Index profiling of anisotropic graded-index planar waveguides from effective indices

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We present a method for recovering the refractive-index profile of an anisotropic graded-index waveguide from the effective indices by using a cubic spline interpolation function. The first and second derivatives of cubic splines are continuous to ensure a smooth index profile, which is consistent with practical graded-index distributions. A straightforward iteration with an exact dispersion equation to verify the interpolated profile makes this method easy and reliable for application. This approach is proved by numerical analysis of several typical index distributions and experimental examples showing that the refractive-index profiles in anisotropy can be reconstructed close to the exact profile. Waveguides with both more modes (more than four guiding modes) and fewer modes (two to four) can be universally profiled with good accuracy. © 2005 Optical Society of America

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1. INTRODUCTION

The refractive-index profile plays a crucial role in a graded-index waveguide, as it can provide significant information about the waveguide's propagation properties; thus determination of the profile has attracted considerable interest. Besides isotropic optical waveguides, anisotropic materials such as $LiNbO_3$, $LiTaO_3$, and $KTiOPO_4$ (KTP) have also been widely used to fabricate optical waveguides.[1–7] The most commonly used methods, such as the inverse Wentzel–Kramers–Brillouin (IWKB) method[8] and the improved IWKB method,[9] are employed to reconstruct the index profile from measured effective indices. However, WKB theory is an approximate method appropriate only for the analysis of isotropic waveguides, so that it will unavoidably limit the accuracy of the inverse methods and will restrict their application to the TM mode of anisotropic waveguides. When the mode number is less than five, usually the IWKB method cannot yield reliable results. In this paper an interpolation method using a cubic spline function,[10] based on an exact analytic transfer matrix (ATM) method,[11] is introduced to recover the refractive-index profile from the effective indices. The cubic splines have a profile that is quite smooth, and the first and second derivatives at each interpolation point are continuous. With an iterative procedure this method can recover the exact index profile with rather good accuracy.

2. RECOVERY PROCESS

A. Exact Analysis for Anisotropic Graded-Index Waveguide

In an anisotropic planar waveguide, when the principal axes of anisotropy are parallel to the rectangular axes in the coordinate system of the waveguide, the dielectric tensor can be depicted in diagonal form as

$$\varepsilon = \varepsilon_0 \begin{pmatrix} {n_x}^2 & 0 & 0 \\ 0 & {n_y}^2 & 0 \\ 0 & 0 & {n_z}^2 \end{pmatrix}, \qquad (1)$$

where ε_0 is the permittivity in free space and n_x, n_y, and n_z are the refractive indices for the electrical field polarized parallel to the x, y, and z axes of the coordinate system, respectively. In the following analysis we take the z axis as the propagation direction and assume that the refractive index varies with the x axis and that the waveguide materials are lossless.

For graded-index anisotropic planar waveguide with a refractive-index profile of the arbitrary form

$$n_x(x) = \begin{cases} n_{sx} + \Delta n_x f_1(x/D_1) & (x \geqslant 0) \\ n_{cx} & (x < 0) \end{cases},$$

$$n_y(x) = \begin{cases} n_{sy} + \Delta n_y f_2(x/D_2) & (x \geqslant 0) \\ n_{cy} & (x < 0) \end{cases},$$

$$n_z(x) = \begin{cases} n_{sz} + \Delta n_z f_3(x/D_3) & (x \geqslant 0) \\ n_{cz} & (x < 0) \end{cases}, \qquad (2)$$

where n_{sx}, n_{sy}, n_{sz} and n_{cx}, n_{cy}, n_{cz} are the refractive indices of the substrate and the cover layer, respectively, $\Delta n_x, \Delta n_y$, and Δn_z are index modulations and $f_1(x/D_1)$, $f_2(x/D_2)$, and $f_3(x/D_3)$ are index profile functions, as shown in Fig. 1, the dispersion equation can be obtained based on an ATM method in explicit form as

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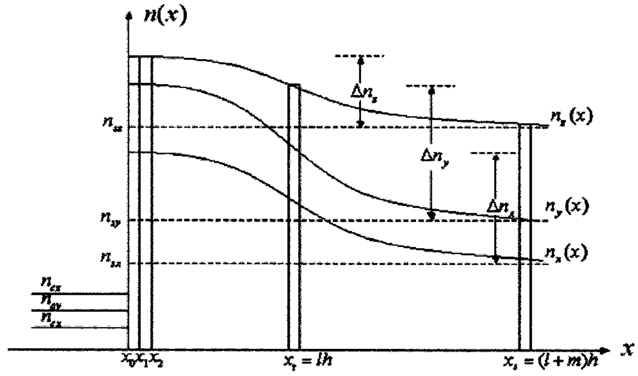

Fig. 1. Graded-index anisotropic planar waveguide with arbitrary index profile.

$$\int_0^{x_t}\kappa(x)\mathrm{d}x+\int_0^{x_t}\frac{p(x)f(x)}{p^2(x)+\kappa^2(x)}\left|\frac{\mathrm{d}[\kappa(x)/f(x)]}{\mathrm{d}x}\right|\mathrm{d}x$$
$$=N\pi+\tan^{-1}\left[\frac{f_0}{f_c}\frac{p_c}{\kappa_0}\right]+\frac{\pi}{2}(N=0,1,2,\ldots). \quad (3)$$

Here x_t is the turning point, and the propagation constant β can be calculated from $\beta=k_0n_x(x_t)$ (for the TM mode) or $\beta=k_0n_y(x_t)$ (for the TE mode):

$$\kappa(x)=\begin{cases}\kappa^{\mathrm{TM}}(x)=\dfrac{n_z(x)}{n_x(x)}[k_0{}^2n_x{}^2(x)-\beta^2]^{1/2} & \text{TM mode}\\ \kappa^{\mathrm{TE}}(x)=[k_0{}^2n_y{}^2(x)-\beta^2]^{1/2} & \text{TE mode}\end{cases}.$$

The function $p(x)$ is determined by the differential equation

$$\frac{\mathrm{d}[p(x)/f(x)]}{\mathrm{d}x}=\frac{\kappa^2(x)+p^2(x)}{f^2(x)},\quad p(x_t)=p_t.$$

Here

$$f(x)=\begin{cases}n_z{}^2(x) & \text{TM mode}\\ 1 & \text{TE mode}\end{cases}.$$

Beyond x_t, p_t is characterized as an equivalent attenuation vector; $f_0=f(0)$, $\kappa_0=\kappa(0)$, and

$$p_c=\begin{cases}p_c^{\mathrm{TM}}=\dfrac{n_{cz}}{n_{cx}}(\beta^2-k_0{}^2n_{cx}{}^2)^{1/2} & \text{TM mode}\\ p_c^{\mathrm{TE}}=(\beta^2-k_0{}^2n_{cy}{}^2)^{1/2} & \text{TE mode}\end{cases},$$

$$f_c=\begin{cases}n_{cz}{}^2 & \text{TM mode}\\ 1 & \text{TE mode}\end{cases}.$$

More details about this ATM analysis of anisotropic graded-index waveguides are in presented Ref. 11.

B. Smooth Interpolation with Cubic Spline Functions

The index profile is recovered from a series of effective indices $n_i(i=1,2,\ldots,k)$ of the graded-index waveguide, which can be measured by the m-lines method.[12] A set of increasing coordinates $x_i(i=1,2,\ldots,k)$ is assigned arbitrarily to mode index $\{n_i\}$, and the surface index is $n_0(x=0)$, which is unknown and should be determined. Now we have a sets of points $[(n_0,0),(n_1,x_1),(n_2,x_2),\ldots,(n_k,x_k)]$. These points can be interpolated by cubic spline functions with a smooth profile. In order to work out the unknown surface index n_0, the point (n_1,x_1) is selected from the sets of points. So Thus the series of points $[(n_0,0),(n_2,x_2),\ldots,(n_k,x_k)]$, except point (n_1,x_1), are used to fit the cubic splines. When $x\geqslant x_k$, an exponentially attenuated profile is assumed; thus, according to the interpolation theory for the cubic spline function, the index profile can be described as follows:

$$n(x)=M_0\frac{(x_2-x)^3}{6h_1}+M_2\frac{x^3}{6h_1}+\left(n_0-\frac{M_0h_1{}^2}{6}\right)\frac{x_2-x}{h_1}$$
$$+\left(n_2-\frac{M_2h_1{}^2}{6}\right)\frac{x}{h_1},\quad 0\leqslant x\leqslant x_2,$$

$$n(x)=M_i\frac{(x_{i+1}-x)^3}{6h_i}+M_{i+1}\frac{(x-x_i)^3}{6h_i}+\left(n_i-\frac{M_ih_i{}^2}{6}\right)\frac{x_{i+1}-x}{h_i}$$
$$+\left(n_{i+1}-\frac{M_{i+1}h_i{}^2}{6}\right)\frac{x-x_i}{h_i},$$

$$x_i\leqslant x\leqslant x_{i+1},\ i=2,3,\ldots,k-1,$$

$$n(x)=n_s+b\exp(-ax),\quad x\geqslant x_k, \quad (4)$$

where $h_1=x_2$, $h_i=x_{i+1}-x_i$ $(i=2,3,\ldots,k-1)$, and $M_i(i=0,2,\ldots,k)$ is the second derivative of $n(x)$ at the sets of points $[(n_0,0),(n_2,x_2),\ldots,(n_k,x_k)]$; n_s is the refractive index of the substrate. Parameters a and b of the exponential profile beyond x_k are determined by two points $[(n_k,x_k),(n_{k+1},x_{k+1})]$, where $x_{k+1}\gg x_k$ and $n_{k+1}=n_s+\varepsilon$; ε is very small. It is proved by calculation that an x_{k+1} of $5x_k$ to $10x_k$ and ε of 1×10^{-10} to 1×10^{-7} will have little influence on the final results. Reasonably and technically, we set $x_{k+1}=5x_k$ and $\varepsilon=1\times10^{-7}$. The series of second derivatives M_i $(i=0,2,\ldots,k)$ is determined by the following system of linear equations:

$$\begin{bmatrix}2 & 1 & & & \\ \mu_2 & 2 & \gamma_2 & & \\ & \ddots & \ddots & \ddots & \\ & & \mu_{k-1} & 2 & \gamma_{k-1}\\ & & & 1 & 2\end{bmatrix}\begin{pmatrix}M_0\\ M_2\\ \vdots\\ M_{k-1}\\ M_k\end{pmatrix}=\begin{pmatrix}d_0\\ d_2\\ \vdots\\ d_{k-1}\\ d_k\end{pmatrix}, \quad (5)$$

where

$$\mu_i=\frac{h_{i-1}}{h_{i-1}+h_i},\quad \gamma_i=1-\mu_i(i=2,3,\ldots,k-1),$$

$$d_0=\frac{6}{h_1}\left[\frac{n_2-n_0}{h_1}-n'(0)\right],$$

and $n'(0)$ is the first derivative of $n(x)$ at the surface $x=0$; $n'(0)$ will be given and may be changed, which will be discussed in detail below. Here

$$d_2 = 6\frac{\frac{n_2-n_0}{h_1} - \frac{n_3-n_2}{h_2}}{-x_3}, \tag{6}$$

$$d_i = 6\frac{\frac{n_i-n_{i-1}}{h_{i-1}} - \frac{n_{i+1}-n_i}{h_i}}{x_{i-1}-x_{i+1}}, \quad i=3,\ldots,k-1, \tag{7}$$

$$d_k = \frac{6}{h_{k-1}}\left[n'(x_k) - \frac{n_k-n_{k-1}}{h_{k-1}}\right], \tag{8}$$

where $n'(x_k)$ is the first derivative of $n(x)$ at $x=x_k$, which is equal to the first derivative of the exponential profile at $x=x_k$ under the continuous condition, and $n'(x_k)=-ab\exp(-ax_k)$.

Because the surface index n_0 is unknown, we need another known condition added to the system of linear equations so that all of the unknown parameters can be solved. This added condition is that the point (n_1,x_1) lies on the curve from $(n_0,0)$ to (n_2,x_2), which can be depicted as

$$n_1 = M_0\frac{(x_2-x_1)^3}{6h_1} + M_2\frac{{x_1}^3}{6h_1} + \left(n_0 - \frac{M_0{h_1}^2}{6}\right)\frac{x_2-x_1}{h_1} + \left(n_2 - \frac{M_2{h_1}^2}{6}\right)\frac{x_1}{h_1}. \tag{9}$$

Finally, for an arbitrarily given series of $\{x_i\}$, the index distribution can be fitted with a very smooth profile according to the continuous first and second derivatives of all cubic spline functions, even at the interpolation points $[(n_2,x_2),(n_3,x_3),\ldots,(n_{k-1},x_{k-1})]$.

C. Iterative Recovery Process

For an anisotropic waveguide, the TE mode indices are determined only by the profile of $n_y(x)$, as is implied in Eq. (3), whereas the TM mode indices are jointly decided by $n_z(x)$ and $n_x(x)$. From a series of measured TE or TM mode indices, $n_y(x)$ or $n_x(x)$ can be interpolated with the cubic spline function introduced above. The profile of $n_z(x)$ needs to be investigated for a practical situation, and it might be equal or a partial to $n_x(x)$ or $n_y(x)$, depending on the waveguide fabrication processes. Thus, for an arbitrarily given series of $\{x_i\}$, the profile of $n_x(x)$ or $n_y(x)$ and $n_z(x)$ can be obtained with interpolation and practical assumptions. Then we use the dispersion equation given in Subsection 2.A to solve the interpolated index distribution, and we get a new series of corresponding effective indexes $n_i^{\mathrm{cal}}(i=0,1,\ldots,k)$. Simultaneously, a new series of $\{x_i\}$ is obtained by calculation. We define and calculate the departure of the effective indices between calculated values and exact values as $\Delta=\Sigma_{i=0}^{k}(n_i^{\mathrm{cal}}-n_i)^2$. We can evaluate this deviation; if it is still large enough, we substitute the new series of $\{x_i\}$ into Eq. (4), and a new index profile can be fitted by interpolation onto the new series of points. The Series's effective indexes $\{n_i^{\mathrm{cal}}\}$ and $\{x_i\}$ can be determined by solution of the new index distribution in the waveguide by the ATM method. Repeating the above approach, the deviation Δ will become smaller and smaller; that is, this iteration process is convergent, and the profile is approaching the real profile. When Δ is close to zero, the refractive-index profile is finally acquired.

It should be noted that for facility in the iteration procedure the initial series of $\{x_i\}$ should be chosen so that the waveguide of the fitting profile has enough guiding modes. We can choose $\{x_i\}$ as an arithmetic series, and the interval is chosen to be 5λ–8λ, where λ is the wavelength in air.

In the previous discussion we noted that $n'(0)$, the first derivative of $n(x)$ at the surface $x=0$, is given and may be altered. For a given $n'(0)$, the obtained profile may be impractical. Because the second derivative can reflect the concave and the convex character of the curve, the practicability of the index distribution can be judged by investigation of the series of second derivatives M_i $(i=0,2,\ldots,k)$, because for a practical refractive-index profile the signs of $\{M_i\}$ have special rules. By careful investigation of numerous practical graded-index profiles, we propose the following criteria; either (1) every sign of $\{M_i\}$ before the first positive sign should be negative, and every sign of $\{M_i\}$ after the first positive sign should be positive, or (2) all signs of $\{M_i\}$ are positive.

As we know, for most graded-index profiles, such as Gaussian, error-function, Fermi, and exponential profiles, $n'(0)\leq 0$. First we set $n'(0)=0$, and under this value we can get a convergent profile. Then, if the signs of $\{M_i\}$ in the profile satisfy the criteria, the practical index profile is achieved; if the signs of $\{M_i\}$ don't satisfy the criteria, $n'(0)$ should be decreased until $\{M_i\}$ from the calculated profile meet the criteria. Simulation results prove that from a series of effective indexes $\{n_i\}$ the index distribution can be precisely recovered, very close to the exact profile, with the iteration approach and the proposed criteria.

3. NUMERICAL RESULTS AND COMPARISONS

To investigate the reliability of this method, we give some typical examples of Ti-diffused and annealed proton-exchanged (APE) lithium niobate waveguides with Gaussian and error-function profiles. The cover layer is air with an index of $n_a=1.0$. All numerical simulations are performed with a wavelength of 0.6328 μm. First we consider Ti-diffused Z-cut lithium niobate waveguides with index distributions of Gaussian profile. Lithium niobate is an uniaxial crystal; thus for a Z-cut sample $n_x(x)=n_e$, $n_y(x)=n_z(x)=n_o$, and for an X-cut sample $n_y(x)=n_e$, $n_x(x)=n_z(x)=n_o$. Ti-diffusion technology will universally increase the ordinary and the extraordinary refractive indices, so a Ti-diffused waveguide will support both TE and TM modes. As mentioned above, the TE mode indices are determined by only the profile of $n_y(x)$; thus $n_y(x)$ can be recovered first. From the relation $n_y(x)=n_z(x)$, the profile of $n_z(x)$ is immediately obtained; then $n_x(x)$ can be recovered from the TM mode indices, as there is only one unknown variable left in Eq. (3) for the TM mode. The first example of a Ti-diffused lithium niobate waveguide is given by[13] $n_y(x)=n_z(x)=n_o=2.286+0.009\exp(-x^2/D^2)$, $n_x(x)=n_e=2.2+0.014\exp(-x^2/D^2)$, where $D=4.5$ μm supports four TM and three TE modes, and $D=3$ μm supports two TM and two TE modes. The recovered results are shown in Figs. 2(a) and 2(b), respectively. It can be seen that the recovered profiles agree quite well with the exact distributions, although there are only two to four guiding modes, especially in the guiding region. In Fig. 3 the profile calculated beyond the last mode does not coincide with the real situation very well because an exponential distribution of the mode field is assumed beyond the last guide mode.

The next examples are implemented in APE lithium niobate waveguides with Gaussian and error-function profiles. The Proton-exchange process increases the extraordinary index in the guiding layer but decreases the ordinary index; thus only TM modes can be stimulated in Z-cut samples and TE modes in X- and Y-cut substrates. As no mode will be guided in the ordinary index profile, accurate determination of the ordinary index distribution will require other techniques, such as transmission spectrum analysis and radiation mode measurement.[14,15] After annealing, the typical change of the ordinary index Δn_o is approximately -0.2–$0.4\,\Delta n_e$, and we set $\Delta n_0 = -(1/3)\Delta n_e$ in the following simulation. For an APE lithium niobate waveguide with the profile[13] $n_e = 2.2 + 0.01\exp(-x^2/5^2)$, $n_o = 2.286 - 0.004\exp(-x^2/5^2)$, a Z-cut sample will support four TM modes with effective indices of 2.2074, 2.2044, 2.2020, and 2.2004, and an X-cut sample will support four TE modes with effective indices of 2.2074, 2.2043, 2.2018, and 2.2003. The recovered profiles of the two samples are shown in Figs. 3(a) and 3(b), respectively. Figure 3(c) exhibits the results of another

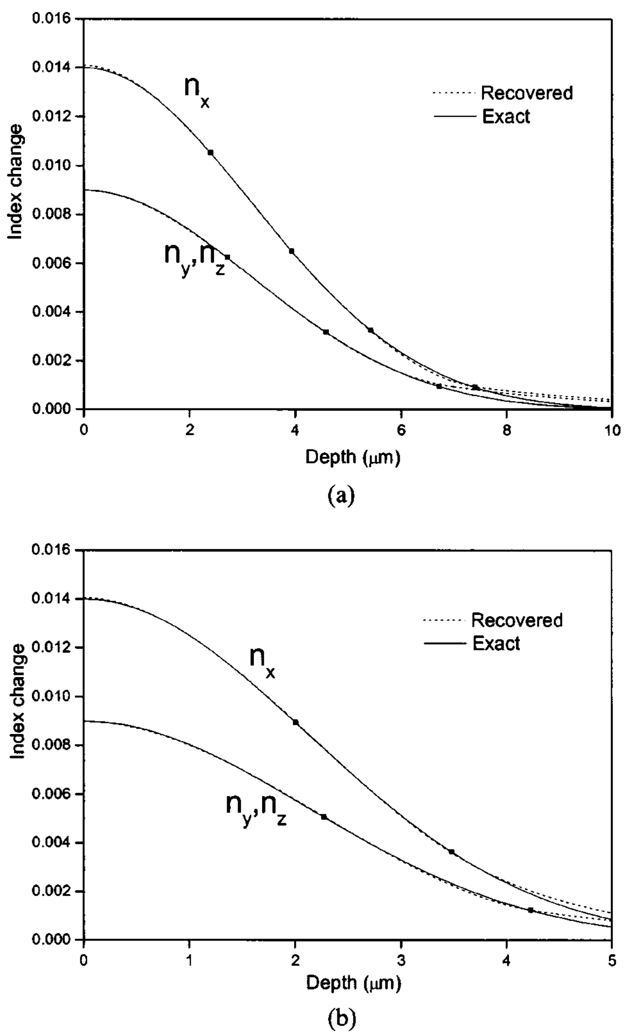

Fig. 2. Gaussian distribution and recovered index profiles of Ti-diffused Z-cut lithium niobate waveguides. (a) $D = 4.5\ \mu$m, supporting four TM and three TE modes; (b) $D = 3\ \mu$m, supporting two TM and two TE modes.

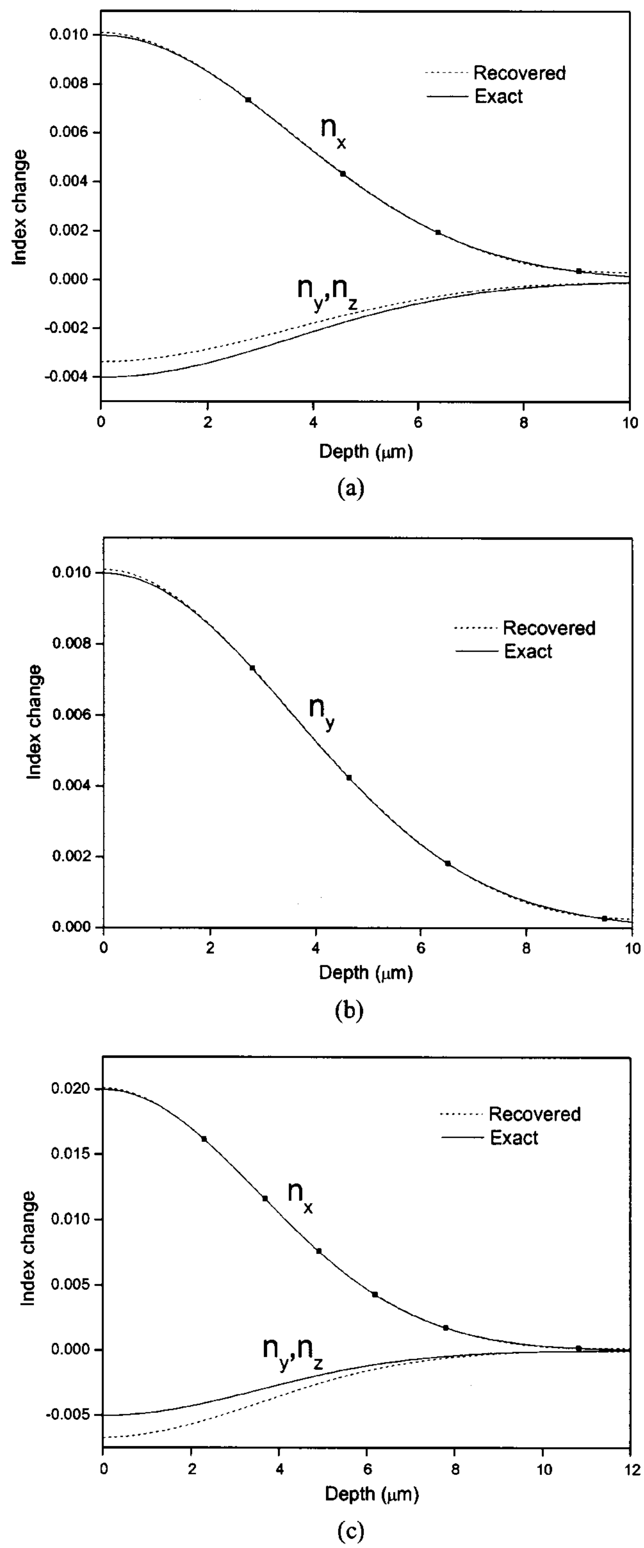

Fig. 3. Gaussian distribution and recovered index profiles of APE lithium niobate waveguides. (a) Z-cut, four TM modes; (b) X-cut, four TE modes; (c) Z-cut, six TM modes.

Z-cut APE waveguide with a profile of $n_e = 2.2 + 0.02 \times \exp(-x^2/5^2)$, $n_o = 2.286 - 0.005\exp(-x^2/5^2)$, which can support six TM modes. As depicted in the three graphs, the recovered extraordinary index profiles are also in good agreement with the exact distributions. The departure is greater in the ordinary index profiles because no mode information for the ordinary index distribution is given. A Z-cut APE lithium niobate waveguide with an error-function profile is further introduced to investigate the reliability of the current method. The error-function profile is given by

$$n_e(x) = 2.2 + \frac{\Delta n}{2}\left[\mathrm{erf}\left(\frac{0.9+x}{3.5}\right) + \mathrm{erf}\left(\frac{0.9-x}{3.5}\right)\right] \Big/ \mathrm{erf}\left(\frac{0.9}{3.5}\right),$$

$$n_o(x) = 2.286 - 0.25 \times \frac{\Delta n}{2}\left[\mathrm{erf}\left(\frac{0.9+x}{3.5}\right) + \mathrm{erf}\left(\frac{0.9-x}{3.5}\right)\right] \Big/ \mathrm{erf}\left(\frac{0.9}{3.5}\right),$$

with $\Delta n = 0.04$ stimulating five TM modes and $\Delta n = 0.01$ stimulating three TM modes. Similar good results are

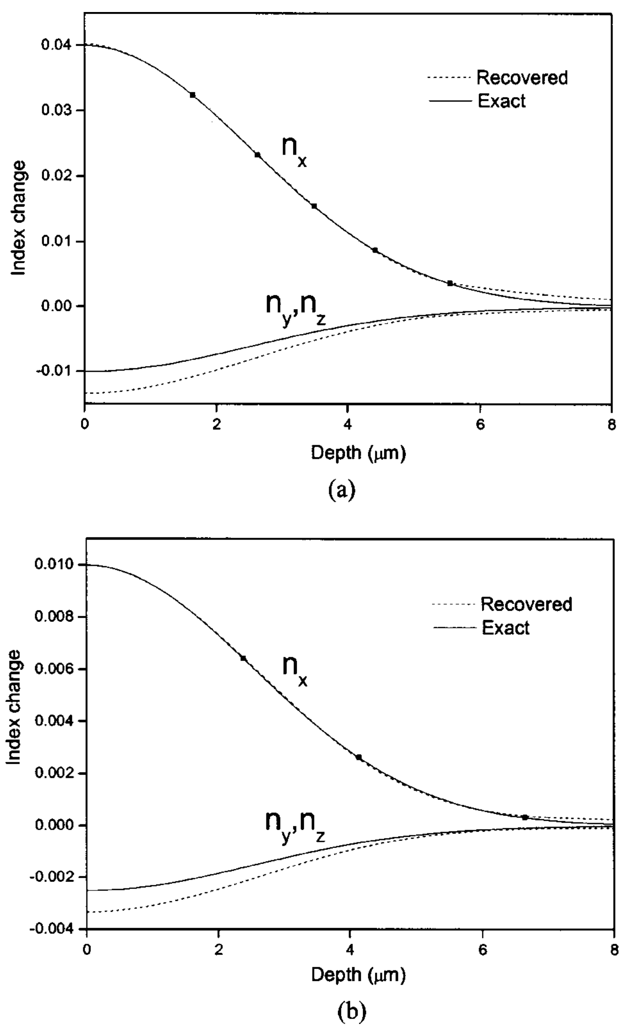

Fig. 4. Error function distribution and recovered index profiles of APE lithium niobate waveguides. (a) $\Delta n = 0.04$, supporting five TM modes; (b) $\Delta n = 0.01$, supporting three TM modes.

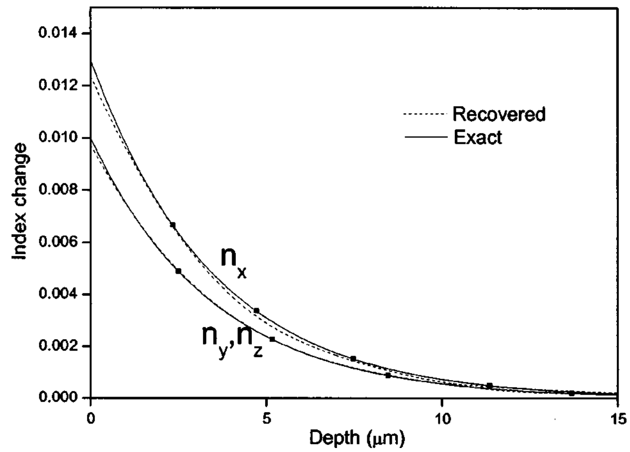

Fig. 5. Exponential distribution and recovered index profiles of a hypothetical Z-cut lithium niobate waveguide, supporting four TE and four TM modes.

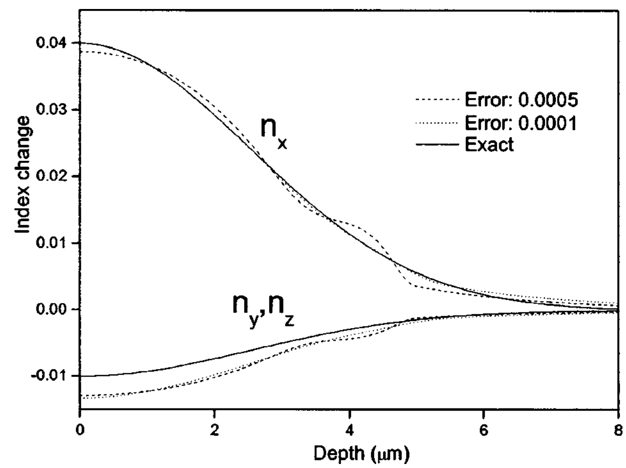

Fig. 6. Recovered error function profiles with errors of 1×10^{-4} and 5×10^{-4} added to even-order mode indices.

separately depicted in Figs. 4(a) and 4(b), where good agreement can be also seen between the recovered and the exact extraordinary index profiles. To further testify the to universality of the technique, we assume an exponential profile in a Z-cut lithium niobate waveguide, as $n_y(x) = n_2(x) = n_o = 2.286 + 0.01\exp(-x/3.5)$, $n_x(x) = n_e = 2.2 + 0.013\exp(-x/3.5)$, which can guide four TE and four TM modes. As can be seen in Fig. 5, the retrieved results also agree quite well with the real profiles.

As the experimental values measured usually have inevitable errors, it is necessary to study the sensitivity of the current method to experimental errors. Generally, we artificially add errors of 1×10^{-4} and 5×10^{-4} to the even-order mode indices from the above error-function profile [Fig. 4(a), $\Delta n = 0.04$] for investigation. As is shown in Fig. 6, this method can stand a typical error of 1×10^{-4}. When the error increases, an oscillatory character is exhibited in the recovered profiles.

Finally, an experimentally fabricated Z-cut lithium niobate waveguide is profiled after diffusion of a 100-nm ZnO film at 1000°C for 45 min.[5] At 632.8 nm, three measured guiding mode indices for the ordinary refractive index are 2.2876, 2.2869, and 2.2864. Figure 7 gives the profile recovered from the measured indices by our method and the

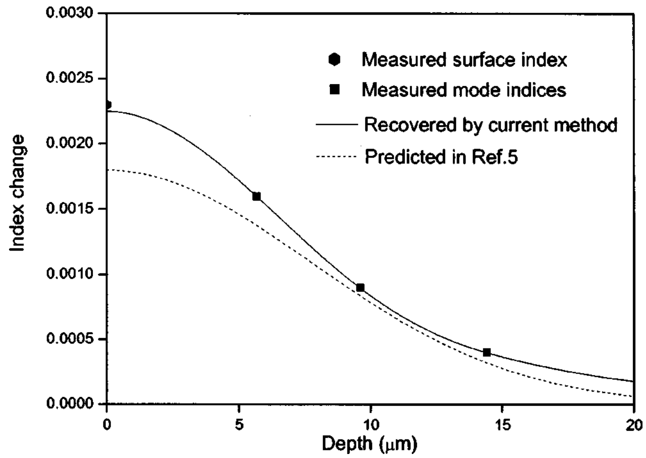

Fig. 7. Comparison of retrieved ordinary index profiles of a *Z*-cut lithium niobate waveguide diffused with 100-nm ZnO film at 1000°C for 45 min. The data are from Ref. 5.

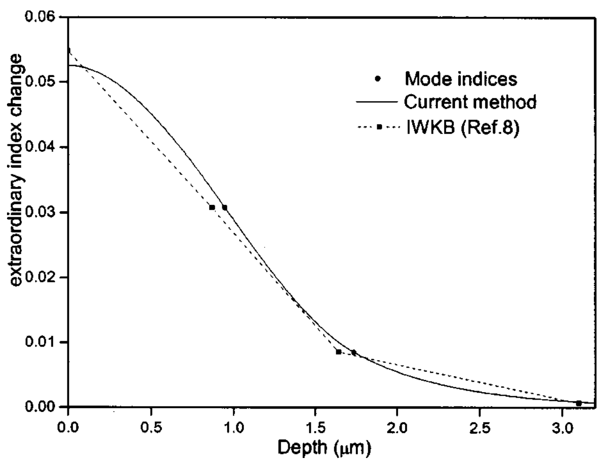

Fig. 8. Comparison of the recovery of the extraordinary index profile in an APE *Y*-cut lithium niobate waveguide obtained after proton exchange in benzoic acid at 230°C for 3 min and subsequent annealing at 350°C for 1 h in air.

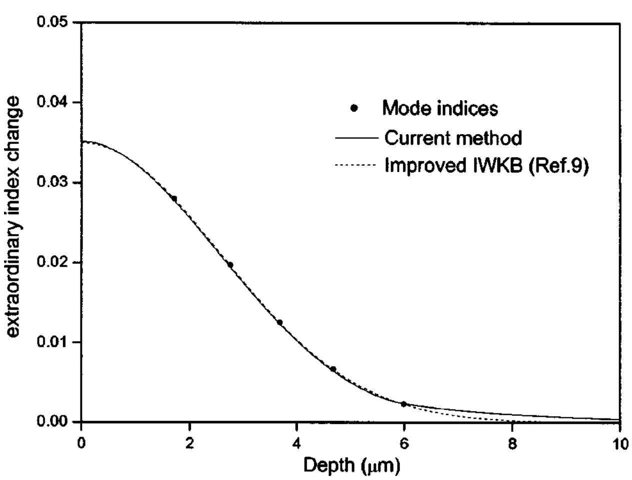

Fig. 9. Comparison of the recovery of the extraordinary index profile in an APE *Z*-cut lithium niobate waveguide proton exchanged in benzoic acid at 160°C for 10 h and subsequently annealed at 330°C for 24 h in air.

predicted profile from Ref. 5. The surface index change obtained by the current method is 2.2×10^{-3}, very close to the measured data of 2.3×10^{-3}. As is shown in Fig. 7, the predicted profile from Ref. 5 is quite different from the measured mode indices, and we believe the profile recovered by the current method with all experimental data is more credible, as long as the experimental data has good accuracy. The second experimental example is implemented in an APE *Y*-cut lithium niobate waveguide obtained after proton exchange in benzoic acid at 230°C for 3 min and subsequent annealing at 350°C for 1 h in air.[2] The extraordinary index profiles recovered by the current technique are compared with the IWKB method[8] in Fig. 8. We can see that the current method can yield more reliable results than the IWKB method in a waveguide with fewer modes. Figure 9 gives another example from an APE lithium niobate waveguide proton exchanged in benzoic acid at 160°C for 10 h and subsequently annealed at 330°C for 24 h in air, which can support five modes.[3] In the profiling of waveguides that can support more than four guiding modes, the improved IWKB method[9] usually can have good results. As is depicted in Fig. 9, our method can still deal well with such waveguides.

4. CONCLUSIONS

In conclusion, reliable recoveries of refractive-index profiles for different polarizations of graded-index anisotropic waveguides have been demonstrated. With cubic spline interpolation functions based on an exact ATM method and simple iterative approaches, the profiles can be smoothly recovered with good accuracy. This method can uniformly predict multimode waveguides with more modes and even with fewer modes reliably from the effective indices. The explicit analysis provides a reliable and convenient technique for the determination of the graded-index profile in an anisotropic planar waveguide.

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