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► **To cite this version:**

Clement Deleau, Han Cheng Seat, Helene Tap, Frederic Surre, Olivier D Bernal. Integrated Silicon Nitride Horizontal Long Period Grating for Refractometric Gas Sensing applications. 2020 IEEE International Instrumentation and Measurement Technology Conference (I2MTC), May 2020, Dubrovnik, Croatia. pp.1-6, 10.1109/I2MTC43012.2020.9129170 . hal-03547247

HAL Id: hal-03547247

<https://hal.science/hal-03547247v1>

Submitted on 31 Jan 2022

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Integrated Silicon Nitride Horizontal Long Period Grating for Refractometric Gas Sensing applications

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Abstract—We designed an integrated long period grating based on the horizontal periodic tapering of a silicon nitride channel waveguide. The structure is studied for gas sensing applications, using Styrene AcryloNitrile sensitive layer. Simulation results from the proposed architecture show high sensitivity beyond 1700 nm/RIU using a wavelength interrogation method centered at 1550 nm for a 20 μm large and 300 μm long structure.

Keywords—Integrated photonics, gas sensor, modeling, long period grating, coupled local mode theory.

I. INTRODUCTION

For the past two decades, long period fiber gratings (LPFGs) have been intensely investigated for communication [1] and sensing applications [2]. A wide diversity of LPFG-based systems has been demonstrated and used in various applications, such as optical filters [3], gain flatteners, polarization couplers, multiplexers and particularly refractometric sensors [4-7]. However, to the best of our knowledge, the design of these structures is typically limited to standard dimensions and intrinsic parameters of the host fibers, rendering them unsuitable for integration and optimization.

Following the enormous impact of integrated electronics on our society, integrated photonics have been subject to an exponentially growing interest since its earliest inception as laser diode devices for telecommunication applications in the 1960s and is now widely studied for the design of original, power-efficient and high-resolution compact sensors. In 2003, Tsoi and al. [8] demonstrated the first integration of a long period waveguide grating (LPWG) having similar properties to conventional LPFGs. The LPWG architecture using a periodic perturbation of the width or height of the waveguide enables strong coupling between the fundamental mode and a copropagating cladding mode. It can thus be designed to **selectively perform coupling under specific conditions**, making them very interesting candidates for in-situ chemical monitoring. Using a suitable functionalizing chemical layer for the cladding window surrounding the LPWG core, the detection and quantification of a specific analyte has been demonstrated through various techniques [4,5,7].

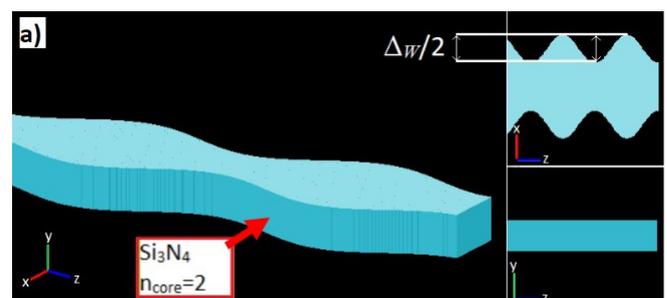
The fabrication of index-modulated structures required for long period gratings can be performed through local corrugation [9], tapering [6], laser irradiation, ultraviolet inscription, arc discharge [10]. We propose here to introduce a grating perturbation on the fundamental mode of a simple channel waveguide through a smooth periodic change of the waveguide width. Unlike binary gratings, this type of grating enables smooth power coupling and can be studied under the slowly-varying envelope approximation assumptions. The design is studied to analyze the LPWG response to a change of analyte concentration through the change of the sensing material refractive index.

This paper is organized in three parts. First, in Section II, the general design of the horizontal LPWG is presented and compared to other reported types of LPWG. In Section III, the Coupled Local-Mode Theory (CLMT) [11] is used to introduce and describe the principle of the LPWG's mechanism. This approach is formulated as a proof-of-concept but can subsequently be extended to accurately model the LPWG response and characteristics [12,13]. In Section IV, CLMT is applied on our structure and an EigenMode Expansion (EME) method is performed with Lumerical suite tools as a comparison and simulation results of the sensor's sensitivity are discussed. Finally, in section V, two fabrication methods are proposed.

II. ARCHITECTURE

A. Proposed structure

The proposed LPWG sensor structure consists of a periodically-modulated (along the z-axis) channel width (x-axis) waveguide inside of a polymeric sensing region as illustrated in Figure 1.



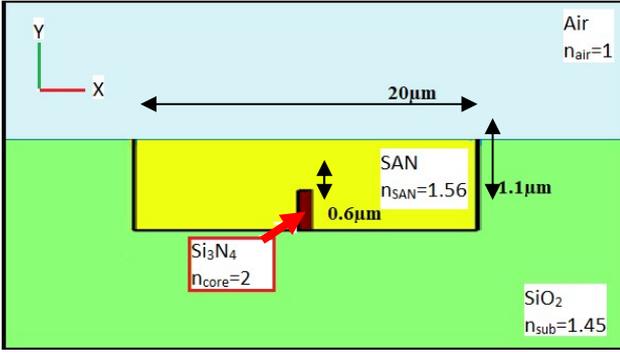


Fig. 1. (a) Horizontal LPWG core profiles and (b) cross-sectional material architecture where the Si_3N_4 and the Styrene AcryloNitrile (SAN) are the core and cladding waveguides respectively

As explained in the next section using CLMT [11], the excitation of the coupling phenomenon between core and cladding modes is performed via a periodic modification of the local modes along the propagation z -axis. Two different grating types can allow this mechanism. The most common grating is one with a local index variation inscribed in the waveguide or core [1,10]. It usually requires a specific and complex apparatus as well as accurate calibration on each material to be engraved. The second grating structure, more commonly employed in integrated photonics structures, are corrugated waveguides [9,14], which can be achieved by an additional vertical etching step to create relief, leading to optical coupling to cladding modes above the waveguide core. On the contrary, our structure is designed to incorporate a horizontal modulation via a periodic waveguide width variation and the design of a specific cladding box. Hence, no further process step is necessary. This is advantageous since the modulation pattern is directly drawn on the layout.

B. Materials and dimensions

The sensing mechanism is based on the coupling between two different modes; the fundamental core mode, HE₁ of effective index $n_{\text{eff},1}$, and an n^{th} cladding mode of effective index $n_{\text{eff},n}$, which is mostly confined in the cladding which can later be functionalized to a specific chemical. Since grating-assisted coupling involves coupling the core mode to higher-order modes, which are modes with lower effective indices, the following condition must be fulfilled to have mode confinement

$$n_{\text{core}} > n_{\text{eff},1} > n_{\text{clad}} > n_{\text{eff},n} > n_{\text{sub}} > n_{\text{air}}$$

where n_{core} , n_{clad} , n_{sub} and n_{air} are the refractive indexes of the Si_3N_4 waveguide core, the cladding, the SiO_2 substrate, and the air respectively.

A specific set of materials and structure dimensions must then be considered to allow both standard manufacturing process and functionalization for potential gas sensing. Silicon nitride (Si_3N_4 or more commonly SiN) is employed for its ease of growth in the domain of integrated photonics and optical properties (i.e. for its relatively medium index contrast with silicon oxide). The sensitive layer employed as cladding must be a porous polymer, in which the gas is soluble. In addition, the sensitivity and selectivity can be enhanced by employing supramolecular compounds which have a cage-like structure within which molecules can be reversibly trapped [21]. For example, Cryptophane-A which presents the smallest relative cavity, a methane trap, can be incorporated into a Styrene

AcryloNitrile (SAN) film of index $n=1.56$, forming the sensing layer of a Mach-Zehnder-based methane sensor [15,16]. It is referred to here as cladding, as it almost entirely encompasses the Silicon Nitride core (Fig. 1.(b) and 2.(a))

Figure 1. (b) describes the cross-sectional refractive index profile of the LPWG, with $n_{\text{core}}=2$, $n_{\text{clad}}=1.56$, $n_{\text{sub}}=1.45$, $n_{\text{air}}=1$. A sensing window thickness of $\sim 1 \mu\text{m}$ allows uniform and relatively quick diffusion of the gas species to be detected as demonstrated in [5,7,8,15]. The cladding and waveguide are respectively designed to have a 20 and 0.8 (w_{core}) μm width and a 1.1 μm and 0.6 (h_{core}) μm thickness to ensure single mode propagation only within the core while allowing multiple higher order modes within the cladding. Moreover, the cladding dimensions determine the maximum order of the propagating cladding modes, which directly influences the coupling strength, as demonstrated later in section III and IV. The maximum width variation Δw (see Fig. 1. (a)) and grating length period Ω are chosen to be 0.6 μm and 8.76 μm , respectively (Fig. 1 a) so that Ω corresponds to the standard LPG phase-matching condition [11,12,13] on the propagation constants $\beta_j(z)$ and $\beta_l(z)$ of the two modes to couple at the resonance wavelength around 1550 nm:

$$\beta_j(z=0) - \beta_l(z=0) = \frac{1}{\Omega}, \quad (1)$$

Here, coupling occurs between the fundamental HE₁, and higher order propagating cladding modes, out of which one exhibits a higher coupling at a specific wavelength as described in the next section. More precisely, it will be further shown that only odd cladding modes can be coupled to the fundamental mode through the LPWG. Their respective effective indices and profiles were simulated with Lumerical, as shown in Fig. 2 for 2 higher-order modes only, to calculate the resonant grating period. We see that for the two multi-modes, most of the optical field is confined into the SAN, therefore called cladding-modes. These modes thus become inherently more affected by a change of the SAN refractive index n_{clad} . Using eq. (1), the resonance wavelength can be approximated by the average of the values of each coupled-mode effective indices along z -propagation. Note, however, that the real resonance wavelength values will be slightly shifted as the functions of the mode effective indices versus core width are not linear.

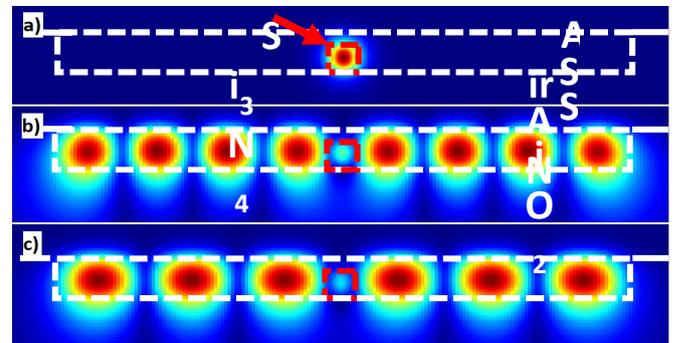


Fig. 2. Mode profiles at 1550 nm for Fundamental (a) HE₁ mode, and cladding (b) HE₉ and (c) HE₇ modes calculated with Lumerical mode solver

III. LPG MODEL

Different methods have been used to model the light propagation when introduced into the LPG. However, certain types of simulation methods find difficulty to model accurately this type of sensor as the behavior of the distribution of light is very continuous and highly depends on small structure variations.

A. Finite-Difference Time-Domain

As an example, Finite-Difference Time-Domain (FDTD) gives an interesting insight of the overall sensor mechanism as shown in Fig 3, where coupling happens between HE₁ and HE₇, but its high dependence on fine discretization makes it inadequate for accurate modeling in our case using our computing resources. The need for both high temporal and mesh resolution over a relatively large area, especially at the interfaces where refraction happens, leads to large memory needs, otherwise simulations will present larger numerical errors than other methods. However, comparing Fig. 3. (a) and (b) clearly illustrates that, only at resonance, most of the optical power is transferred from the core mode to the higher order cladding mode after a brief propagating length.

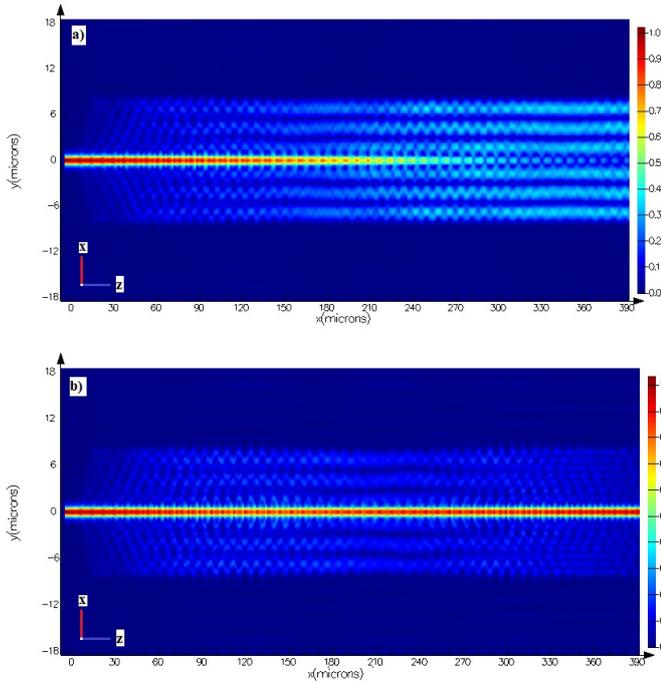


Fig. 3. (a) Illustration of the intensity distribution seen from above at resonance (b) Normalized intensity distribution seen from above with a slightly different cladding index

To circumvent these computing issues, two different methods can be used instead: the common EigenMode Expansion method and, more specific to our LPG application, the CLMT [11].

B. Eigenmode Expansion method

The Eigenmode expansion method (EME), also referred to as mode matching method, is a rigorous technique used for modeling waveguides [17,18], which relies on a scattering parameter superposition approach to calculate the amplitude of each mode at any propagation distance. This technique has very good efficiency for periodic and/or long

components and provides flexible post-calculations analysis. It is thus ideal for modeling long period grating-based systems [18] as, due to the structure periodicity, it is possible to calculate the structure scattering parameters from one single period. The method is available in various commercially available software such as Lumerical© suite tools, which was used to simulate the results presented on fig. 2.

Figure 2. shows (a) the fundamental mode profile and (b)-(c) the profile of two cladding modes that can couple to the fundamental mode at certain conditions. The grating period is longitudinally divided into 40 block objects and the guided mode calculation considers 40 modes per block similarly to [12].

C. Coupled Local-Mode Theory application

On the other hand, the CLMT application is performed through the characterization and calculation of the continuous refraction at the interfaces between the core and sensing window, which provides a **more physical model** on the coupling behavior in the LPG. The application of the theory was performed through Matlab© and COMSOL© linked scripts.

Conventional Coupled Mode Theory (CMT)[11] is usually used to describe the coupling between modes when small perturbations are assumed and modes remain almost unchanged along the propagation direction. Further, the general coupled mode equations are restricted to weakly guiding waveguides where polarization effects are ignored. CMT can thus model very accurately the first category of LPGs mentioned in Section II, where the waveguide dimensions remain constant and only local refractive indices are modified. However, in the presence of significant cross-sectional dimension modulations [13], CMT can no longer be applied, and a more specific approach, such as CLMT [11], is required. CLMT achieves good results [12,13] when used to describe structures with large but slowly varying non-uniformities along the waveguide and can thus be potentially used to describe our structure. In this section, a brief introduction to CLMT is formulated together with a method to calculate coupling coefficients. It will allow better understanding of the structure behavior and provide more insight to further optimize the design architecture.

Generally, there is no exact solution to Maxwell's equations for propagation along a perturbed waveguide. It is, however, possible to obtain accurate approximations of modes within local regions, known as local modes [11] which superpose to form the transverse field components as

$$\Phi_t(x, y, z) = \sum_j \{b_j(z) + b_{-j}(z)\} \hat{\phi}_{ij}(x, y, \beta_j(z)), \quad (2)$$

where $\hat{\phi}_{ij}$ represents the orthonormal electric or magnetic transverse field profiles of the j^{th} mode, and $b_{\pm j}(z)$ are both modal amplitude and phase for forward (+) or backward (-) propagation.

The coupling behavior between local modes is formulated by the general coupled local-mode equation [11]

$$\frac{db_{\pm j}}{dz} \mp i\beta_j b_{\pm j} = \sum_j \left\{ C_{\pm j,l} b_l + C_{\pm j,-l} b_{-l} \right\}, \quad (3)$$

with C_{jl} the coupling coefficient between the local modes j and l which can be expressed as [11]

$$C_{jl} = \frac{1}{4} \left(\frac{\epsilon_0}{\mu_0} \right)^{\frac{1}{2}} \frac{1}{\beta_j - \beta_l} \int_{A_\infty} \hat{e}_j^* \cdot \hat{e}_l \frac{\partial n^2}{\partial z} dA, \quad j \neq l; \quad C_{jj} = 0 \quad (4)$$

The squared index component of the horizontal grating structure can be expressed here as

$$n^2(x, y, z) = \begin{cases} n_{clad}^2 & y > \frac{h_{core}}{2} \\ n_{core}^2 (1 - \Delta_n H(x - \rho(z))) & |y| \leq \frac{h_{core}}{2} \\ n_{box}^2 & y < -\frac{h_{core}}{2} \end{cases}, \quad (5)$$

with $\Delta_n = 1 - \frac{n_{clad}^2}{n_{core}^2}$, $\rho(z) = \frac{\Delta_w}{4} \sin\left(\frac{2\pi z}{\Omega}\right) + \frac{w_{core}}{2}$ and

where $x = y = 0$ at the center of the waveguide. H denotes the Heaviside function and ρ the periodic width variation of the LPWG along the z axis. By substituting eq. (5) into (4), we obtain the coupling coefficient for local modes of an integrated horizontal grating in the form of

$$C_{jl}(z) = \frac{1}{4} \left(\frac{\epsilon_0}{\mu_0} \right)^{\frac{1}{2}} \frac{n_{core}^2 \Delta_n}{\beta_j - \beta_l} \frac{d\rho(z)}{dz} \begin{bmatrix} \frac{h_{core}}{2} \\ -\frac{h_{core}}{2} \\ \int_{-\frac{h_{core}}{2}}^{\frac{h_{core}}{2}} ((\hat{e}_j^* \cdot \hat{e}_l)_{x=\rho(z)}) dy \\ \frac{h_{core}}{2} \\ + \int_{-\frac{h_{core}}{2}}^{\frac{h_{core}}{2}} ((\hat{e}_j^* \cdot \hat{e}_l)_{x=-\rho(z)}) dy \\ -\frac{h_{core}}{2} \end{bmatrix}, \quad (6)$$

with $C_{jj} = 0$.

Further, the transverse electric field at the interfaces of a step-index waveguide of relatively high index contrast is discontinuous, which complicates the calculation of the integrand. A bypass method [11] is to recognize that $n^2 e_t$ is continuous across the interfaces. As a result, the transverse component of the integrand can be replaced by

$$\left(\frac{n^2 \hat{e}_{t,j}^*}{n_{core}^2} \right) \cdot \left(\frac{n^2 \hat{e}_{t,l}}{n_{clad}^2} \right)$$

As previously mentioned, one of the main advantages of this CLMT compared to the EME method consists in providing a better insight of the phenomena taking place in the LPWG. In particular, important LPWG properties can be deduced from this equation (eq. 6): (1) only coupling of the fundamental mode to odd cladding modes is possible as the even mode coupling coefficients are null; (2) the coupling amplitude can be increased by modifying the grating amplitude Δ_n and period Ω (via ρ) or by optimizing the field superposition at the waveguide interfaces. The increase of the coupling coefficient amplitude fastens the rate at which energy is exchanged between modes, as described in eq. (3), thereby reducing the minimum required LPWG's length to achieve maximum coupling.

To obtain a good estimation of the remaining integral in $C_{jl}(z)$ (eq. 6), COMSOL mode-solver, based on finite-element method, can be used as it allows a convenient way to extract the interface fields of each modes, their effective indices, and Poynting vectors for normalization. Ten cross-sections were simulated by sweeping the waveguide width between minimum and maximum values to constitute a dataset of values. These calculations are only required over half a period of the 3D model because of the structure's periodicity. This dataset is then transferred to Matlab, coupling coefficients are calculated and extracted, and only then, the LPG geometry is taken into account to model energy distribution. Another advantage of the proposed model based on CLMT is that using this predetermined dataset, any LPG geometry can be designed and simulated easily. CLMT only requires a dataset of coupling coefficients for given cross-sections and directly calculates energy distribution as a function of $C_{jl}(z)$, while EME superposes each mode to calculate scattering parameter between each section.

IV. SIMULATION RESULTS

A. Model validation

Figure 4 shows the cladding mode power versus the propagating length along the LPWG for different wavelengths obtained with both CLMT and EME techniques. It clearly shows that comparable results can be achieved with the CLMT. In addition, here, the highest order propagating mode (HE9, for our LPWG's dimensions) shows higher coupling than any lower order modes (e.g. HE7) at their respective resonant wavelengths (HE9@1540nm and HE7@1484nm), as previously demonstrated by the CLMT equations, due to a higher field product integrand at the core/cladding interface. This results in a reduced LPWG's length to achieve maximum coupling. The "HE9 normalized power" at wavelengths 1550nm and 1525nm clearly describes the coupling behavior of the LPWG when the injected wavelength drifts from the resonance, resulting in a reduction of the coupled energy at a the optimal sensor length (the shortest length where coupling reaches its peak at resonance), $L_{opt} = 300\mu\text{m}$ here.

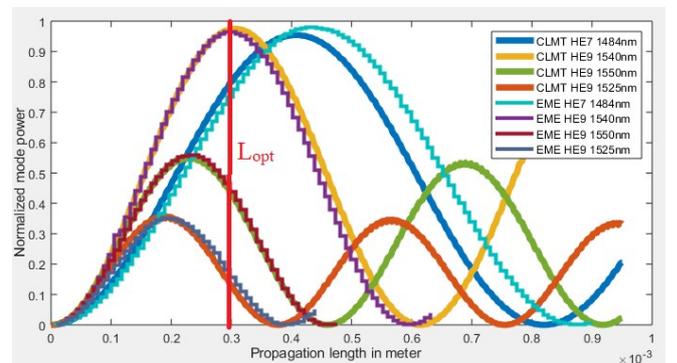


Fig. 4. Cladding mode normalized power versus propagation length (SI) for HE7 and HE9 modes at different wavelengths simulated by CLMT application and EME

B. Sensor sensitivity

The system interrogation can be performed through the wavelength interrogation method [4-7]. The refractive index

sensing mechanism relies on the disruption of the resonance of the LPWG which occurs when the cladding mode propagation constant changes. As a main difference with typical LPFG chemical sensors, which usually involve SPR as the cladding material cannot be modified easily, the cladding mode here is mostly confined in the sensing layer incorporated with the selective transducer. It is expected to lead to a relatively large modification of the mode propagation constant when the material index changes, i.e. analyte-induced perturbations, which enhances sensor sensitivity.

Figure 5. (a) shows the coupling spectra for different cladding refractive indices. From these results, the sensitivity can be calculated (cf. Fig. 5. (b)). The average sensitivity is found to be 1768nm/RIU (refractive index unit).

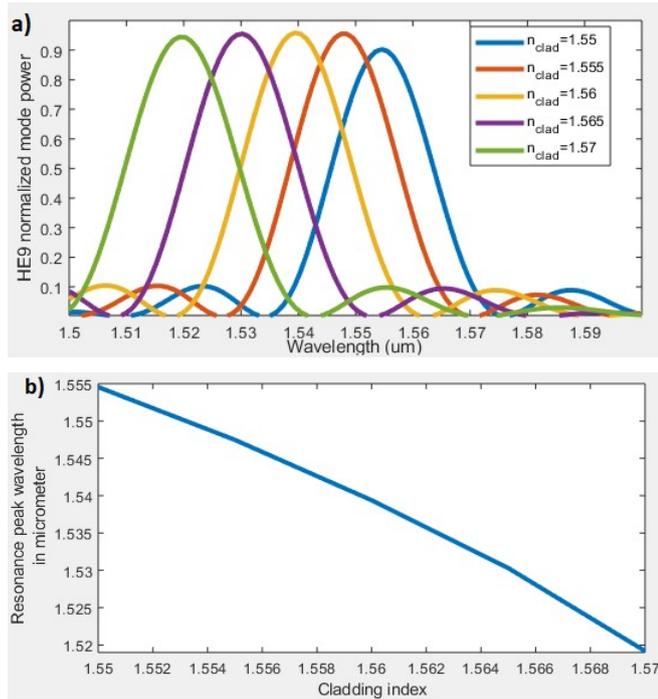


Fig.5. (a) HE9 normalized mode power spectra for a 33 periods long grating at different cladding refractive indices, calculated with EME method and (b) resulting resonance peak shift for wavelength interrogation

As it is difficult to measure the output spectra of the higher mode the measurement is made directly at the output of the core, which allows to get the same wavelength via detecting a dip in the light in the core.

We assume here that the output core intensity is equal to the input intensity minus the coupled energy to cladding modes along propagation, which could easily be measured using grating couplers, for example.

One can also notice a LPG peak is larger than other resonance peak found in integrated optics, which prevents it from large linewidth source issues.

V. FABRICATION PROPOSALS

This new type of integrated refractometric sensor is based on a specific coupling mechanism which allows several profile configurations, and therefore multiple realization processes. As described in the first section, the effective indices of each region must respect a certain relationship. Two different approaches can be employed to fabricate the LPWG.

A first method would be to simply create an opening into the buried core of a photonic chip and cover it with a sensing film to fill the etched region as seen in Fig. 6. (a). A downside to this method is the lack of control of the thickness of the film at certain areas where the cladding could form a rib multi mode waveguide instead of a strip one. It could simply be bypassed to a certain extent by performing spin coating to different speeds until the thickness reaches a value corresponding to a desired $n_{eff,n}$ of the rib cladding mode.

A second method (Fig. 6. (b)) currently being investigated would be to perform lithography on the polymer layer, creating polymer waveguides encompassing the core waveguide. (19) This type of structure could also be translated to an electro optical multi-mode coupler, enabling selected coupling of the fundamental mode into a specific higher order mode.

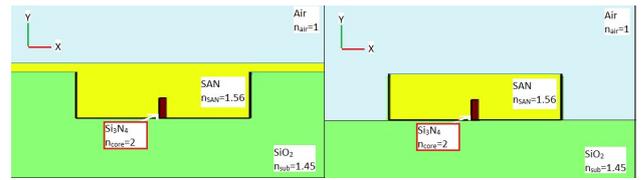


Fig. 6. (a) Rib cladding structure and (b) Strip cladding structure

VI. CONCLUSION

We have presented a new sensor architecture based on a long period horizontal grating structure. We have also proposed to describe the LPWG using the CLMT which provides more insight on the physics of the structure. For example, it indicates that a higher index contrast and therefore higher n_{core} values could increase the coupling, rendering the architecture an interesting candidate for silicon on-chip integration. This approach has been successfully compared to and verified using a standard method based on EME. Moreover, CLMT is more flexible to common grating profile modulations [12,20] as we work on the reconstruction of the coupling coefficient shape along propagation. The calculated overall sensor sensitivity reaches 1768 nm/RIU, and further improvement could increase the sensitivity to over 2000nm/RIU. Based on [21], from the achieved Mach Zehnder sensitivity of 0.768 mrad/ppm, the SAN and Cryptophane layer sensitivity to methane in terms of RIU/ppm can be estimated to be approximately 6.3 nRIU/ppm. As a result, using a similar sensitive layer with our proposed LPG architecture, an 11 fm/ppm theoretical wavelength sensitivity could be expected. This new type of design appears promising and can benefit from improvements or hybridations, potentially involving new sensing mechanisms, like plasmonics [18] or photonic crystals [22].

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