Design of a 2D TiO_2 Photonic Crystal Waveguide Sensor

E. Jardinier, G. Pandraud, H.T.M. Pham, P.J. French and and P.M. Sarro

Abstract— **A photonic crystal waveguide working in the visible and in the ultra violet is presented for sensing. The sensor is applied to Refractive Index (RI) measurements. The sensitivity at different wavelength is presented for both air holes and air core configurations of photonic crystal waveguide (PCW) made of TiO_2. It is shown that by using Atomic Layer Deposition (ALD) the expected sensitivity of the air core configuration outperforms the previously reported results.**

Index Terms— **Microsensors, Propagation, Optical planar waveguides, Sensitivity.**

I. INTRODUCTION

Photonic crystals (PC) are artificial optical materials with a periodic modulation of the refractive index. Depending on the exact periodic modulation PCs may posses a photonic bandgap. Thus, a given bandwidth of light cannot be transmitted through such a material. A wide range of devices based on bulk PCs have been presented for biosensing where the incident light perpendicular to the PC is reflected and measured. Such a method has been used for protein [1] or antibodies [2] detection.

Planar PCs in which the light is guided along defects, such as missing rows of holes or rods can be designed to obtain a very high and spatially selective sensitivity to changes in RI superior to bulk devices. The basic property of a PCW is that a given bandwidth of light can be guided in the waveguide. As in a standard waveguide, the light is confined by the film thickness vertically and by the PC horizontally. The sensing properties of PCW have already been exploited for different simple parameters. Applications of PCW include nanofluidic tuning [3] and RI measurements [4], however they have not been used for biosensing in the visible and the ultra violet. Further compare to bulk PC biosensors, PCW sensors are ultra-compact and can be integrated with both additional optical and electronic components onto one single chip. We present in this paper a 2D Finite-Difference-Time-Domain (FDTD) modeling of a PCW made of TiO_2. We describe the fabrication of air core TiO_2 PCWs by ALD and compare its modeled sensitivity to the one of a air holes device.

II. PHOTONIC CRYSTAL WAVEGUIDE CONFIGURATION

Among the great variety of deposition processes and technologies, ALD has been receiving increased attention due to its ability to deposit very thin layers at low temperatures with precise thickness and stress control and exceptional uniformity and conformality. For example, TiO_2 can be deposited by ALD and presents the characteristics of being transparent in the visible as well as having a high refractive (n=2.47). Further ALD has proven to be the appropriate technique to produce air core PCs has shown in Fig. 1 [5].

At first an Anodic Aluminum Oxide (AAO) template is prepared on a substrate Fig.1. a). It consists of a periodic array of holes with a hexagonal lattice. The TiO_2 is then deposited by ALD, layer by layer, into the AAO pores Fig.1. b). The deposition rate is of about 0.5 Angstrom per cycle. Later the upper TiO_2 is removed by polishing Fig.1. c) and the AAO template is selectively etched to obtain a periodic array of TiO_2 rods Fig.1. d). The used etchant can be phosphoric acid or KOH, both being selective for AAO against TiO_2.

The line defect to produce a PCW is made by photolithography in the AAO template. To unsure the single-mode condition for a TE polarized incident light, the waveguide thickness where the line defect is introduced, is chosen to be smaller then 100 nm.

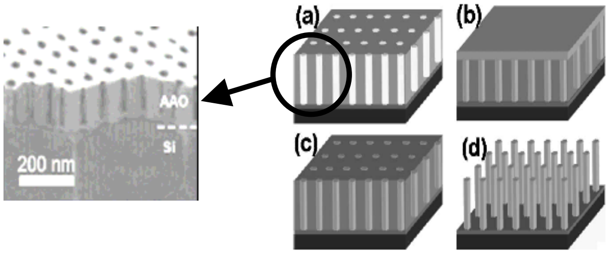


Fig. 1. Different fabrication steps to produce TiO2 pillars from an AAO template by ALD.

E. Jardinier is with Ecole Nationale Superieure D'Electronique et de Radioelectricite de Grenoble, 23 Rue des Martyrs BP 257, 38016 Grenoble, cedex 1.

G. Pandraud is with the Kavli Institute of Nanoscience, Delft University of Technology, 1 Lorentzweg, 2628 CJ Delft, The Netherlands; Phone: 0031 15 2781602; Email: g.pandraud@tudelft.nl

H.T.M Pham and P.M. Sarro are with Electronic Components, Technology and Materials, Delft University of Technology, 17 Feldmannweg, 2628 CT Delft, The Netherlands.

P.J. French is with Electronic Instrumentation Laboratory, Delft University of Technology, 4 Mekelweg, 2628 CD Delft, The Netherlands.

III. MODELING

Fig. 2. shows the PCW simulated using a 2D FDTD package and the corresponding index profiles for both air holes and air core structures. It consists of a hexagonal lattice in which the three central rows are removed.

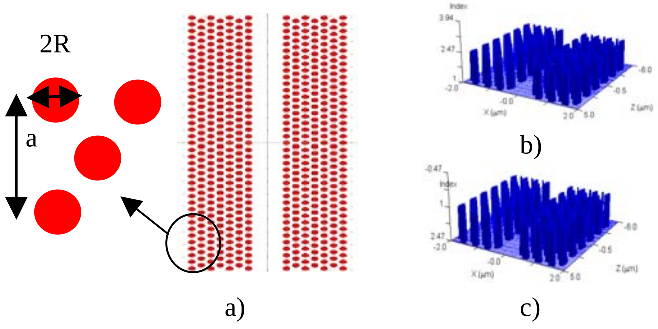


Fig. 2. a) Photonic crystal waveguide configuration ; b) The refractive index profile of a air core TiO_2 PCW ; c) The refractive index profile of a air holes TiO_2 PCW

At first, simulations are performed to optimize the lattice constant a and the rods radius R (Fig. 2.). The interesting property of PCW is the sudden drop in transmission where the transmission of the fundamental mode is no longer possible. A sharp change in transmission is a clear advantage for the actual sensor operation as it is simple to detect and gives the possibility for precise detection even for spectrum with a high degree of noise.

Four lattice constant were investigated, a = 130nm, 260nm, 390nm and 520 nm and for each of them the radius varies as r = 0.2a, 0.3a and 0.4a. Those dimensions are compatible with the dimensions of the AAO templates fabricated at Delft University of Technology [6]. They are also close to the ones usually used in PCW designs made of silicon.

The launched light is a continuous wave (CW), of Gaussian shape, of transverse electric polarization (TE), with a power normalized at 1. The output signal is collected in X=0 at the end of the device (Fig. 2.). Both structures presented in Fig. 2. b) and c) are studied and the results are presented in the following.

A. *Air holes PCW*

Fig. 3. shows the transmission spectrum of a air holes PCW for two sets of lattice parameters and hole radius. It presents a sharp drop at the lower band edge with potential high sensitivity in the UV region. However, a deeper study showed that there is no shift in wavelength while the refractive index of the cover is changing. This assumption has to be verified by experiments as it is very likely that we are reaching the limits of the FDTD software package.

The upper band edge highlights a second possible working point of the system. It is situated in the near infrared range where PCW biosensors have already been reported.

However by varying the refractive indexes of the surrounding medium (Fig. 4), we can access the sensitivity of this PCW configuration.

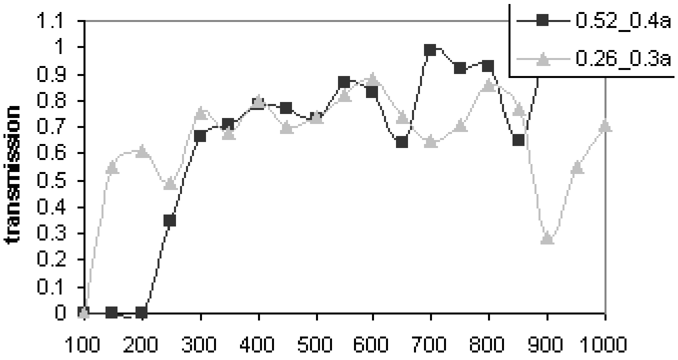
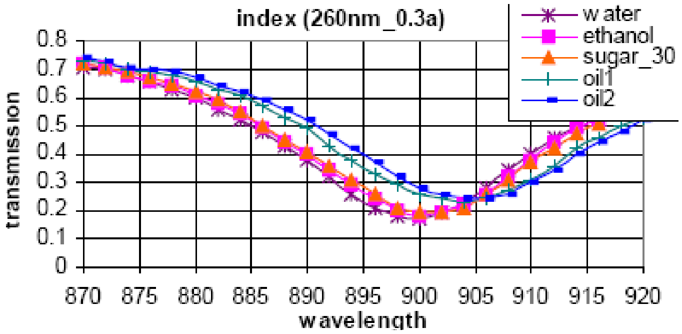


Fig. 3. Calculated transmission sprectra for TE-like polarization vs. wavelength from a air holes TiO_2 PCW in water with a=0.52/R=0.4a and a=0.26/R=0.3a



Solution	Refractive index
Water	1.33
Ethanol	1.36
Sugar 30%	1.38
Oil1	1.48
Oil2	1.518

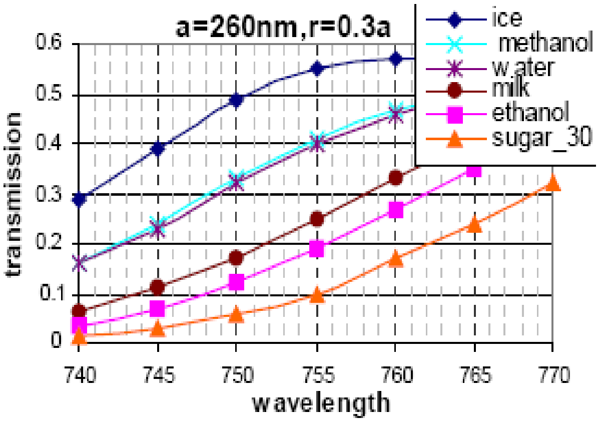
Fig. 4. Calculated transmission sprectra for TE-like polarization vs. wavelength from a air holes TiO_2 PCW in water with a=0.26/R=0.3a and for different refractive indexes.

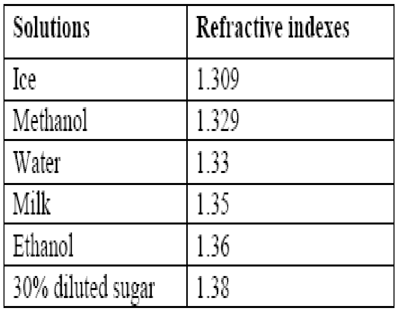
B. *Air core PCW*

Fig. 5. shows a working point of such a device when the core refractive index is varying. These PCW structures allow sensing in the visible range where sources are easy to find and cheap. The detection can also easily been integrated to as silicon absorbs in the visible. In Fig. 6 is shown a second working point that this time allows sensing in the extreme UV range.

C. *Sensitivity comparison*

Fig. 7 shows the sensitivity of the above structures. The change in wavelength is plotted against the change in refractive index. The points are all taken from the curves of Fig. 4 and 5 at a transmission level of 0.3. It shows that the most sensitive structure is the air hole PCW.





Solutions	Refractive indexes
Ice	1.309
Methanol	1.329
Water	1.33
Milk	1.35
Ethanol	1.36
30% diluted sugar	1.38

Fig. 5. Calculated transmission sprectra for TE-like polarization vs. wavelength from a air core TiO_2 PCW in water with a=0.26/R=0.3a.

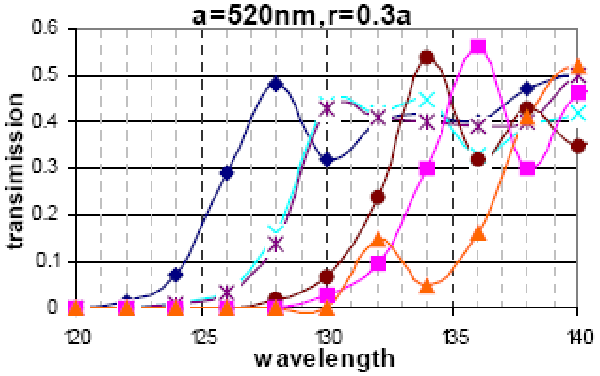


Fig. 6. Calculated transmission sprectra for TE-like polarization vs. wavelength from a air core TiO_2 PCW in water =0.52/R=0.3a giving a working point in the ultra violet.

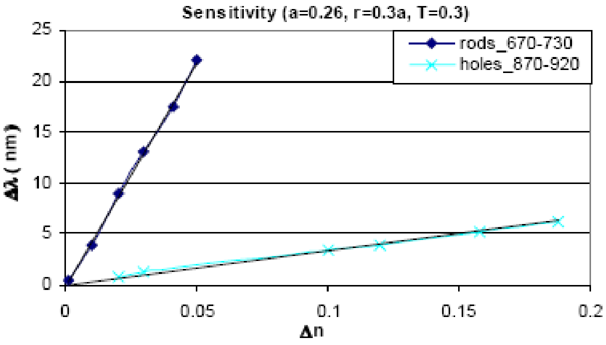


Fig. 7. Sensitivity comparison between air holes and air core TiO_2 PCW in water with a=0.26/r=0.3a at a transmission of 0.3.

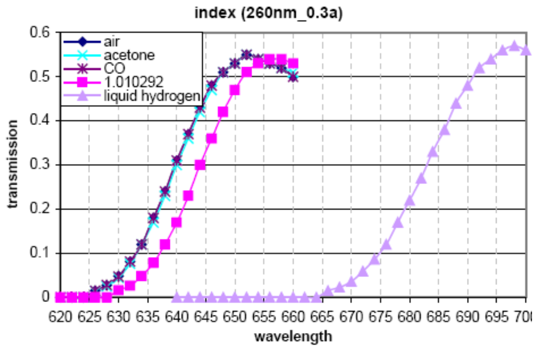
D. *Gas sensing*

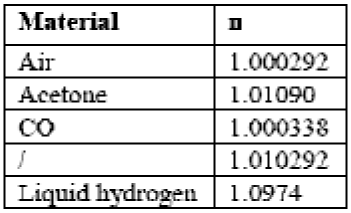
If we assume that the minimum detectable change in wavelength is in the order of 100 pm [7], from Fig. 6 we can estimate the minimum detectable change in RI. For the structure where a=260 nm and r=0.3a and in the case of a air core PCW, this minimum is found to be 0.00023 meaning that even gases can be detectable (with changes in refractive indexes of gases varying from 0.001 to 0.000001 [8]).

The previous estimation is based on the simulated results obtained for liquid so to confirm the hypothesis we performed simulations with gases for a structure having a=260 nm and R=0.3a. Fig. 8 shows the shift in wavelength obtained for different refractive indexes. The wavelength range has experienced a small shift compare to the study with liquids but stays in the visible and with a maximum of transmission of about 60 %. The sensitivity is plotted in Fig. 9.

IV. CONCLUSION

We have presented a photonic crystal waveguide used for RI measurements fabricated using ALD TiO_2. We have shown that it is a good candidate for sensing applications from the UV to the near infrared. By comparing a air holes structure to a air core structure we found out that by far the more sensitive one is the air core configuration with a sensitivity as high as 0.002 nm^{-1}. Such structure presents also a sensitivity higher than air holes biosensors made of silicon that exhibits a sensitivity of 0.0157 nm^{-1} [9]. We have also shown that a basic straight waveguide can also be used as gas sensor.





Material	n
Air	1.000292
Acetone	1.01090
CO	1.000338
/	1.010292
Liquid hydrogen	1.0974

Fig. 8. Calculated transmission sprectra for TE-like polarization vs. wavelength from a air core TiO_2 PCW in air with a =0.26/R=0.3a.

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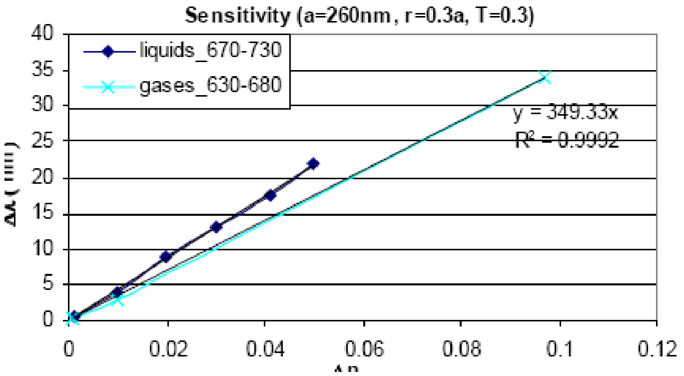

Fig. 9. Sensitivity comparison between a gas detection and a liquid detection for a air core TiO_2 PCW with a=0.26/r=0.3a at a transmission of 0.3.

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