Synthesis of Titanium Indiffused LiNbO₃ Waveguides with Desired Modal Fields
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ABSTRACT
In this paper we report a procedure based on variational approximation, to obtain the refractive index profile and in turn the process parameters for fabrication of waveguide from the desired modal field. We have illustrated our procedure by the design of a diffused channel waveguide for optimum coupling to a standard communication grade fiber.

Keywords: Diffused Channel waveguides, Variational method, Fabrication of diffused channel waveguides

1. INTRODUCTION
In the design of optical waveguides and waveguide-based devices, it is often required to synthesize waveguides with a desired modal field. It is often important to design the modal field and corresponding refractive index profile of the waveguide that compose the device, as the important characteristics of optical waveguides such as spot-size, single mode condition and coupling coefficients can be predicted once the index profiles and modal fields are known. In this paper we report a procedure based on variational approximation, to obtain the refractive index profile and in turn the process parameters for fabrication of waveguide from the desired modal field.

We have illustrated the use of the procedure in the design of waveguides with modal fields for optimum coupling efficiency between a typical communication grade fiber and waveguide. In optical systems that contain integrated optical components, coupling efficiency between the fundamental mode of the diffused channel waveguide of an integrated optical circuit and the optical fiber that is connected to the circuit plays an important role in insertion loss considerations. The estimation of coupling efficiency requires the knowledge of the modal fields of both the fiber and waveguide. Since, in general, analytical solutions are not possible for diffused channel waveguides, one has to use either approximate methods like Effective-Index method or numerically intensive methods like finite difference, finite element or Beam propagation techniques. In all these methods, modal fields are obtained as numerical data. We have, instead used appropriately defined closed form expressions for modal fields of channel waveguide based on the variational method, for the optimum design of a diffused channel waveguide.

2. CLOSED FORM SEPARABLE CHANNEL WAVEGUIDE FIELDS
The typical refractive index profile obtained by Titanium diffusion into LiNbO₃ waveguides can be described as

\[ n^2(x, y) = n_s^2 + 2n_x \Delta n \exp\left(\frac{x}{w}\right) f\left(\frac{y}{h}\right) \]

\[ = n_c^2 \quad y < 0 \]

where \( n_s \) is the substrate index with \( g(x/ w) = \exp(-x^2 / w^2) \), \( f(y/h) = \exp(-y^2 / h^2) \) and \( \Delta n \) is the maximum refractive index change of the diffused channel waveguide. One can define, in general, a suitable separable field \( \psi(x, y) = X(x)Y(y) \) for a diffused channel waveguide. It has been shown that for the best separable field \( Y(y) \) corresponds to the modal field of a \( y \)-slab waveguide with a planar index distribution \( n^2(y) \) defined as

\[ n^2(y) = n_s^2 + K + 2n_x \Delta n_y f\left(\frac{y}{h}\right) \]

\[ = n_c^2 \quad y < 0 \]  \hspace{1cm} (y > 0) \]

where \( \Delta n_y = \Delta n \int g(x/ w)X(x)^2 dx \) and \( K \) is a constant. Similarly the best separable \( X(x) \) corresponds to the following symmetric \( x \)-slab waveguide with the planar index distribution \( n^2(x) \).

\[ n^2(x) = n_s^2 + K + 2n_y \Delta n_x g(x/ w) \]  \hspace{1cm} (y < 0) \]

where \( \Delta n_x = \Delta n \int f(y/ h)Y(y)^2 dy \) . Here \( \Delta n_y \) and \( \Delta n_x \) are equivalent relative index differences along the two directions.
The solution for the planar waveguide defined in the x and y direction can be obtained by the scalar variational analysis as

\[ Y(y) = \frac{1}{\sqrt{h d_x}} \left( 1 + \frac{\gamma_y}{h} y \right) \exp \left( -\alpha_y \frac{y^2}{h^2} \right) \quad y > 0 \]
\[ = \frac{1}{\sqrt{h d_y}} \exp \left( \gamma_x \frac{y}{h} \right) \quad y < 0 \]

where \( \gamma_y \) and \( \alpha_y \) can be expressed in closed form as a function of a normalized \( V \) parameter in y direction, \( V_y = k_0 h \sqrt{2 n_s \Delta n} \) asymmetry parameter, \( p = (n_s^2 - n_c^2)/2 n_s \Delta n \), where \( k_0 = 2\pi/\lambda_0 \) is the free space wave number and \( d_y = \frac{1}{2\gamma_y} + \frac{1}{2\alpha_y} \sqrt{\frac{\pi}{2} \left( 2 + \gamma_y^2 + \frac{\gamma_y^2}{8\alpha_y^2} \right)} \sqrt{\frac{\pi}{2}} \)

Similarly

\[ X(x) = \frac{1}{\sqrt{h d_x}} \exp \left( -\alpha_x \frac{x^2}{w^2} \right) \quad \text{for all } x \]
\[ = \frac{1}{\alpha_x} \sqrt{\frac{\pi}{2}} \quad \text{and } \alpha_x \text{ defines the width of the Gaussian field in } x \text{ direction can be expressed as} \]
\[ \alpha_x(V_x) = a_0 + a_1 V_x + a_2 V_x^2 \]

where \( V_x = k_0 h \sqrt{2 n_s \Delta n_x} \)

3. FIBER TO WAVEGUIDE COUPLING EFFICIENCY

The coupling efficiency between the fiber and waveguide is given by

\[ \eta = \int \psi_1(x, y) \psi_2(x, y) \, dx \, dy \]

here \( \psi_1 \) is the normalized waveguide modal field as defined above and \( \psi_2 \) is the modal field of the optical fiber. For the single mode fiber placed at \( (0, \xi) \) the fiber modal field can be approximated to a Gaussian given by

\[ \psi_2(x, y) = \sqrt{\frac{2}{\pi \omega_f}} \exp \left( -\frac{x^2 + (y - \xi)^2}{\omega_f^2} \right) \]

where \( \omega_f \) is the spot size of the fiber and is typically a function of \( V \) number and radius of the fiber.

By use of separable fields in x and y directions the coupling efficiency can be written as a product

\[ \eta = \eta_x \eta_y \]

Using the closed form modal field, we get analytical expressions for the coupling efficiency as

\[ \eta_x = \frac{I}{w \omega_f d_x} \sqrt{\frac{2}{\pi}} \quad \text{and} \quad \eta_y = \frac{J}{h \omega_f d_y} \sqrt{\frac{2}{\pi}} \]

where \( I \) is given by

\[ I = -\frac{1}{\sqrt{\omega_f^2 + \alpha^2}} \left( \frac{\alpha^2}{\omega_f^2} \right) \]

and \( J \) is

\[ J = \frac{\exp \left( -\frac{z^2}{\omega_f^2} \right) \left[ \exp(k_1^2) \left( \sqrt{\pi} k_2 (1 + \text{erf}(k_1)) + h \sqrt{\pi} \gamma_x \xi (1 + \text{erf}(k_1)) + k_2 \omega_f \gamma_y \xi \right) \right]}{\omega_f} \]

with \( k_1 = k_0 h \sqrt{\Delta n_x} \) and \( k_2 = k_0 h \sqrt{\Delta n_y} \).
with \( k_1 = \frac{\xi}{\sqrt{\omega_f^2 + \frac{\alpha_s^2}{\omega_f^2} + \frac{1}{\alpha_s^2}}} \) and \( k_2 = \sqrt{h^2 + \alpha_s^2 \omega_f^2} \).

For optimizing the position of the fiber \((0, \xi)\), we have to maximize the coupling efficiency with respect to \( \xi \), or obtain \( \xi = \xi_m \), which is the value of \( \xi \) at which \( \frac{d\eta_v}{d\xi} = 0 \).

The design now requires that both \( \eta_x \) and \( \eta_y \) to be maximized. However in an attempt to do so we realized that both cannot be maximized independently since, the parameters are eventually limited by the diffusion process in fabrication, as discussed in the next section.

4. OPTIMIZING THE REFRACTIVE INDEX PROFILE AND DETERMINING FABRICATION PARAMETERS

The coupling between waveguide and fiber can be maximized by an optimization of waveguide profile parameters, \( \Delta n \), \( h \) and \( w \). It is possible to tailor the waveguide profile within certain limits by adjusting the fabrication parameters, thickness and width of the Ti stripe, temperature and duration of diffusion and crystal cut.

The titanium diffused waveguides in lithium niobate, or the Ti: LiNbO\(_3\) waveguides, are formed by the in-diffusion of the titanium dopant into the lithium niobate host. To form a waveguide, a stripe of titanium is deposited on the LiNbO\(_3\) substrate. For a given stripe width, which we identify with the waveguide width, the amount of titanium is characterized by the stripe thickness before diffusion \(8,9\). The index distribution can be characterized by diffusion constants, diffusion temperature, diffusion time and a diffusion temperature coefficient. Moreover, since the lithium niobate crystal is anisotropic, the refractive index depends on the crystal cut and light polarization. We have used TE polarization in a z-cut LiNbO\(_3\) corresponding to the ordinary index \( n_o \).

The graded refractive index \( n(x, y) \) obtained by the diffusion process, is a sum of the bulk crystal index \( n_s = n_o \) and the diffusion-induced index change \( \Delta n(x, y) \),

\[
\Delta n(x, y) = d_o c_o^2 F_o \left[ \text{erf} \left( \frac{w_s}{2D_x} \left( 1 + \frac{2x}{w_s} \right) \right) + \text{erf} \left( \frac{w_s}{2D_x} \left( 1 - \frac{2x}{w_s} \right) \right) \right]^2 \exp \left( -\frac{y^2}{2D_y} \right) \tag{10}
\]

where, for the ordinary (o) index distributions the dispersion factor is \( d_o (\lambda) = \frac{0.67 \lambda^2}{\lambda^2 - 0.13} \) and the wavelength is measured in microns. The distribution constant \( F_o = 1.3 x 10^{-25} \, \text{cm}^3 \) and the distribution power factor \( \gamma = 0.55 \). The profile parameters include the profile constant \( c_o \), the titanium stripe width before diffusion \( w_s \), the lateral diffusion length \( D_x \) and the diffusion length in depth \( D_y \). The lateral diffusion length \( D_x = 2 \sqrt{t D_{o,x} \exp(-T_0/T)} \) and the diffusion length in depth \( D_y = 2 \sqrt{t D_{o,y} \exp(-T_0/T)} \) are functions of the diffusion time \( t \) and the diffusion temperature \( T \). The temperature coefficient \( T_0 = 30300 \text{Kand} \) the diffusion constants \( D_{o,x} \) and \( D_{o,y} \) are specific for lithium niobate substrate. The profile constant \( c_o = \pi c_m \sqrt{\pi D_y} \) is a combination of the stripe thickness before diffusion \( \tau \), the dopant constant \( c_m = 5.67 x 10^{22} \, \text{cm}^{-3} \) and the diffusion length in depth \( D_x \) described earlier.

The above profile is equivalent to Eq. (1) with \( h = D_x / \sqrt{\gamma} \) and \( w \) obtained by the relation

\[
\left\{ \text{erf} \left( \frac{w_s}{2D_x} + \frac{\sqrt{\gamma} w}{D_s} \right) + \text{erf} \left( \frac{w_s}{2D_x} - \frac{\sqrt{\gamma} w}{D_s} \right) \right\} \left[ 2 \text{erf} \left( \frac{w_s}{2D_s} \right) \right] = e^{-1} \tag{11}
\]

Now by solving above equation for a given strip width \( w \), one can get the relationship between profile width \( w \) and \( D_s \), which in turn is related to \( h \) as \( D_x \) and \( D_s \) are related to each other. Hence for different stripe widths one obtains the possible waveguide profile depth, \( h \) corresponding to a waveguide width \( w \). Fig 1 shows the variation of \( h \) with \( w \).
for various stripe widths (corresponding to a typical value of $D_{oh}=D_{ov}=0.023 \text{cm}^2/\text{s}$). Keeping this constraint in mind $\eta_x$ and $\eta_y$ have to be maximized.

From x slab: $\eta_x$ is a function of $w, \alpha_x$ and $\omega_f$ i.e.,

$$\eta_x = G[w, \alpha_x(V'), \omega_f]$$

(12)

As $\omega_f$ is known, $\eta_x$ is optimized by an appropriate choice of $\alpha_x$. Once $\alpha_x$ is chosen for a given $w$, $X(x)$ is now defined and $\Delta n_x(w)$ can be obtained from the closed form relation of Eq (6). In an attempt to maximize coupling efficiency along the $x$ direction, $\eta_x$, to unity by an appropriate choice of $\alpha_x(V') = w/\omega_f$ for a typical communication fiber, we realized that the corresponding $w$ resulted in an $h$ which reduced efficiency in the $y$ direction $\eta_y$ to a small value. Hence, it was necessary to compromise on the choice of $w$; we restricted the choice so as to obtain $\eta_x > 0.90$. With this choice it became possible to find an appropriate $h$. Once $w$ and $h$ are defined, one can write

$$\Delta n_y = \Delta n \int g(x/w) X(x)^2 \, dx$$

so $\Delta n = \Delta n_y / P$ where $P$ is a constant and $\Delta n_y = \Delta n \int f(y/h) Y(y)^2 \, dy$ gives $\Delta n = \Delta n_x / Q(\Delta n_x)$. With these equations $\Delta n_y$ is obtained and hence $\Delta n$ and $Y(y)$ gives $\eta_y$ for optimum coupling efficiency. Fig. 2(a) and (b) shows the variation of $\Delta n$ with $w$ and $h$ at respectively at different values of strip widths.

Finally, Fig. 3 shows the product $\eta = \eta_x \eta_y$ as a function of profile width $w$ at different stripe widths. It is seen that maximum efficiency can be obtained at a stripe width of 2µm and profile width of 6µm corresponding to a profile depth of 5.89µm.
Thus this analysis gives us all the important parameters $h$, $w$ and $\Delta n$, required to define the refractive index profile of the desired diffused channel waveguide. Once the three parameters are known, the stripe thickness before diffusion $\tau$, diffusion time $t$ and the diffusion temperature $T$ can be defined as

$$t = \frac{D_y^2}{4D_{ov} \exp \left(\frac{-T_0}{T}\right)}$$  \hspace{1cm} (12)

$$\tau = \left(\frac{\Delta n}{d}\right)^{1/2} \cdot \frac{1}{2F_{erf} \left(\frac{w}{2D_x}\right) \sqrt{\pi D_y}}$$  \hspace{1cm} (13)

The fabrication parameters for the waveguide defined above are obtained as titanium stripe thickness before diffusion $\tau = 0.226 \mu m$, diffusion time $t = 7.65$ hrs and the diffusion temperature $T = 1027^\circ C$. By simulating this waveguide on BPMCAD$^{10}$ software and finding the coupling efficiency by simulation, we also confirmed that the above parameters corresponded to a maximum coupling efficiency of about 0.91.

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