# An Iterative Method for Optical Reconstruction of Graded Index Profiles in Planar Dielectric Waveguides

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***Abstract*—A nondestructive technique for the reconstruction of refractive index profiles in planar waveguides is presented and analyzed. The approach is based on the integral scattering equations, which permit to relate the refractive index of an inhomogeneous layer to the reflected field intensity at different incidence angles. From this formulation, an iterative algorithm is developed, such as at each iteration step the problem is formulated as the minimization of a functional representing the error between the measurements and the model data. The recovered profile is then used to improve the validity of the approximation in performing the next step. In this approach, the unknown index profile is represented as the sum of a finite series of basis functions avoiding to select *a priori* the particular functional form (e.g., Gaussian function, complementary error function, etc). The practical effectiveness of this approach is demonstrated by numerically simulating the measurements for different planar waveguides. The influence of measurement uncertainty and noise on the stability of the technique is also evaluated.**

***Index Terms*—Optical waveguides, refractive index profiling.**

## I. INTRODUCTION

THE CHARACTERIZATION of the refractive index profiles of planar waveguides has a fundamental importance for the determination of their optical properties. In fact, features such as band-width, mode pattern and coupling efficiency are related to the refractive index profile. Refractive index profiling also permits to study the "physics" of the waveguides fabrication process and to develop adequate analytical process models useful to relate the process itself to the optical parameters. Several methods have been developed in order to determine the waveguide refractive index: transmitted near-field intensity profiles [1]–[3], the measurements of effective indexes ("$m$-lines") [4]–[7], interferometric methods [8]. Recently, the ellipsometry has also been successfully employed, however a good agreement with "$m$-lines" method has been found only at depths above 0.5–0.6 $\mu$m [9].

Among these, the most widely used are the effective indexes measurements with different reconstruction algorithms: inverse Wentzel–Kramers–Brillouin (IWKB) [4], [5], finite differences methods [6], reflectivity methods [7]. However, when the number of the modes is low (e.g., single-mode waveguides) the reconstruction, using effective indexes measurements, becomes very difficult. In order to overcome this limitation, new techniques making use of a combination of the effective indexes measured for both mode types [transverse electric (TE) and transverse magnetic (TM)] and multiple wavelength methods, have been proposed; nevertheless, they have the disadvantage of requiring the knowledge of the dispersion properties of the waveguide substrate, as well as the dispersion properties of the coupling prism used to measure of the effective indexes [5].

In this paper, a nondestructive technique for the reconstruction of index profile in single- or multimode dielectric planar waveguides is presented and analyzed in detail. This technique allows the reconstruction of the refractive index profile of nonguiding structures as well, so representing a powerful tool in the characterization of the fabrication processes.

The approach is based on the scattering integral equations. In particular we expand the scattered field intensity in a power series about the reference profile and stop the series to the first-order term. This permits to linearly relate the field intensity reflected by the waveguide to the refractive index profile. Starting from this formulation a Newton–Kantorovitch type iterative algorithm is developed [10]. Differently from the reconstruction methods usually used in diffraction tomography, as the distorted Born iterative method (DBIM) [11], [12], which needs both the amplitude and phase of the reflected field, this new approach only requires the knowledge of the field intensity reflected by the sample, immersed in a suitable matching liquid, at different angles. At each iteration step the problem is formulated as the minimization of a quadratic functional representing the error between the measurements and the model data, the recovered profile is hence used to improve the validity of the approximation and to perform the next step. In order to carry out the minimization, the unknown refractive index profile is expressed as the sum of a finite number of polynomials. The choice of the above approach has two advantages: first it does not require to fix in advance the analytical form (e.g., Gaussian function, error function, etc.) [13] of the refractive index profile and it can be done without the need of a large number of unknowns, as usually happens when step functions are used (multilayer modeling) [12]. Second, it is not restricted to waveguides allowing to reconstruct also nonguiding structures.

The numerical simulations performed show the effectiveness of the method. Reconstructions in presence of noise have also been carried out in order to test the robustness of the algorithm.

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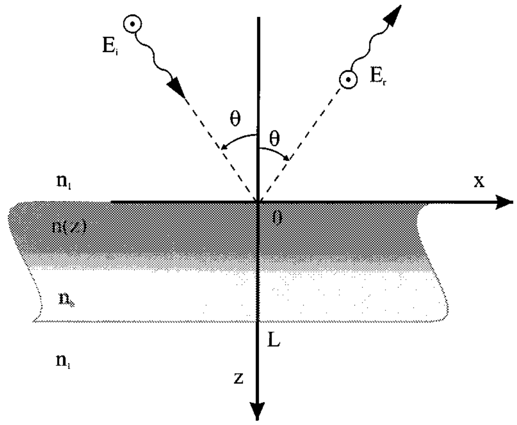


Fig. 1. Geometry of the problem.

## II. The Scattering Integral Equations

The waveguide considered is depicted in Fig. 1. It is immersed in a matching liquid with a refractive index $n_1$. The substrate and waveguide refractive indexes are $n_s$ and $n(z)$, respectively. The waveguide is illuminated, from an angle $\theta$ varying in the set $\Theta = [\theta_{\min}, \theta_{\max}]$, by a plane wave $E_i$ with the electric field vector perpendicular to the plane of incidence and wavelength $\lambda$ (in the vacuum).

The refractive index profile can be expressed as the superposition of a reference profile $n_b(z)$, also called "background profile," and a perturbation $\chi$, called "contrast function," defined as

$$\chi(z) = n^2(z) - n_b^2(z). \tag{1}$$

The total electric field $E_r$ reflected at a fixed distance $\bar{z}$ can be written as the sum of two contributions: the field reflected by the reference profile $E_b$ and the field reflected by the perturbation, called "scattered field" $E_s$

$$E_r(\bar{z};\theta) = E_b(\bar{z};\theta) + E_s(\bar{z};\theta) \quad \bar{z} < 0. \tag{2}$$

Using the integral formulation of the scattering, $E_s$ can be expressed as [14]:

$$E_s(\bar{z};\theta) = k_0^2 \int_0^L G(\bar{z}, z';\theta)\chi(z')E(z';\theta)\,dz' \tag{3}$$

where $k_0 = 2\pi/\lambda$ is the wavenumber of the vacuum, $G(\bar{z}, z';\theta)$ is the Green's function, that is the solution of following equation [14]:

$$\frac{\partial^2 G(z,z';\theta)}{\partial z^2} + n_b^2(z)k_0^2 G(z,z';\theta) = -\delta(z-z') \tag{4}$$

and $E$ is the total field inside the waveguide and the substrate, depending upon the contrast $\chi$ according to the equation [14]

$$E(z';\theta) = E_{ib}(z';\theta) + k_0^2 \int_0^L G(z', z'';\theta)\chi(z'')E(z'';\theta)\,dz'' \qquad 0 \le z \le L \tag{5}$$

$E_{ib}$ being the field inside the structure when only the reference profile exists.

Because the scattered field depends on the product between the contrast function $\chi$ and the total field $E$ [see (3)], and the latter depends also on the contrast [see (5)], the relation between the contrast function and the scattered field is nonlinear and difficult to solve. However, if $\chi(z) \ll n_b^2(z)$ (weak scattering approximation) it can be linearized by approximating the total internal field by $E_{ib}$ [14], so that (3) may be rewritten as

$$E_s(\bar{z};\theta) \cong E_{sl}(\bar{z};\theta) = k_0^2 \int_0^L G(\bar{z}, z';\theta)\chi(z')E_{ib}(z';\theta)\,dz'. \tag{6}$$

The last equation establishes a linear relationship between the scattered field (in the so-called distorted Born approximation) and the refractive index profile, and it has been widely used [14] in order to reconstruct the refractive index starting from the knowledge of $E_s$ at different wavelengths and/or different directions of incident field. However, the weak scattering approximation poses limits both on the difference between the refractive index profile and the reference profile and on its size [15]. In order to overcome these limits, several linear iterative techniques have been developed in literature [11], [12]. In particular, the distorted Born iterative method (DBIM), "equivalent" to the Newton–Kantorovitch method [16], has been used for the reconstruction of nonweak scattering profiles [12]. However, the reconstruction methods usually used in diffraction tomography (DBIM, etc.) [11], [12], [16] require the knowledge of the reflected field $E_s$, this implies that both amplitude and phase of the field must be measured. These requirements have limited the practical application of diffraction tomography at optical frequencies. In fact, this requires methods quite complicate from an experimental point of view [17], although the phase of the scattered field at optical wavelength can be indirectly measured. In order to overcome these disadvantages we have developed a new technique that requires only the knowledge of the reflected field intensity.

## III. Reconstruction Method

Let us consider the total intensity reflected by the sample

$$\begin{aligned} I(\theta) &= |E_r(\theta)|^2 = |E_b(\theta) + E_s(\theta)|^2 \\ &= |E_b(\theta)|^2 + 2\,\Re\text{e}\{E_s(\theta)E_b^*(\theta)E_b^*(\theta)\} + |E_s(\theta)|^2 \end{aligned} \tag{7}$$

where $\Re\text{e}\{\cdot\}$ denotes the real part of the corresponding complex argument.

If $\chi(z) \ll n_b^2(z)$, which implies to assume that the waveguide is a weak perturbation with respect to the reference profile, we can approximate $E_s$ with the scattered field $E_{sl}$ in the distorted Born approximation given by (6). Substituting $E_s \cong E_{sl}$ in (7) and neglecting the second-order term [the third term of left-hand side of (7)] we obtain

$$I(\theta) \cong |E_b(\theta)|^2 + 2\,\Re\text{e}\{E_{sl}(\theta)E_b^*(\theta)\}. \tag{8}$$

This expression represents a linear approximation of the reflected field intensity and can also be obtained by a direct linearization of the operator (7) through its expansion in a power series about the reference profile $n_b$ and stopping the series to the first-order term.

Equation (8) permits to linearly relate the refractive index profile to the reflected intensity and can be used in order to reconstruct the refractive index profile from the knowledge of the reflected intensity $I$. However, the weak perturbation poses limits on the reconstructable profiles similar to the ones posed by the distorted Born approximation. So a method just based on the solution of (8) is not reasonable for dielectric waveguide characterization.

Starting from these considerations a Newton–Kantorovitch type algorithm has been developed. The iterative algorithm starts from an initial reference profile and solve (8), the solution found is then used to improve the reference profile for the next linearization and so on.

Because no *a priori* assumptions are made on the unknown profile, we can choose, as starting reference profile, the refractive index profile existing before the waveguide fabrication

$$n_{b0}(z) = \begin{cases} n_1 & z < 0 \\ n_s & 0 \le z \le L. \\ n_1 & z > L \end{cases} \tag{9}$$

However, it must be underlined that in practical cases the substrate thickness falls usually in the millimeter range and the two substrate surfaces are not perfectly parallel to each other [18]. This means that, unless time consuming and complicate fabrication procedure are followed, the substrate cannot be regarded as a Fabry–Perot interferometer. In the above situation, the infinite series of reflections coming from the backside of the substrate does not emerge at the same angle as the reflection coming from the front surface [19]. A suitable detection apparatus (see Fig. 4) can easily filter out those stray beams, so that the substrate can be regarded as a semi-infinite.

The hypothesis of a semi-infinite substrate leads to assume the following reference profile:

$$n_{b0}(z) = \begin{cases} n_1 & z < 0 \\ n_s & z \ge 0 \end{cases}. \tag{10}$$

In this case, both the Green's function and internal total field have an analytical closed form [22].

The unknown refractive index profile is expressed as a superposition of a finite number $M$ of basis functions, defined in the region $D = [0, d]$ $(d \le L)$ where significant variation occurs

$$\chi(z') = \sum_{m=0}^{M} a_m P_m \left( \frac{z' - d/2}{d/2} \right) \quad z' \in D \tag{11}$$

$P_m$ being the Legendre polynomial of order $m$ [20]. The number $M$ of the Legendre polynomials and the extension $d$, used in the reconstruction procedure, can be "guessed" relying on the *a priori* information about the technological process employed to realize the profile under analysis [13]. Anyway, in order to take into account the unavoidable differences between the expected profile and the actual one, the "step-by-step" procedure illustrated in [21] can be used.

At each step, we have to find the solution of a linear system of equations

$$I_i = |E_b(\theta_i)|^2 + 2\,\mathrm{Re}\left\{ \sum_{m=0}^{M} a_m \gamma_m(\theta_i) E_b^*(\theta_i) \right\} \tag{12}$$

where

$$\gamma_m(\theta_i) = k_0^2 \int_0^d G(z, z'; \theta_i) E_{ib}(z'; \theta_i) P_m \left( \frac{z' - d/2}{d/2} \right) dz' \tag{13}$$

where $I_i$ being the field intensity samples, taken at $N$ different angles $\theta_i$ in the set $\Theta = [\theta_{\min}, \theta_{\max}]$, with $N \ge M$. The number of independent measurements $N$, useful for the reconstruction, can be estimated following the analysis performed in [22].

The solution of the system (12) is searched, in a least-squares sense, as the minimum of the following functional:

$$\Phi = \sum_{i=1}^{N} \frac{(F_i(\underline{a}) - I_i)^2}{I_i} \tag{14}$$

where $\underline{a} = (a_0, a_1, \ldots, a_M)$ and

$$F_i(\underline{a}) = |E_b(\theta_i)|^2 + 2\,\mathrm{Re}\left\{ \sum_{m=0}^{M} a_m \gamma_m(\theta_i) E_b^*(\theta_i) \right\}. \tag{15}$$

The functional $\Phi$ represents the "distance" between the field intensity samples and the calculated one for an estimated contrast profile $\chi$.

The recovered contrast profile $\chi_1$ is used to update the reference profile

$$n_{r1}(z) = \sqrt{n_{r0}^2(z) + \chi_1(z)}. \tag{16}$$

The updated reference profile is used to perform a new linearization of the operator (7) and calculate the Green's function and internal total field to be used in the next step [see (6)]. The procedure stops when the difference between two successive recovered profiles is negligible. The flowchart of the reconstruction algorithm is illustrated in Fig. 2.

The advantage of this technique is that the expansion of the unknown profile in basis functions allows to face the problem without fixing the shape of the doping profile itself. A polynomial base has been chosen in order to avoid the need of a large number of unknowns as usually happens when pulse functions are used (multilayer modeling) [12]. Furthermore, the method is not restricted to waveguides, it allows the reconstruction of the refractive index profile of nonguiding structures as well, so representing a powerful tool in the characterization of the fabrication processes.

Even if this approach permits to improve the reconstruction quality as compared to the Born methods [21], it presents some limits that are strictly related to the initial linear approximation. In fact, if the refractive index profile represents a too strong perturbation with respect to the starting reference profile, the algorithm could not converge, as for the DBIM [12]. The validity of the linear assumption can be improved by increasing the wavelength (leading to a decrease of the spatial resolution) or by a

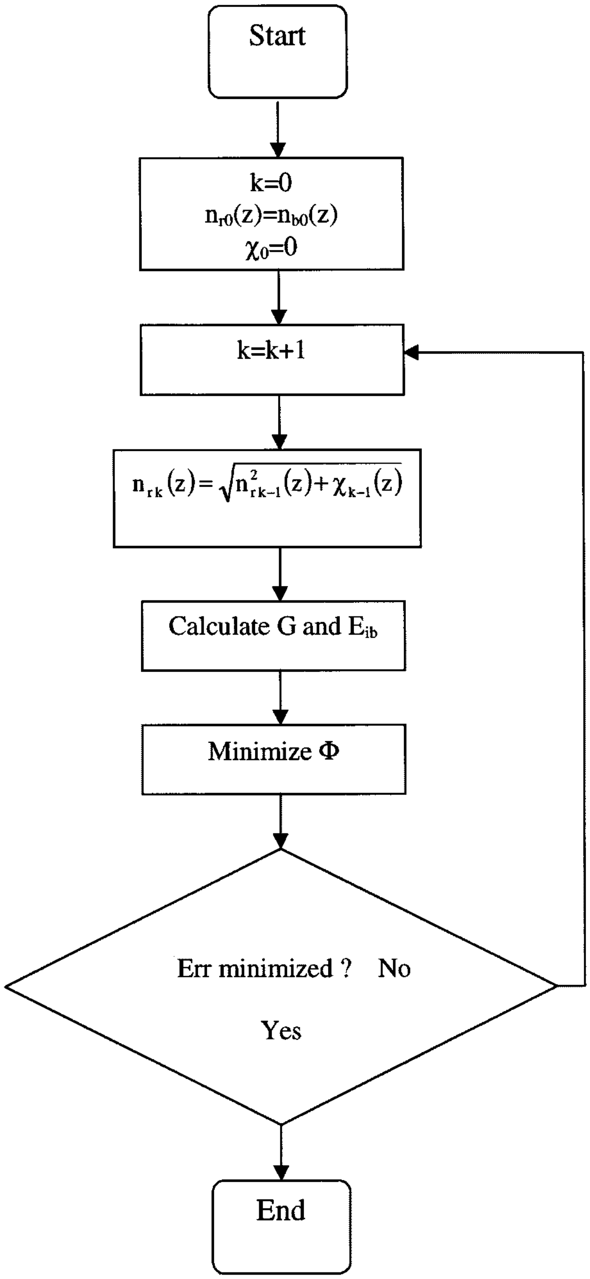


Fig. 2. Flow chart of the reconstruction algorithm.

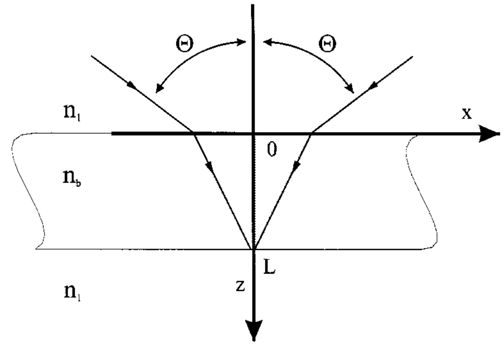


Fig. 3. Refraction effect at the interface between the substrate and the surrounding medium.

suitable choice of the starting reference profile (if *a priori* information on the unknown profile are available). In this work we have chosen to test the methods in the worst case assuming, as starting reference profile, the refractive index profile existing before the waveguide fabrication.

Before proceeding any further, let us briefly discuss the necessity of a matching liquid. Usually, in the literature, the unknown profile is supposed to be embedded in a homogeneous space (Born approximation). This means that in order to reproduce the above condition a suitable matching fluid, whose refractive index is as close as possible to the one of the substrate $n_s$, is needed [17], [23]. If we assume as the reference profile a nonhomogenous space near to the true profile, the matching liquid seems to be no longer necessary. However, the validity of the linear approximation depends not only on the product of the waveguide size and the refractive index difference between the waveguide itself and the reference profile (as it occurs in the Born approximation), but also on the refractive index difference between the substrate and the surrounding media [22]. This can be explained by taking into account for the refraction effect at the interface between the two media. In fact, in order to well reconstruct an index profile, it is necessary that the angle of view $\Theta$ approaches to $\pi/2$, however the refraction at the interface can induce a drastic reduction of the "effective" angle of view inside the substrate (see Fig. 3) [22]. The use of a matching liquid permits to overcome this problem and a suitable choice of it can also simplify the measurements. In fact, if the refractive index of the liquid is greater than the refractive index of the waveguide, the "effective" angle of view approaches to $\pi/2$ for $\Theta < \pi/2$. This allows to avoid the measurements at grazing incidence, which are difficult to perform. We would like to underline that measurements with matching fluids are often performed in the characterization of optoelectronic materials (see f.i. [8], [17], [23], [24]). Regarding our propose, a practical way to set up the experiment is shown in Fig. 4. This arrangement allows the rotation of the sample without the realignment of the detector, so it is particularly suitable for variable angle measurements. The optical system placed in front of the detector, made up by a couple of lenses and a field stop, guarantees an excellent off-axis rejection, so filtering out the spurious reflections from the backside of the substrate.

## IV. Numerical Results

The effectiveness of the proposed approach has been verified performing several reconstructions starting from synthetic measurements for different waveguides, with or without noise. We suppose that the waveguide analyzed was obtained by an ion-exchange process in a soda-lime glass substrate with a refractive index $n_s = 1.5115$. The wavelength of the incident field is $\lambda = 0.6328$ $\mu$m and the incident angle $\theta$ varies in the set $\Theta = [15°, 71°]$. The range of the incident angles and the number of the samples $N$ are estimated by the refraction index of the substrate, the refraction index of the matching liquid and the thickness of the reconstruction region $d$. A detailed analysis on the choice of the measurements angles and on the samples number useful for the reconstruction is performed in [22]. As a

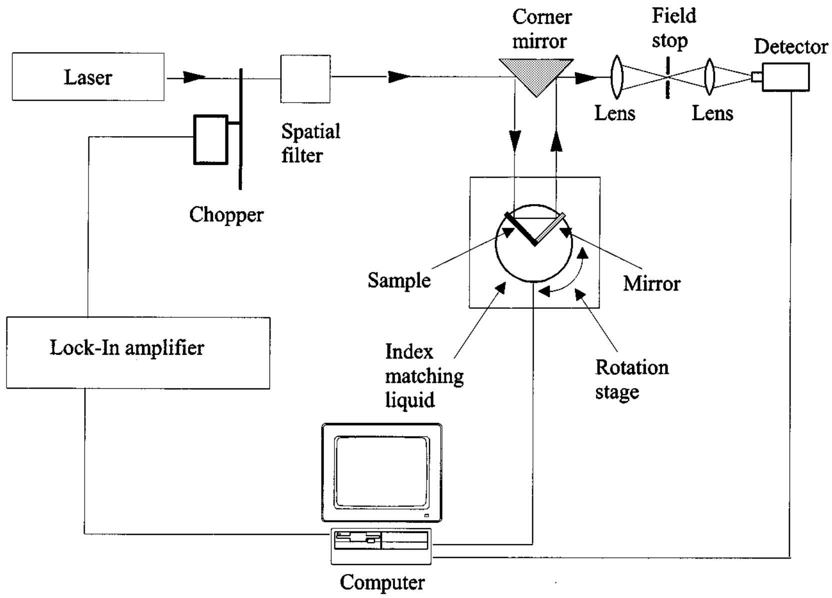


Fig. 4. Proposed experimental setup.

matching liquid a mixture of bromonaphtalene and ethanol [20] with a refractive index $n_1 = 1.5969$ is considered.

In the reconstruction procedure the number $M$ of the Legendre polynomials and the extension $d$ of the region where significant variation occurs have been "guessed" relying on the *a priori* information about technological process employed so that the estimated profile can be represented by means of the polynomials expansion with a rms error lower than 0.01%. This allows to avoid the necessity of a "step-by-step" procedure [21], so reducing the computational burden. In the case of ion-exchange process $M$ and $d$ can be easily estimated from the exchange time [13].

The waveguides considered are chosen in order to test the reconstruction algorithm with different index changes and different depths, so various doping ions ($Cs^+$, $Ag^+$, $K^+$) are employed.

In the first example, a $Cs^+/Na^+$ ion exchange is considered. In this case complementary error function profiles are obtained [13], in particular we assume as refractive index profile

$$n(z) = 1.5115 + 0.03\,\mathrm{erfc}\left(-\left(\frac{z}{\sigma}\right)^2\right)$$

with $\sigma = 1.2\ \mu$m.

The result of the reconstruction process, with $M = 7$ and $d = 3\ \mu$m, is depicted in Fig. 5. As it can be seen, the reconstructed profile agrees well with the exact one. In order to analyze the convergence characteristics of the results we have also performed the reconstruction changing the number $M$ from 3 up to 9. The results with $M = 3$ and $M = 4$ are depicted in Fig. 6. In Fig. 7 the mean square error versus the number $M$ of the Legendre polynomials used in the reconstruction procedure is plotted.

In the second case, a $Ag^+/Na^+$ ion exchange with a Gaussian profile is considered [13]. The assumed refractive index profile is

$$n(z) = 1.5115 + 0.085\exp\left(-\left(\frac{z}{\sigma}\right)^2\right)$$

with $\sigma = 0.7\ \mu$m.

In this case we choose $M = 8$ and $d = 2\ \mu$m. The result of the reconstruction process is depicted in Fig. 8.

Successively, we apply the technique to a refractive index profile obtained by a $K^+/Na^+$ ion exchange. The analyzed profile is

$$n(z) = 1.5115 + 0.0084\exp\left(-\left(\frac{z}{\sigma}\right)^2\right)$$

with $\sigma = 1.63\ \mu$m.

At the considered wavelength this profile supports only one propagation mode. In this case, $M = 8$ and $d = 4\ \mu$m have been used (see Fig. 9 curve $\#1$).

In order to show the capability of the technique in the fabrication process monitoring, we consider the same ion exchange process as above, but now the depth of the refractive index profile is smaller ($\sigma = 0.9\ \mu$m), as a consequence of a shorter exchange time. In this case we have that the profile obtained is a nonguiding structure so it cannot be characterized with other classical methods. The result of the reconstruction with, $M = 8$ and $d = 2.5\ \mu$m, is shown in Fig. 9 curve $\#2$. Furthermore, the influence of the refractive index variation on the reflected intensity is also shown in Fig. 9 where, in the inset, we report the intensity profiles as function of incidence angle corresponding to both the analyzed refractive index profiles.

Finally, we analyze the influence of the measurements uncertainty, which can limit the accuracy of the method. The principal limiting factors are the knowledge of the matching liquid and substrate refractive indexes, as well as the unavoidable measurement noise on the reflected intensity.

As far as the knowledge of the matching liquid refractive index is concerned, it is possible to measure its value, by means of commercially available high resolution refractometers, with an accuracy of $\pm 2 \cdot 10^{-5}$. We have verified that this error does not affect the reconstruction.

The problem of the substrate refractive index is slightly more complicate. In fact, the accuracy in the measurements of its refractive index achievable by standard techniques is about $\Delta n =$

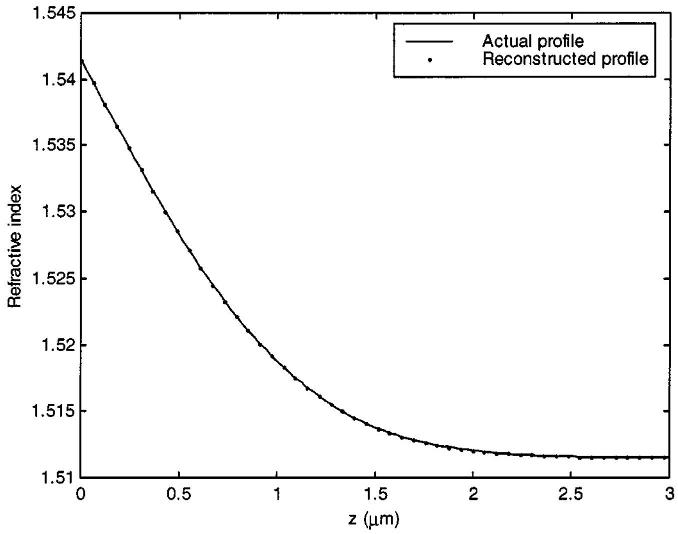


Fig. 5. Actual (solid line) and reconstructed (dotted line) refractive index profiles for the $Cs^{+}/Na^{+}$ waveguide.

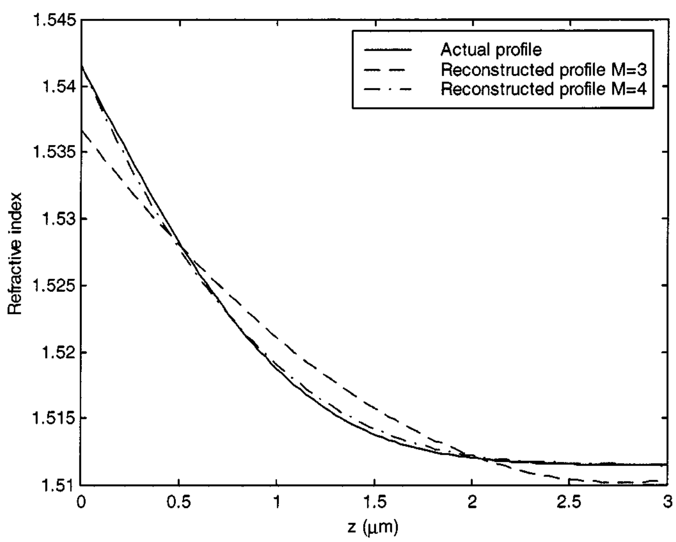


Fig. 6. Actual profile (solid line), reconstructed profile with $M = 3$ polynomials (dashed line) and reconstructed profile with $M = 4$ polynomials (dash dotted line) for the $Cs^{+}/Na^{+}$ waveguide.

$\pm 10^{-4}$ [8]. This can affect the profile reconstruction, as shown in Fig. 10, even if its influence is not serious and the algorithm is stable also when the uncertainty is greater than $10^{-4}$.

The stability of the reconstruction algorithm against noise presence has been verified by performing several reconstructions with uniform white noise added to the simulated measurements. A noise level of one or two percent is reasonable for this kind of measurements. Other authors have successfully performed measurements with about 2% of noise level [23]. Furthermore, we believe that a synchronous detection, as suggested in the experimental configuration of Fig. 4, is able to significantly improve the signal-to-noise ratio (SNR). In Fig. 11, the results of the reconstructions, for the $K^{+}/Na^{+}$ waveguide, with 0.5%, 1%, and 2% of noise are reported.

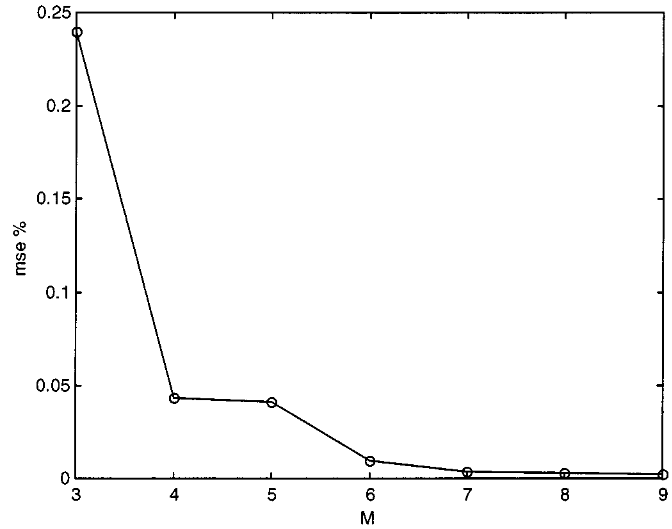


Fig. 7. Mean-square error (mse) versus the number $M$ of polynomial, used to represent the profile.

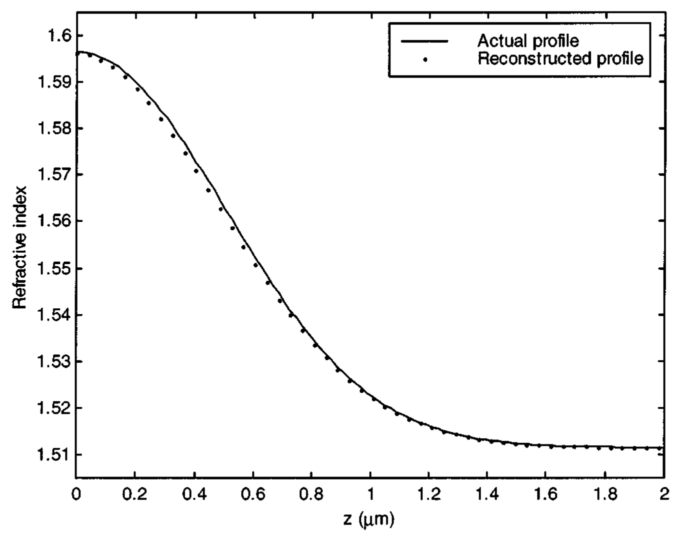


Fig. 8. Actual (solid line) and reconstructed (dotted line) refractive index profiles for the $Ag^{+}/Na^{+}$ waveguide.

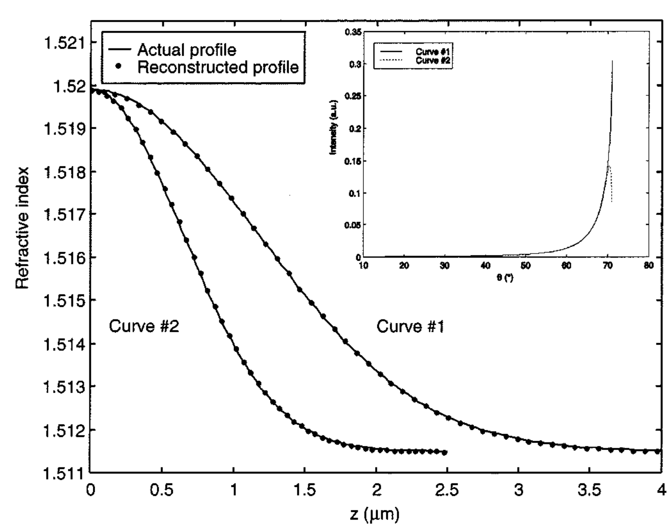


Fig. 9. Actual (solid line) and reconstructed (dotted line) refractive index profiles for the $K^{+}/Na^{+}$ waveguide (curve #1) and reconstructed profiles for the nonguiding structure (curve #2).

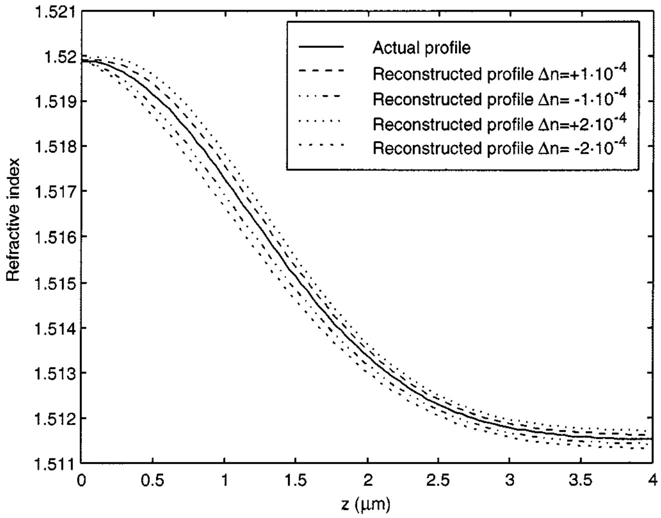


Fig. 10. Actual profile and reconstructed profiles with a substrate refractive index accuracy $\Delta n$ varying from $-2 \cdot 10^{-4}$ to $2 \cdot 10^{-4}$ for the $K^+/Na^+$ waveguide (curve #1).

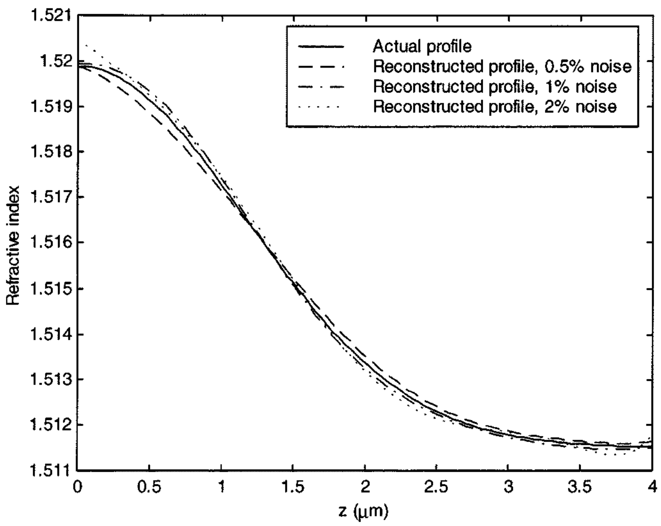


Fig. 11. Actual profile (solid line), reconstructed profile with 0, 5% noise (dashed line), reconstructed profile with 1% noise (dash dotted line), and reconstructed profile with 2% noise (dotted line) for the $K^+/Na^+$ waveguide.

## V. Conclusion

A new method useful for the characterization of planar waveguides and their fabrication processes is presented and analyzed. The approach is based on a Newton–Kantorovitch type iterative algorithm and requires only the knowledge of the field intensity reflected by the sample at different angles. The method permits to reconstruct the refractive index profile also of mono-modal waveguides and nonguiding structures without the *a priori* knowledge of its analytical expression. The numerical results show that the proposed approach is able to retrieve the refractive index profile with relatively high accuracy and that it is stable in presence of noise.

However, the waveguides that can be analyzed with this method should not represent a too strong perturbation with respect to the starting reference profile. If large waveguides must be characterized a suitable choice of starting reference profile is required.

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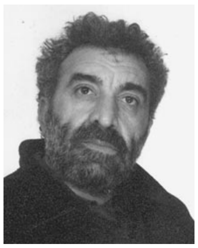

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