in Fig. 2(b) shows the case \( \theta_i = \phi_i = \pi/4 \). Regardless of the choice of angles \( \theta_i \) and \( \phi_i \), clear linear polarization of fields \( \mathbf{E} \) and \( \mathbf{H} \) is found by using Eqs. (7)–(10) together with D components defined by Eq. (28). The roots, \( n_1^*, \ldots, n_5^* \), are recognized as modal indices for TE and TM modes: \( n_1^* = n_{TE0}, n_2^* = n_{TM0}, n_3^* = n_{TE1}, \) and \( n_4^* = n_{TM1} \). Also, the modal indices can easily be verified by using formulas for thin-film dielectric waveguides. The root \( n_5^* = n_1 = 2.2 \) is the false one. It indeed brings \( \det[\hat{M}(n^*)] \) to zero and corresponds to a nonzero set of magnitudes \( D \). However, this is the degenerate case of all \( k \), in Eqs. (15)–(18) being simultaneously equal to zero. It eventually results in zero strength of fields \( \mathbf{E} \) and \( \mathbf{H} \); that is, no waveguide mode corresponds to this root. Such roots can be easily ruled out. In any case, to identify the polarization of a particular mode, we must find the fields. A zero field would indicate the false root. From the author’s experience in running this algorithm, such false roots are rather rare and typically found at \( n^* \) equal to one of the indices characterizing the layers. So they do not change while, e.g., wavelength or layer thickness is varied. It becomes another simple rule to filter out the false roots. From a practical point of view, the false roots represent no substantial difficulty in analysis of waveguide modes, although it would be helpful to develop a simple rule to filter them out without calculating fields or modal index derivatives.

**B. Surface Modes at the Interface with Positive Uniaxial Crystal**

Another textbook example for testing the validity of the proposed algorithm is the surface mode at the interface between an isotropic medium and a positive uniaxial crystal. \(^{10,11} \) Because the structure under consideration is rather simple (single interface), an electrodynamic description of such modes could be done analytically. In the present approach, we take \( N = 0 \). Equations (24)–(27) are reduced to

\[
D_{00}(f_0^*)_r + D_{01}(f_1^*)_r = D_{10}(f_0^*)_r + D_{11}(f_1^*)_r, \tag{30}
\]

where, as in Section 2, \( f \) stands for \( \mathbf{e} \) or \( \mathbf{h} \) and \( \tau = x \) or \( y \), so that Eq. (30) contains four equations. The material parameters have been taken from Ref. 11: The substrate is rutile \((n_{s1} = 2.5837 \text{ and } n_{s2} = 2.8719 \text{ at wavelength } \lambda = 0.6328 \text{ } \mu \text{m})\), and the cladding index is an arithmetic average of the rutile indices: \( n_{c0} = n_{c0} = 2.7278 \). The surface mode exists within a narrow range of angles \( \phi_1 \). For \( \theta_1 = 90^\circ \) (optical axis is parallel to the interface), the surface mode was found for \( \phi_1 \) in the range from \( \phi_{\text{min}} = 42.464^\circ \) to \( \phi_{\text{max}} = 42.976^\circ \). For smaller angles \( \theta_1 < 90^\circ \), the range of \( \phi_1 \) suitable for the existence of the surface mode is even narrower. The function \( \det[\hat{M}(n^*)] \) for \( \theta_1 = 90^\circ \) and \( \phi_1 = 42.7^\circ \) is shown in Fig. 3(a). At this angle the modal index is \( n_1^* = 2.728206 \). At \( \phi_1 = \phi_{\text{max}} \) the modal index is approaching the index of the cladding, and at \( \phi_1 = \phi_{\text{min}} \) it is greater than \( n_{c0} \) (\( n^* \approx n_{c0} + 1.35 \times 10^{-3} \) in this example). Modal index versus \( \phi_1 \) is shown in Fig. 3(b).

**C. Surface Modes at the Metal–Uniaxial-Crystal Interface**

Another textbook example of a surface wave is a surface plasmon at the interface between metal and dielectric. For isotropic dielectrics the plasmon’s modal index is known to be

\[
n^* = \left( \frac{\varepsilon_m \varepsilon_d}{\varepsilon_m + \varepsilon_d} \right)^{1/2}, \tag{31}
\]

where \( \varepsilon_m \) and \( \varepsilon_d \) are dielectric permittivities of metal and dielectric media, respectively. The plasmon can only have a TM polarization and exist if \( \text{Re}(\varepsilon_m + \varepsilon_d) < 0 \). Here we apply the proposed algorithm for simulation of plasmon waves at the interface between metal and uniaxial crystal. Let us note that a structure containing a metallic layer is essentially lossy and that the modal index becomes a complex value. Some peculiarities of the
proposed algorithm resulting from the complex nature of the modal index are discussed in Subsection 3.F. Here it is emphasized that the algorithm is suitable for simulation of surface waves at metallic interfaces. We consider a gold–lithium-niobate material system at a wavelength of $\lambda = 1.55 \text{ m}$.

An infrared (IR) wavelength is more convenient for such examples because of the better optical properties of most metals in the IR spectral range compared with those in the visible range. We set the cover index to $n_0 = 0.559 + 0.19.81j$ (gold) and the substrate index to $n_1 = 2.21$ and $n_2 = 2.14$ (LiNbO$_3$) and calculate the complex-valued modal index of the plasmon wave for different orientations of the optical axis with respect to the propagation direction ($\theta_1 = 0, \phi_1 = 0$ to $\pi/2$). The simulation results are presented in Fig. 4. At $\phi_1 = 0$ (plasmon direction is parallel to the optical axis), both real and imaginary parts of the numerically calculated modal index coincide with the numbers given by Eq. (30), assuming that $\epsilon_2 = n_2^0$. The nonzero imaginary part of the modal index is associated with absorption in a metal cover. At angles $\phi$ approaching $60^\circ$, losses are significantly increased because of leakage to the substrate (dashed curve in Fig. 4). This is a peculiarity of a uniaxial crystal, and it certainly does not happen for an isotropic substrate. Losses versus angle shows a rather wide resonant peak, which indicates a phase matching between the plasmon and the wave leaking into the substrate. The real part of the modal index shows a corresponding resonant behavior in the vicinity of the peak absorption angle (solid curve in Fig. 4). At $\phi_1$ approaching $90^\circ$, the real part of the plasmon’s modal index becomes equal to the ordinary index of the substrate, and losses vanish, which indicates that at these conditions the plasmon becomes an ordinary wave propagating parallel to the surface with infinitely small confinement in a metal cover.

To prove that the absorption peak is indeed associated with the leakage, rather than with absorption in metal, similar calculations have been performed for an idealized metal structure with no absorption [set $\text{Re}(n_0) = \text{Re}(n_0)$ $= 0$ in the previous calculations]. At these conditions losses sharply appear for angles greater than $49^\circ$. For smaller angles losses are exactly equal to zero because there is no absorption and no leakage. The real and imaginary parts of the plasmon’s modal index are shown in Fig. 4 by the dotted and dotted–dashed curves, respectively.

D. Dielectric Anisotropic Structure

Now we consider a dielectric anisotropic structure. The modes are hybrid in the general case. Nevertheless, if all the optical axes are kept within the plane containing the direction of the mode propagation and the normal to the surface ($\phi = \pi/2$), simple geometrical consideration of ellipsoids of refractive indices allows for clear separation of TE- and TM-polarized modes. Moreover, the TE modes are determined by ordinary indices only. To observe this in the model, we set the substrate indices to $n_0 = 2.7278$ and $n_1 = 2.5837$; the film indices are increased by 0.02, that is, $n_{o2} = 2.23$ and $n_{e2} = 2.16$; the film thickness is $t_1 = 5 \text{ \mu m}$; and the cladding is air ($n_{o0} = n_{e0} = 1$). This set of parameters re-
with the coupling coefficient controlled by an external electro-optical modulators employs a directional coupler and calculate modal indices as a function of \( \theta \). Numerical results are shown in Fig. 5(a). The plot shows that the TE and TM modes are clearly separated. At \( \theta \approx 66^\circ \), modal indices for the TE1 and TM0 modes become equal: \( n_{TM0}^f = n_{TE1}^f \). The plot shows no anticrossing behavior around this point, which indicates no coupling between the modes.

Hybrid modes appear when \( \phi_0 \neq \pi/2 \) and \( \theta_0 \neq 0 \). Figure 5(b) shows the case \( \theta = \pi/2 \). We keep \( \phi_0 = \phi_2 = \phi \) and calculate modal indices as a function of \( \phi \). The modes are hybrid except for \( \phi = 0 \) and \( \phi = \pi/2 \). At \( \phi = 0 \) the modes are TM0, TM1, TE0, and TE1 in the order of descending modal index. At \( \phi = \pi/2 \) the modes are TE0, TM0, TE1, and TM1, given in the same order. At \( \phi \approx 66.6^\circ \) the dispersion curves show clear anticrossing with \( \Delta n^* = 0.0025 \). This indicates strong coupling between the TM1 and TE0 modes (coupling coefficient \( K = \pi \Delta n^* / \lambda \approx 50 \text{ cm}^{-1} \)), which is also treated as formation of hybrid polarized modes. At a larger angle (\( \phi > 80^\circ \)), the anticrossing of the dispersion curves TM0–TE0 and TM1–TE1 is much smaller (1.7 \( \times 10^{-5} \) and 1.4 \( \times 10^{-4} \), respectively), which shows much weaker mode coupling. No TE1 mode was found in the range \( 40^\circ < \phi < 74^\circ \), which simply indicates that the waveguide in this case does not satisfy the cutoff condition for TE1. The dashed curve in the plot corresponds to the values of \( n^* \) that bring \( |\det(M(n^*))| \) to a local minimum, although it is not a solution of Eq. (29).

Coupling between the TE and TM modes can be used in optoelectronic devices. One of the schemes for LiNbO\(_3\) electro-optical modulators employs a directional coupler with the coupling coefficient controlled by an external voltage. The TE–TM coupling described above allows for a more elegant design using a single waveguide. With properly adjusted waveguide parameters, total polarization conversion will take place at zero voltage, while, by applying the controlling signal, one can detune the resonance so that polarization of the input signal will remain unchanged.

E. Two-Layer Anisotropic Structure

Let us consider an anisotropic waveguide film covered by a protective film. The film parameters are chosen to be close to those in a practical situation. Amorphous silica film, for example, could be used on top of a fragile and hygroscopic crystal such as BaB\(_2\)O\(_4\) (BBO) to protect the waveguide from damages. Because deposition of a film usually takes place at relatively high temperature, thermal expansion creates tension at room temperature and makes the film a uniaxial material with the optical axis normal to the surface. The thermal-stress-induced birefringence of oxide films is often big enough to make the TM modal index higher than the TE index, which can never happen for an isotropic film. Let us take \( n_{e1} = 1.45, n_{e3} = 1.455, \) and \( t_2 \) varying from 0 to 0.5 \( \mu \text{m} \). Then, to have a realistic estimate, we take the indices for Y-cut BBO waveguide film at the wavelength \( \lambda = 0.633 \text{ \mu m} \) from Ref. 12 (\( n_{e2} = 1.691, n_x = 1.560 \)) and assume an optical barrier layer with lower indices (\( n_{e3} = 1.561, n_{e0} = 1.521 \)) right below the waveguide layer. We take the waveguide layer thickness \( t_2 = 0.5 \mu \text{m}, \) which corresponds to a single-mode waveguide, and the cover film thickness \( t_1 = 0.2 \mu \text{m}. \) In this model we assume that the optical barrier layer is thick enough to neglect light tunneling to the substrate. To emphasize the role of birefringence in the cover film, we calculate modal indices in the structure with isotropic cover film with index \( n_1 = (n_{e1} + n_{e3})/2 \). The simulation results are shown in Fig. 6. We again keep \( \theta_2 = \theta_3 = \pi/2 \) and plot modal indices versus \( \phi \) (\( \phi_2 = \phi_3 = \phi \)). In the cladding and the cover layer, \( \theta_0 = \theta_1 = \phi_0 = \phi_1 = 0. \) TE0–TM0 anticrossing is observed at \( \phi = 74.25^\circ \) with \( \Delta n^* = 9.1 \times 10^{-4} \) (coupling strength of 45 cm\(^{-1}\)). When birefringence in the covering film is neglected, the error in the modal index may be as large as

![Fig. 5. Modal indices of an anisotropic waveguide versus guided-mode propagation direction.](image-url)
However, in the vicinity of TE–TM coupling, both cases show almost identical results [Fig. 6(b)], which could be attributed to a rather symmetric mixing of TE and TM polarized modes at $\phi = 74.25^\circ$. Accurate simulation of modal indices in such structures is certainly required for precise design and analysis of waveguide-based nonlinear optical devices.

### F. Lossy Modes

An example of a lossy waveguide would be a structure with a metal layer. In practical applications it occurs in electro-optical devices, when controlling voltage is applied to a structure through electrodes placed close to the guiding layer. Gold is usually a good choice for the electrodes because of its high conductivity and strong light reflection from its surface, which means weak penetration of light in a metal layer and, consequently, low absorption. Another similar example would be a plasmon mode at the metal–dielectric interface. Applicability of the proposed algorithm for the analysis of such structures is illustrated in Subsection 3.C.

Another possible reason for optical losses is leakage to a substrate that has an index of refraction that is greater than the modal index. Leaky modes in anisotropic structures have been studied previously.\textsuperscript{13,14} The guiding layer in such systems is separated from the substrate by a low-index buffer. Light tunneling through the buffer results in optical losses.

All these cases are covered by the proposed approach; naturally, they result in the complex roots of Eq. (29), while the overall algorithm remains basically unchanged. The complex roots may be found, for example, by scanning over the Re($n^*$) axis and keeping Im($n^*$) equal to zero. This may reveal the approximate roots of the equations Re[$\det(M(n^*))$] = 0 and Im[$\det(M(n^*))$] = 0. Then one can use, e.g., Newton’s algorithm to find the complex roots of Eq. (29). Other methods of numerical analysis of Eq. (29) are certainly possible. This issue is beyond the scope of the present analysis.

As a numerical example, the calculation of losses in a BBO waveguide is presented (Fig. 7). We take all the parameters identical to those mentioned above and assume variable thickness $t_3$ of the buffer layer and the substrate indices $n_o = 1.661$ and $n_e = 1.561$.

### 4. ADDING THE THIRD DIMENSION

Assumptions (13) and (14) allowed us to consider a rather general case of guided modes in a uniaxial multilayer. We now can find the modal indices and modal field distributions for guided modes propagating in any given direction within the waveguide layers. These modes are plane in the sense that their fields do not vary along the in-plane direction normal to the in-plane wave vector. Adding the third dimension to the problem would extend the model and allow for simulating such important phenomena as propagation of converging and diverging waves in a uniaxial waveguide. This analysis for anisotropic media is more difficult than that for isotropic materials. The difficulty of the anisotropic case is associated with
the rather complex dependence of the wave vector on the propagation direction. In addition, the direction of the energy propagation does not necessarily coincide with the wave vector. As a result, for example, a diverging wave will have wave fronts with variable radius of curvature and variable intensity along the wave front. A possible way of doing such an analysis would be to present a converging (diverging) wave as a continuous set of the plane modes propagating in different directions. Integrating over the set, one can find the intensity distribution in any desirable area. The most crucial step in this approach will be to formulate the orthogonality condition for the plane modes, which will result in an algorithm for decomposition of a converging (diverging) wave into a set of the plane modes. Detailed consideration of these questions is beyond the scope of this paper.

5. CONCLUSION

In conclusion, an algorithm has been proposed to simulate guided modes in a multilayer structure made of uniaxial layers with each layer characterized by its own ordinary and extraordinary index and direction of optical axis. The electric and magnetic fields in each layer are presented as a superposition of ordinary and extraordinary waves, which are coupled at the interfaces between the layers. Some classical examples are considered by using the proposed algorithm, including isotropic and anisotropic structures and surface waves at the interface between isotropic and positive uniaxial materials.

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