

Design and Analysis of Silicon Antiresonant Reflecting Optical Waveguides for Evanescent Field Sensor

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Abstract—Silicon based antiresonant reflecting optical waveguides (ARROW's) have been designed in order to obtain a high sensitive optical transducer for sensing applications. The designed sensor has an integrated Mach–Zehnder interferometer configuration. The optical waveguides that form its structure have to verify two conditions: monomode behavior and high surface sensitivity. In this paper, we present a theoretical modeling of the propagation characteristics and surface sensitivity of the ARROW structure.

Index Terms—Antiresonant reflecting optical waveguide (ARROW) theoretical design, evanescent wave sensors, Mach–Zehnder interferometer, silicon technology.

I. INTRODUCTION

ONE IMPORTANT step in the development of chemical sensors is the design and fabrication of a physical transducer capable of transform, in an efficient way, a chemical or biological reaction in a measurable signal [1]. There are several physical methods to obtain this transducing signal like those based on amperometric, potentiometric or acoustic systems. However, transducers that make use of optical principles offer more attractive characteristics such as the immunity to electromagnetic interference, the use in aggressive environments and, in general, a higher sensitivity. Moreover, optical sensors based on integrated optics add some other advantages as a better control of the light path by the use of optical waveguides, a higher mechanical stability and a reduced size. In sensors based on the evanescent field, although light travels confined within the optical waveguide, there is a part of the guided mode (called the evanescent field) that interacts with the surrounding environment. When there is a chemical reaction at the waveguide surface, as it can be understood as a refractive index variation, the evanescent field detects this change and induces a modification of the optical properties of the guided mode.

Among the different techniques to detect this variation, we have chosen an interferometric method based on the Mach–Zehnder configuration due to its higher sensitivity

compared to other schemes [2], [3]. For sensing use, the optical waveguides that form the Mach–Zehnder interferometer have to verify two conditions: a monomode behavior and a high surface sensitivity. These characteristics make crucial the design and analysis of the optical waveguides before their fabrication for the development of a high sensitive optical sensor.

In this paper, we will focus on the design of single-mode integrated optical waveguides with a very high surface sensitivity for their application in optical sensors. The waveguides are based on antiresonant reflecting optical waveguide (ARROW) structures and are fabricated with standard integrated circuit (IC) silicon technology. The fabrication and characterization of these sensors has been already performed and results will be published somewhere else.

II. THE ARROW STRUCTURE

The optical sensor is based on the ARROW structure [4]–[7]. The optical confinement of light in these waveguides is based on the total internal reflection at the air-core interface and a very high reflectivity, of 99.96%, at the two interference cladding layers underneath the core. The refractive indexes and thickness of these layers are designed in such a way that they behave as a Fabry–Perot resonator operating at its antiresonant wavelengths. This structure is a leaky waveguide (it does not support guided modes) that have an effective single-mode behavior, that means, higher order modes are filtered out by loss discrimination due to the low reflecting of the interference cladding. Other important features of this structure are that it presents low losses for the fundamental mode; it has polarization selective characteristics, that is, transverse magnetic (TM)-polarized light presents higher losses than transverse electric (TE)-polarized light; there is a large tolerance in the election of the refractive indexes and thickness of the cladding layers. The conventional ARROW—a structure based on silicon technology is depicted in Fig. 1: the core and second cladding are silicon oxide layers with a refractive index of 1.46 and the thickness of the second cladding is half of the core. The first cladding is a silicon nitride layer of $0.12 \mu\text{m}$ and a refractive index of 2.00.

This ARROW waveguiding concept came to solve the two main limitations of the conventional TIR (total internal reflection) waveguides: the reduced dimensions for monomode behavior (an important subject for further technological development and mass-production of the sensors) and the high insertion-losses in the optical-interconnects fiber-waveguide. With ARROW structures we can have monomode behavior with a

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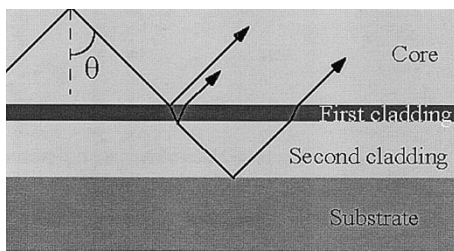


Fig. 1. Conventional ARROW—A structure.

core thickness of the same size as the core of a single-mode optical fiber, suitable for efficient end-fire coupling.

A. Design of the Optical Waveguide for Sensor Application

As we mentioned above, these ARROW structures will be the basis for an integrated evanescent field sensor based on the Mach–Zehnder interferometer. In its integrated version, an optical waveguide is split into two arms and after a certain distance they recombine again. Only one of the arms (sensor arm) will be exposed to the surrounding medium during a certain distance L (interaction length). For that reason, the interferometer has to be covered with a protective layer that will prevent any interaction between the interferometer and the outer medium. In the sensor arm, certain area of length L will be opened to bring into contact the waveguide and the environment. When a change in the refractive index of the outer medium takes place, light that travels through the sensor arm will experience a change in its propagation characteristics via the evanescent field. At the sensor output, light coming from both arms will interfere, showing a sinusoidal variation that can be directly related to the change of the refractive index in the surrounding medium. The protective layer is a 2- μm silicon oxide layer with a refractive index of 1.46. Therefore, the core refractive index has to be higher than 1.46 in order to obtain a guiding structure.

The homogeneity in the deposition processes of the different waveguide layers together with the small dimensions of the sensor (the interferometer arms are separated 100 μm) assures that the optical waveguides of the two interferometer arms are equal and, subsequently, the sensor response will only depend on the refractive index changes that take place at the sensor area. Moreover, a second area of length L can also be opened in the reference arm to keep the optical differences between the branches as small as possible. This will make the device potentially little sensitive to environmental fluctuations (i.e., temperature) that normally limit the performance of a Mach–Zehnder sensor.

Nowadays, as far as we know, there are not commercial programs available for the theoretical study of ARROW's, probably due to the leaky behavior of these structures. For that reason, we had to develop a home-made computational program based in one of the several theoretical methods available for the simulation of the propagation characteristics of the ARROW structure. Among them (multilayer analysis [8], perturbative methods [9], spectral index [10] or nonuniform finite difference method [11], etc.) the latter has demonstrated to have a greater computational efficiency compared to others. This method was used to make a one-dimensional simulation of the effective refractive index and

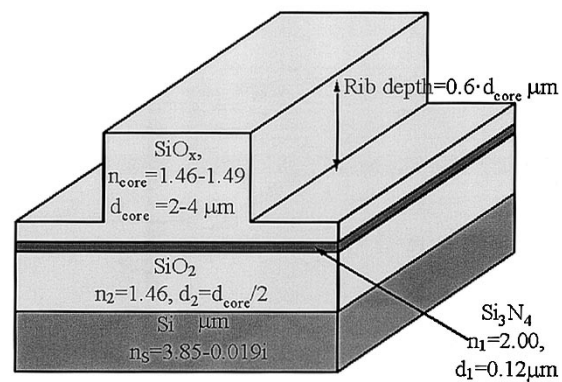


Fig. 2. ARROW structure.

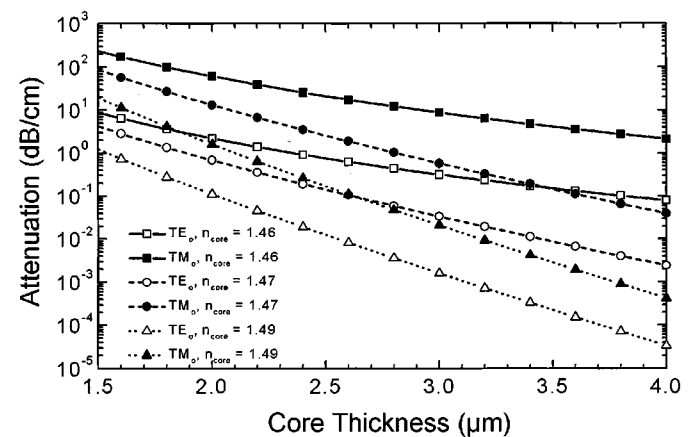


Fig. 3. Attenuation versus core thickness of ARROW structures for the fundamental TE_o and TM_o mode ($n_2 = 1.46, d_2 = d_{\text{core}}/2$).

attenuation losses for a design wavelength of 632.8 nm for the ARROW structure depicted in Fig. 2: the waveguide core is a nonstoichiometric silicon oxide (SiO_x) layer with a refractive index that can be modulated according to x . The technology of growing SiO_x by plasma-enhanced chemical vapor deposition (PECVD) has been developed previously in our group [12] and we are capable of varying the refractive index between 1.46–1.72. The core thickness will be varied between 2–4 μm . The first cladding is a silicon nitride (Si_3N_4) layer with a thickness of 0.12 μm and a refractive index of 2.00 deposited by low-pressure chemical vapor deposition (LPCVD). The second cladding is a Thermally grown silicon dioxide (SiO_2) layer with a refractive index of 1.46 and a thickness of 2 μm . Finally, the waveguide substrate is Silicon with a refractive index of $n_s = 3.85 - j0.01$ at the working wavelength of 632.8 nm.

We evaluated the attenuation losses for the fundamental transverse electric (TE_o) and transverse magnetic (TM_o) modes as a function of the thickness and refractive index of the core. Results can be seen in Fig. 3. As the refractive index of the core increases, attenuation for the fundamental mode decreases. In general, the TM_o mode always present higher losses (more than one order of magnitude) than the TE_o mode due to the presence of the high index first cladding [4]. When the core and second cladding have the same refractive index, losses for the TM_o mode are very high and the device can be considered polarization selective. However, when the core refractive index is

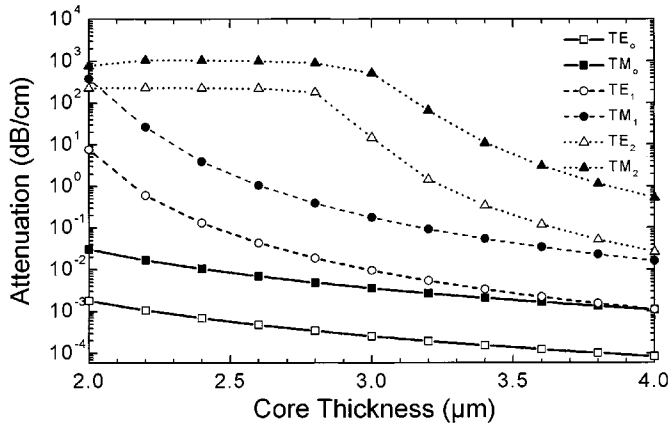


Fig. 4. Attenuation versus core thickness for the three first TE and TM modes of an ARROW structure with a core refractive index of 1.485.

higher than the second cladding refractive index, attenuation for the TM_0 mode decreases being possible, for certain thickness, that both the TE_0 and TM_0 modes propagate through the waveguide structure. Moreover, as the core thickness increases, higher order modes also present lower losses, being possible that the ARROW structure would lose its single-mode behavior. This fact would be a drawback for sensing applications and, therefore, the refractive index of the core has to be precisely controlled. To come to an agreement between a core index value higher than 1.46 and elevated losses for higher order modes, we have chosen a core refractive index of 1.485 (Fig. 4). In this case and comparing with the fundamental TE_0 mode, losses exceed more than one order of magnitude for the TM_0 and first higher order TE_1 mode and more than two for the TM_1 and the second higher order TE_2 mode.

Finally, in order to obtain a lateral confinement of light, a rib structure has to be designed (Fig. 2). Propagation characteristics, as well as lateral single-mode behavior, will depend on the width and depth of the rib. Experimentally, we have observed a good lateral confinement for rib depths in the order of 60% of the core thickness. Regarding the rib width, a lateral dimension lower than $7 \mu\text{m}$ would be enough to obtain a single mode behavior [13].

III. SENSITIVITY CALCULATIONS

For sensing purposes, the optical waveguide structure has to be designed to assure a high sensitivity, that is, the sensor response for changes in the optical properties of the cover medium has to be as high as possible. This sensitivity depends on the strength and distribution of the evanescent field in the outer medium [3], [14], [15]. We can distinguish between two different sensor sensitivities depending on how is the refractive index change in the outer medium.

- 1) if this change is homogeneously distributed in the cover we refer to homogeneous sensing. Sensitivity is related to the power of the guided mode transported in the cover medium [see Fig. 5(a)].
- 2) if there is an adsorption of molecules from a gaseous or liquid sample on the waveguide surface we talk about surface sensing. In this case, sensitivity is related to the

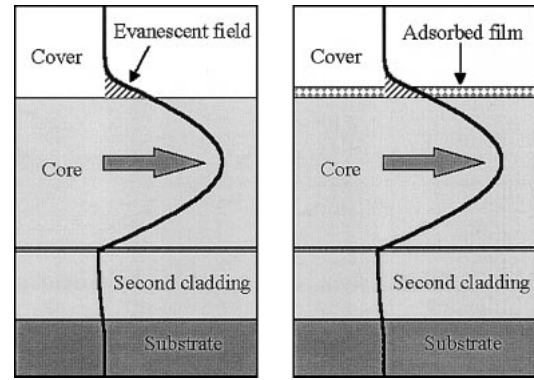


Fig. 5. (a) Homogeneous sensing. (b) Surface sensing.

squared field magnitude at the core-cover interface [see Fig. 5(b)].

In the next sections, we will evaluate sensitivity for a conventional ARROW structure with $n_{\text{core}} = 1.46$ and for an ARROW with a core refractive index of 1.485.

A. Homogeneous Sensing

In this case, sensitivity is evaluated as the rate of change of the effective refractive index of the guided mode, N , under an index change of the outer medium (n_o). The analytical expression for the homogeneous sensitivity is obtained in an analogous way as in references [14] and [15]. Considering a waveguide structure of five homogeneous layers, the E_x field (TE modes) and the H_x field (TM modes) are expressed as superposition of two exponential functions with imaginary arguments for the core, first cladding and substrate. For the second cladding, the arguments are imaginary when the core and second cladding refractive indexes are equal or real when the second cladding refractive index is lower than that of the core. For the cover the argument should be real corresponding to a confined field. By application of the boundary conditions at the waveguide interfaces we obtain a set of linear equations which resolution leads to the modal equation

$$\begin{aligned} \Phi_H = & k_c \cdot d_c + \arctan \left[\left(\frac{n_o}{n_c} \right)^{2\rho} \frac{k_c}{\gamma_o} \right] \\ & - \arctan \left[\left(\frac{n_1^2}{n_c n_2} \right)^{2\rho} \frac{i^\sigma \gamma_2 k_c}{k_1^2} \frac{1}{(\tan(k_2 d_2))^\sigma} \right] \\ = & m \cdot \pi \end{aligned} \quad (1)$$

where

$$\rho = \begin{cases} 0, & \text{TE mode} \\ 1, & \text{TM mode} \end{cases}$$

and

$$\sigma = \begin{cases} 0, & n_2 < n_c \\ 1, & n_2 = n_c \end{cases}$$

and with $k_i = k_o \sqrt{n_i^2 - N^2}$, $\gamma_i = k_o \sqrt{N^2 - n_i^2}$ ($i = c, 1$ or 2) and $k_o = 2\pi/\lambda$. We have assumed that the first cladding thickness verify the antiresonant condition $k_1 \cdot d_1 = (2m + 1)(\pi/2)$. This equation is also known as the

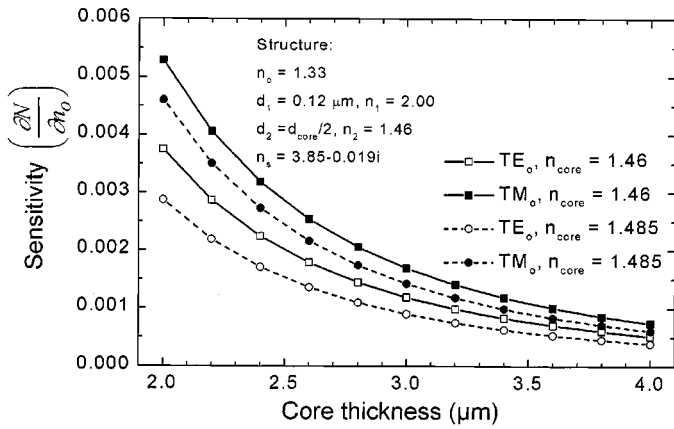


Fig. 6 Homogeneous sensitivity for an aqueous solution ($n_o = 1.33$) for the TE_o and TM_o modes of an ARROW structure with: —(solid line) $n_{\text{core}} = 1.46$ - - (dashed line) $n_{\text{core}} = 1.485$.

transverse resonance condition where the first addend is related to the phase shift that light experiences on the core layer and the second and third addend are the phase shift on the reflections at the core-cover medium interface and at the core-interference cladding interface, respectively. Homogeneous sensitivity can be obtained as the partial derivative $\partial N/\partial n_o$ by implicit differentiation of Φ_H

$$\frac{\partial N}{\partial n_o} = -\frac{\partial \Phi_H/\partial n_o}{\partial \Phi_H/\partial N}.$$

After some algebraic calculations and expressing sensitivity as a function of the fraction of the total power of the guided mode at the cover medium, we obtain

$$\frac{\partial N}{\partial n_o} = \frac{n_o}{N} \cdot \left[2 \left(\frac{N}{n_o} \right)^2 - 1 \right]^\rho \cdot \frac{P_o}{P_T} \quad (2)$$

with

$$\rho = \begin{cases} 0, & \text{TE mode} \\ 1, & \text{TM mode} \end{cases}$$

where

- n_o outer medium refractive index;
- N effective refractive index of the guided mode;
- P_o power of the guided mode at the cover medium;
- P_T total power of the guided mode.

In Fig. 6 (solid line) the sensitivity $\partial N/\partial n_o$ for a conventional ARROW structure with a core refractive index of 1.46 is shown as a function of the core thickness, d_{core} , for the fundamental TE_o and TM_o modes. The cover medium has been considered as an aqueous solution ($n_o = 1.33$). Sensitivity increases as the core thickness diminishes due to a less confinement of light within the core, which implies an increase of the power of the guided mode transported in the cover medium. The dashed line shows the case for an ARROW with $n_{\text{core}} = 1.485$. Now the refractive index difference between the core and the outer medium is higher and, consequently, the guided mode is more confined. This fact implies a decrease in the penetration depth of the evanescent field and, therefore, sensitivity is reduced.

B. Surface Sensing

This sensing scheme is of great interest for the detection of (bio)chemical reactions. The interaction between a receptor molecule adsorbed on the waveguide surface and an analyte can be understood as a mass change in the molecular adlayer and, therefore, as a variation in its refractive index. Surface sensitivity is then related to the value of the evanescent field at the waveguide surface. Assuming that the adsorbed molecules form a homogeneous adlayer of thickness d_ℓ and refractive index n_ℓ , sensitivity is evaluated as the rate of change of the effective refractive index of the guided mode, N , with respect to the thickness of the adsorbed film, d_ℓ . The analytical expressions are obtained by following the same procedure as in the homogeneous sensing case. First, we obtain the modal equation of the waveguide

$$\begin{aligned} \Phi_S &\approx k_c \cdot d_c + \arctan \\ &\cdot \left[\left(\frac{n_o}{n_c} \right)^{2\rho} \frac{k_c}{\gamma_o} \left[1 + \frac{\left(\frac{n_l}{n_o} \right)^{2\rho} \gamma_o^2 - \left(\frac{n_o}{n_l} \right)^{2\rho} \gamma_l^2}{\gamma_o} d_l \right] \right] \\ &- \arctan \left[\left(\frac{n_1^2}{n_c n_2} \right)^{2\rho} \frac{i^\sigma \gamma_2 k_c}{k_1^2} \frac{1}{(\tan(k_2 d_2))^\sigma} \right] \\ &= m \cdot \pi \end{aligned}$$

where

$$\rho = \begin{cases} 0, & \text{TE mode} \\ 1, & \text{TM mode} \end{cases}$$

and

$$\sigma = \begin{cases} 0, & n_2 < n_c \\ 1, & n_2 = n_c \end{cases}$$

and with $k_i = k_o \sqrt{n_i^2 - N^2}$ and $\gamma_i = k_o \sqrt{N^2 - n_i^2}$, assuming that $k_1 \cdot d_1 = (2m + 1)\pi/2$. Subsequently, surface sensitivity is obtained by implicit differentiation of Φ_S

$$\frac{\partial N}{\partial d_\ell} = -\frac{\partial \Phi_S/\partial d_\ell}{\partial \Phi_S/\partial N}$$

and after some algebraic calculations we have

$$\frac{\partial N}{\partial d_\ell} \approx \frac{\gamma_o}{N} \cdot \left[\left(\frac{n_l}{n_o} \right)^{2\rho} \gamma_o^2 - \left(\frac{n_o}{n_l} \right)^{2\rho} \gamma_l^2 \right] \cdot \frac{P_o}{P_T} \quad (4)$$

with

$$\rho = \begin{cases} 0, & \text{TE mode} \\ 1, & \text{TM mode} \end{cases}$$

- n_ℓ refractive index of the adsorbed adlayer;
- P_o power of the guided mode at the cover medium;
- P_T total power of the guided mode.

When the core thickness increases, surface sensitivity decreases due to a higher confinement of the mode within the core layer (see Fig. 7). Again, when the core refractive index is 1.485 (dashed line) the optical power transported in the cover medium is lower than in the case of a conventional ARROW structure (solid line) and, therefore, sensitivity decreases.

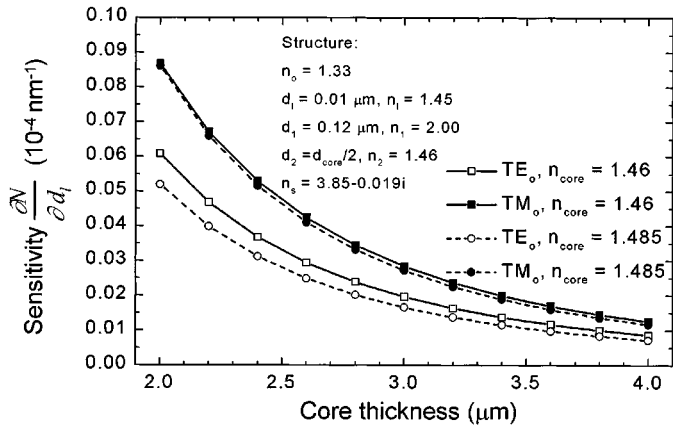


Fig. 7. Surface sensitivity for adsorption of molecules ($n_\ell = 1.45$) from an aqueous solution ($n_o = 1.33$) on the waveguide surface for the fundamental TE_o and TM_o mode versus core thickness for an ARROW structure with: —(solid line) $n_{\text{core}} = 1.46$ - - (dashed line) $n_{\text{core}} = 1.485$.

C. Sensitivity Enhancement

As it has been shown previously [16], sensitivity can be increased by overcoating the surface of the sensor with a high refractive index layer. In Fig. 8, homogeneous and surface sensitivity are shown as a function of the high index layer thickness (with an overlay refractive index of 2.00) for an ARROW structure with a core thickness of 4 μm and refractive indexes of 1.46 and 1.485.

As the overlay thickness increases, the ARROW fundamental mode is transformed progressively to the fundamental mode of a TIR (Total Internal Reflection) waveguide with the high index layer as the core. There is a thickness value where the guided mode is no longer an ARROW mode, but a TIR mode (for $d_{ov} > 40$ nm in Fig. 9). Before reaching this point, the ARROW fundamental mode is distorted in such a way that the field penetration into the cover medium is high compared to the uncoated ARROW and, therefore, sensitivity is enhanced (Fig. 9). Then, it is essential for sensing applications that d_{ov} remains below 40 nm. However, the distortion of the ARROW fundamental mode implies a decrease in the coupling efficiency between the waveguide and the optical fiber. We can also see in Fig. 8 that the overlay thickness where sensitivity is maximum is higher for the TM_o mode than for the TE_o mode.

In Fig. 10 we show the behavior of attenuation as a function of the overlay thickness for the same ARROW structures as in Figs. 8 and 9. Fig. 10(a) shows the attenuation for the fundamental TE_o and TM_o modes for two core refractive indexes of 1.46 and 1.485. We observe the same behavior as in the uncoated case: losses for the TM_o mode are more than one order of magnitude higher than losses for the TE_o mode and, when the core refractive index increases, losses diminish significantly. However, we observe that when the overlay thickness reaches the value where sensitivity is maximum, losses experience a discontinuity. This behavior can be explained in Fig. 10(b). At that thickness, the fundamental ARROW mode is transformed to the fundamental TIR mode, while the first higher order ARROW mode is transformed to the fundamental ARROW mode, with the subsequent abrupt increase of attenuation. At the same transi-

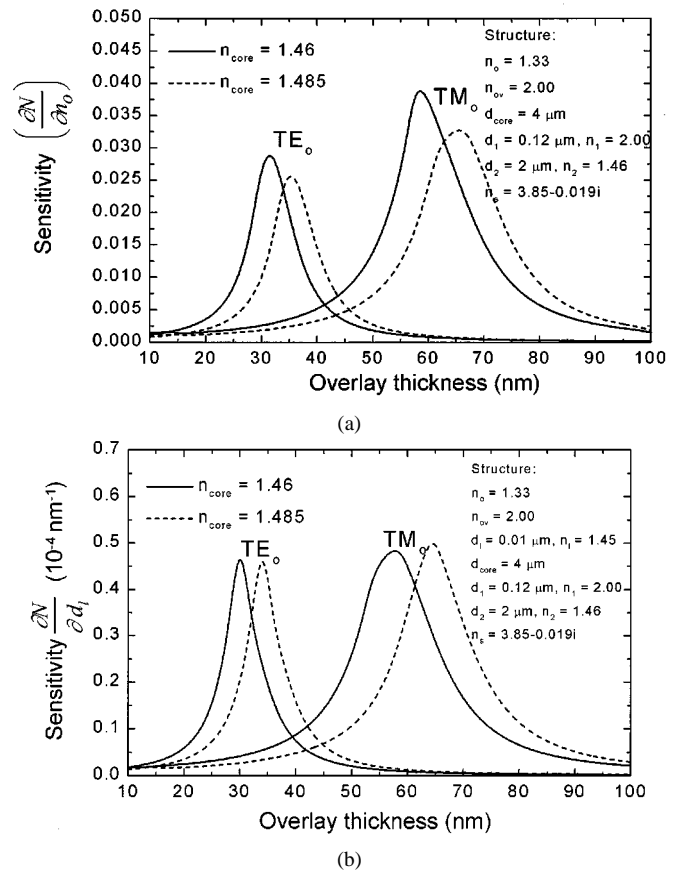


Fig. 8. Sensitivity versus overlay thickness for the TE_o and TM_o modes of an ARROW structure with different core refractive indexes: (a) Homogeneous sensitivity. (b) Surface sensitivity.

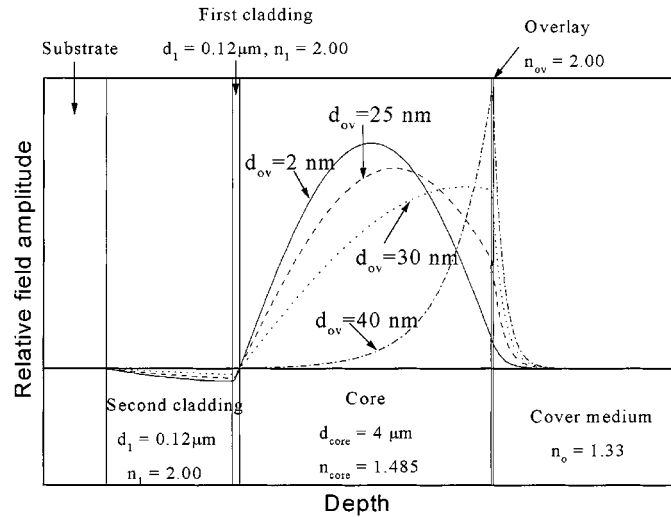


Fig. 9. Transformation of field profile of the fundamental TE_o mode for an ARROW structure (with $n_{\text{core}} = 1.485$ and $d_{\text{core}} = 4 \mu\text{m}$) as the thickness of the overlay increases.

tion point, the second higher order ARROW modes is also transformed to the first order ARROW mode.

IV. DESIGNED STRUCTURES

The optical waveguides that will form the basis of a high sensitive sensor based on the integrated Mach-Zehnder interferom-

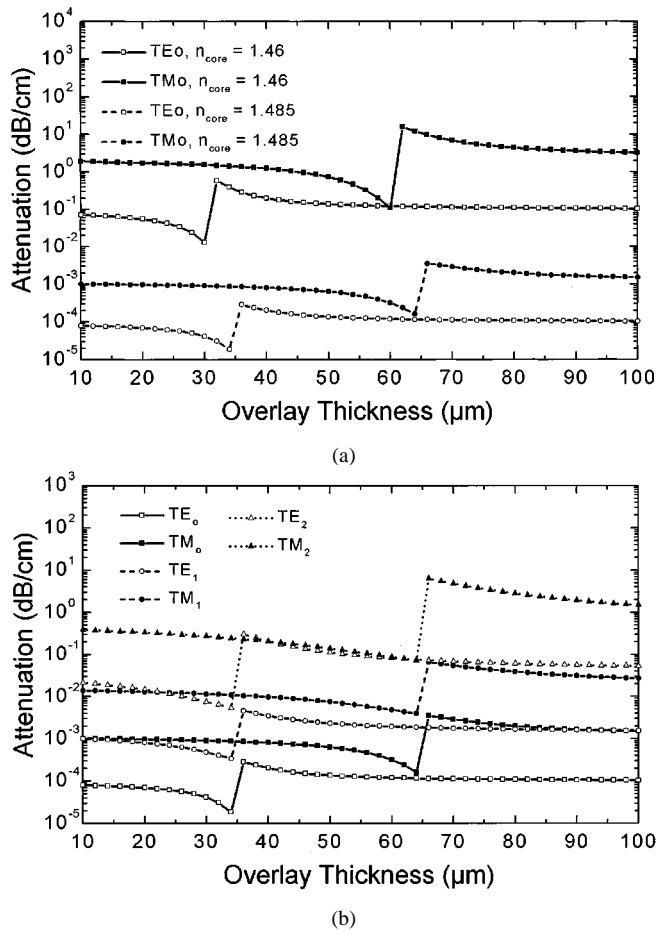


Fig. 10. Theoretical simulation of attenuation versus overlay thickness for: (a) the fundamental TE₀ and TM₀ mode; (b) the three first TE and TM modes of an ARROW structure with a core refractive index of 1.485. In both cases, the structure under study is: $n_o = 1.33$, $n_\ell = 1.45$, $n_{ov} = 2.00$, $d_{core} = 4 \mu\text{m}$, $d_1 = 0.12 \mu\text{m}$, $n_1 = 2.00$, $d_2 = 2 \mu\text{m}$, $n_2 = 1.46$, $n_s = 3.85 - 0.019i$.

eter have to verify two conditions: first, we have to assure their single-mode operation, that will depend on the core thickness and rib parameters (depth and width). Conventional ARROW structures are monomode even for core thickness in the order of a few micrometers. The need of increasing the core refractive index over that of the covering layer (1.46) can affect the waveguide monomode behavior, although it can be controlled with the rib parameters. We will assure this single-mode operation with rib depths in the order of 60% of the core thickness and rib widths lower than 7 μm.

On the other hand, optical waveguides should show a high surface sensitivity. This condition can be obtained decreasing the core thickness, although only to a certain limit (i.e., 2 μm) due to the increasing losses of the fundamental mode for lower core thickness. However, we have shown how sensitivity can be enhanced, more than an order of magnitude, overcoating the waveguide surface with a high refractive index layer.

Taking into account all these conclusions, we have decided to fabricate optical sensors with the following waveguide structure: a silicon substrate with a 2 μm second cladding layer of silicon dioxide ($n_2 = 1.46$) and a 0.12 μm first cladding layer of silicon nitride ($n_1 = 2.00$). The core is a nonstoichiometric silicon oxide layer with a refractive index of 1.485 and a thick-

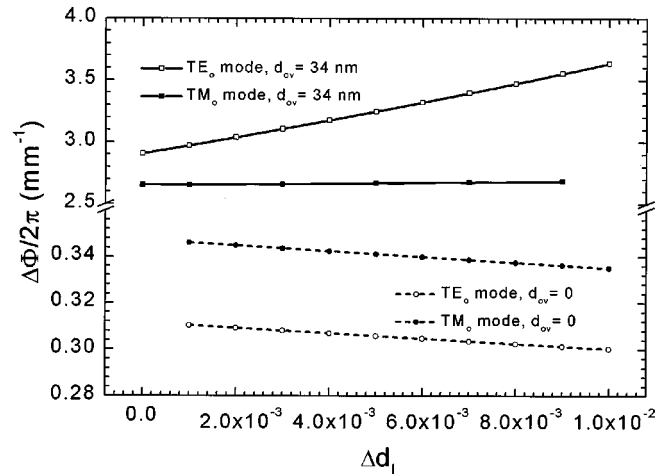


Fig. 11. Phase shift variation in the sensing arm of the Mach-Zehnder interferometer respect to the reference arm (covered with a 2 μm silicon oxide layer of $n = 1.46$) when the thickness of the adsorbed adlayer increases (Δd_ℓ is related to ΔN via the surface sensitivity). The structure under study is: $n_o = 1.33$, $n_\ell = 1.45$, $n_{ov} = 2.00$, $d_{ov} = 34 \text{ nm}$, $d_{core} = 4 \mu\text{m}$, $d_1 = 0.12 \mu\text{m}$, $n_1 = 2.00$, $d_2 = 2 \mu\text{m}$, $n_2 = 1.46$, $n_s = 3.85 - 0.019i$.

ness ranging from 1.5 to 4 μm. The core is overcoated with a silicon nitride layer of 34 nm ($n_{ov} = 2.00$) and with a silicon oxide layer of 2 μm and a refractive index of 1.46. For the chosen overlay thickness, the fundamental ARROW TE₀ mode presents low attenuation, while losses for the TM₀ and higher order modes exceed more than two orders of magnitude. At the same time, sensitivity for the TE₀ mode is much higher than for the TM₀ mode (see Fig. 8). The rib structure has a depth in the order of 60% of the core thickness and different widths from 4 to 8 μm. Concerning the interferometer, several Mach-Zehnder configurations were designed, varying the separation between arms and the Y-junction parameters. Finally, the sensor area has a longitudinal dimension of 6 mm. The optical characterization of such structures will be presented somewhere else.

Finally we present a theoretical simulation of the Mach-Zehnder interferometer behavior for the designed ARROW structure, with an overlay thickness of 34 nm (Fig. 11). We show the phase shift in the sensing arm of the interferometer respect to the reference branch (covered with a 2-μm silicon oxide layer of $n = 1.46$) when there is a variation of the thickness of the adsorbed adlayer (for the surface sensing case). Simulation is performed for the TE₀ and the TM₀ modes and we can appreciate the higher sensitivity of this structure for the TE polarization. We also show, for comparison, the interferometer response when the waveguide is uncoated. It is clear the increase of sensitivity when there is a high refractive index overlay on top of the waveguide.

V. CONCLUSION

ARROW structures are promising waveguides for the development of high sensitive integrated optical sensors. Their fabrication process, based of standard IC Silicon technology, and the large tolerance for the design of the refractive indexes and thickness of the waveguide layers, makes them very appropriate for low-cost mass production. Moreover, they have an effective single-mode behavior even when the core thickness is of the

same order of magnitude as the core of a monomode optical fiber; this characteristic makes them suitable for efficient connection with optical fibers.

For sensing applications, ARROW structures must verify two conditions: they have to be monomode and they should show a high surface sensitivity. To obtain a single mode behavior, we must assure large attenuation losses for the higher order modes. For that reason, the refractive index of the core should be kept under a certain value, i.e., 1.485.

Concerning the second condition, sensitivity increases as the core thickness diminishes. However, we are limited by the attenuation and insertion losses when the size of the core is lower than a certain value, i.e., 2 μm . We have shown how sensitivity can be increased by overcoating the core with a high refractive index layer.

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