



# MODELLING of a two-dimensional photonic crystal with line defect for a laser gas sensor application

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## ABSTRACT

We present the results of a numerical analysis of a two-dimensional photonic crystal with line defect for a laser gas sensor working in a slow light regime. The geometrical parameters of photonic crystals with three different line defects were numerically analyzed: a missing row of holes, a row of holes with changed diameter and air channel. Antireflection sections were also analyzed. The simulations were carried out by MEEP and MPB programs, with the aim to get the values of a group refractive index, transmission and a light-gas overlap as high as possible. The effective refractive index method was used to reduce the simulation time and required computing power. We also described numerical simulation details such as required conditions to work in the slow light regime and the analyzed parameters values' dependency of the simulation resolution that may influence the accuracy of the results.

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## 1. Introduction

Photonic crystals (PhCs) are artificial materials, optical properties of which can be engineered to a wide extent. Of interest for the optical sensor is the possibility of forming absorption spectra and dispersion properties [1–3] according to application requirements. In particular, through manipulation of dispersion the group refractive index, the velocity of light can be slowed down, leading to the so-called “slow light” phenomenon [4,5]. Operation of the gas sensor may be based on absorption spectroscopy where the concentration of the gas is measured through the analysis energy of light absorbed by gas molecules. The use of a slow light phenomenon can enhance the interaction between light and gas medium [6]. However, the increase of the group refractive index ( $n_g$ ) of the crystal is accompanied by changes in the optical field distribution. This, in turn, results in changes of the light-gas overlap ( $\eta$ ) and the transmission coefficients ( $T$ ). The light-gas overlap coefficient is defined as an energy ratio of the electromagnetic field which propagates in air holes of a photonic crystal to the total energy. The coefficient is of 100% if we assume that light is guided outside the material forming a photonic crystal. In this case, theoretically, interaction efficiency is increased by a factor equal to the value of a group refractive index. The third important parameter, for optical gas sensors, is a transmission coefficient which should be maximized to maintain

a good signal-to-noise ratio at the receiver. The unique feature of gas sensors based on photonic crystals is the possibility to obtain high values of all three ( $n_g$ ,  $\eta$ ,  $T$ ) coefficients by a proper design of the photonic crystal structure.

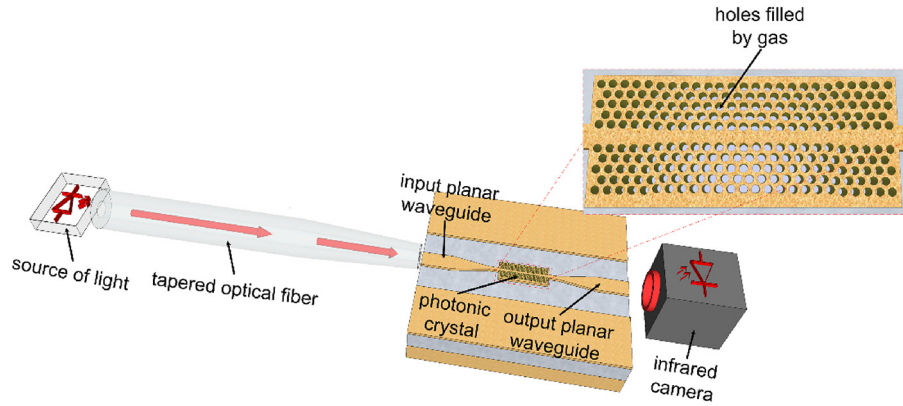
In this paper we present results of an analysis and optimization of the photonic crystal structure, aiming at maximizing the  $\eta$ ,  $n_g$  and  $T$  coefficients, to make the crystal usable in optical gas sensors. An additional calculation complication arises from the fact, that the crystal has to be tuned to a required wavelength of light and an optical band structure has to be taken into account. The band structure should take into account defect modes useful for the optical sensor design. Considering all mentioned requirements and parameters, we define a working point of the device. We choose the working point in the range of a defect mode localized within the photonic band gap. The defect mode occurs because of a disorder introduced into the periodic structure of the photonic crystal. We analyzed a PhC with three types of line defects. For the photonic crystal, we selected a triangular lattice of holes because it provides a greater tolerance of work in the range of a chosen mode. The analysis carried out in this article was performed to optimize the gas sensor, but the method of the analysis can be used while constructing other devices based on photonic crystals.

## 2. The concept of the laser gas sensor

A short description of the concept of the sensor is provided below. Technological details of our laser gas sensor based on a two-dimensional photonic crystal have been presented elsewhere

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**Fig. 1.** The design of gas sensor based on a two-dimensional photonic crystal fabricated in a silicon-on-insulator heterostructure.

[7]. Our sensor, based on a two-dimensional photonic crystal, was fabricated in a silicon-on-insulator heterostructure (SOI) by an e-beam lithography (EBL) and a reactive ion etching (RIE). The gas sensor consisted of a tuneable semiconductor laser, a tapered optical fiber, a 2D photonic crystal working in the slow light regime, and an infrared camera (Fig. 1). The principle of operation of the gas sensor is based on measurements of a single-wavelength light transmission through a photonic crystal which holes are filled with gas. The wavelength of the source of light should correspond to the wavelength of the absorption peak of gas undergoing the detection. The wavelength selected for this work was suitable for a detection of acetylene for which a strong absorption peak occurs at  $\lambda_0 = 1531.588$  nm [8].

The active element of the sensor included a photonic crystal waveguide with input and output strip waveguides and tapered sections between them (Fig. 2). Waveguides consisted of three parts: initial, the widest one ( $W_1 = 15 \mu\text{m}$  and length  $L_1 = 10 \mu\text{m}$ ), intermediate, the longest  $L_2 = 800 \mu\text{m}$  and the final section characterized by width  $W_3$  close to  $1 \mu\text{m}$  and length  $L_3 = 10 \mu\text{m}$ . The tapered optical fibre was used to improve the efficiency of light coupling into an active element of the sensor. Parameters of all the mentioned sections were analyzed and optimized by us for the best sensor operation [7].

The numerical analysis was carried out for photonic crystals with three sorts of line defects including one row of missing holes, one row of holes with changed diameters and an air channel (Fig. 3).

We carried out the numerical analysis with the MEEP (MIT Electromagnetic Equation Propagation) [9] and MPB (MIT Photonic-Bands) [10] packages. The MEEP software, based on a finite-difference time-domain (FDTD) method, was used for transmission and group refractive index characterization of PhC. The MPB software based on definite-frequency eigenstates of Maxwell's equations was used to get photonic band diagrams (PBD) of PhC and to calculate a light-gas overlap.

### 3. Effective refractive index method

In general, the numerical analysis should be performed in three dimensions, where length, width, and thickness of a structure are defined. However, such approach is time-consuming and requires substantial numerical power. The computational requirements are lowered if a 3D model is replaced with a 2D one. For a planar waveguiding structure, a photonic crystal waveguide exhibits refractive index periodicity in two dimensions so that it can be modeled with a good approximation as a two-dimensional structure. The three-dimensional model can be approximated by two-dimensional one, under the condition that refractive index of the guiding material is replaced with an effective refractive index of a planar waveguide

[11,12]. The approach is called Effective Refractive Index method and was used in our analysis. In that method, the photonic crystal fabricated and analyzed numerically is characterized by the effective refractive index which represents both thickness and refractive index of the structure.

The effective refractive indices of the waveguiding modes may be calculated using the mode Eq. (1) of planar waveguides [11]. The equation is solved by finding zeros of the function:

$$\left(\frac{2\pi h}{\lambda}\right) \sqrt{(n_w^2 - N_{eff}^2)} = m\pi + \tan^{-1} \left[ C_1 \sqrt{\frac{N_{eff}^2 - n_c^2}{n_w^2 - N_{eff}^2}} \right] + \tan^{-1} \left[ C_2 \sqrt{\frac{N_{eff}^2 - n_s^2}{n_w^2 - N_{eff}^2}} \right] \quad (1)$$

where  $N_{eff}$  is the effective refractive index of the guiding layer,  $n_w$ ,  $n_s$ ,  $n_c$  are the refractive indices of guiding, top and bottom layer, respectively,  $\lambda$  is the wavelength,  $h$  is the guiding layer thickness,  $m$  is the mode number,  $C_1 = C_2 = 1$  for TE polarization,  $C_1 = n_w^2/n_c^2$  and  $C_2 = n_w^2/n_s^2$  for TM polarization.

The effective refractive index of a guiding layer in which PhC was fabricated was calculated for the wavelength  $\lambda_0 = 1531.588$  nm and the refractive indices  $n_{Si} = 3.48$  [13],  $n_{SiO_2} = 1.44$  [14] (Fig. 4).

Single mode propagation of light through a photonic crystal was obtained for the thickness of a guiding layer equal to or less than 275 nm. The thickness 220 nm was chosen for further analysis. The effective refractive index  $N_{eff}$  was close to 2.74 for the TE polarization for which the gas sensor was designed. The TE polarization was selected because of the availability of the defect mode inside the photonic bandgap (for the triangular lattice 2D PhC) [15].

## 4. Numerical analysis of photonic crystals

The triangular-lattice photonic crystals with three different line defects were analyzed numerically to obtain as high as possible values of transmission, group refractive index, and light-gas overlap. The task definition is straightforward. However, the analysis itself is intricate, extensive and poses several risks. Details on calculating light-gas overlap coefficient, establishing numerical resolution and selecting a working point of the sensor within the slow light regime are described in this paper. Further, a general methodology of modelling photonic-crystal-based devices is provided.

### 4.1. Light-gas overlap coefficient

Modelling software, in general, is composed of three parts: input functions, proper calculation engine, and output functions. The output functions of the MPB software provide values of material

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