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Atomic layer deposition of TiO₂ photonic crystal waveguide biosensors

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Abstract. A photonic crystal waveguide biosensor in the visible is presented for biosensing. 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 TiO₂. It is shown that by using Atomic Layer Deposition (ALD) the expected sensitivity of the air core configuration outperforms the previously reported results.

Keyword: Photonic crystal waveguide, biosensor, ALD.

1. Introduction

Photonic crystals (PC) are artificial optical materials with a periodic modulation of the refractive index. Depending on the exact periodic modulation PCs may possess a photonic bandgap. Thus, a given band width 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. In comparison with 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) modelling of a PCW made of TiO₂. We describe the fabrication of air core TiO₂ PCWs by ALD and compare its modelled sensitivity to the one of an air core device.

2. Photonic-crystal waveguide consideration

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, TiO₂ 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 figure 1 [5]. At first an Anodic Aluminum Oxide (AAO) template is prepared on a substrate figure 1a. 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 figure 1b. The deposition rate is of about 0.5 Angstrom per cycle. Later the upper TiO_2 is removed by polishing figure 1c and the AAO template is selectively etched to obtain a periodic array of TiO_2 rods figure 1d. 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 ensure the single-mode condition for a TE polarized incident light, the waveguide thickness, where the line defect is introduced, is chosen to be smaller than 100 nm.

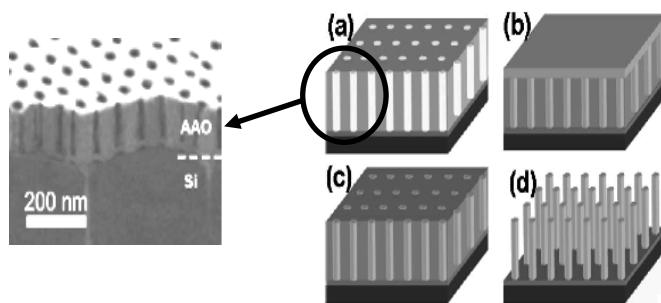


Figure 1. Different fabrication steps to produce TiO_2 pillars from an AAO template by ALD.

3. Modelling

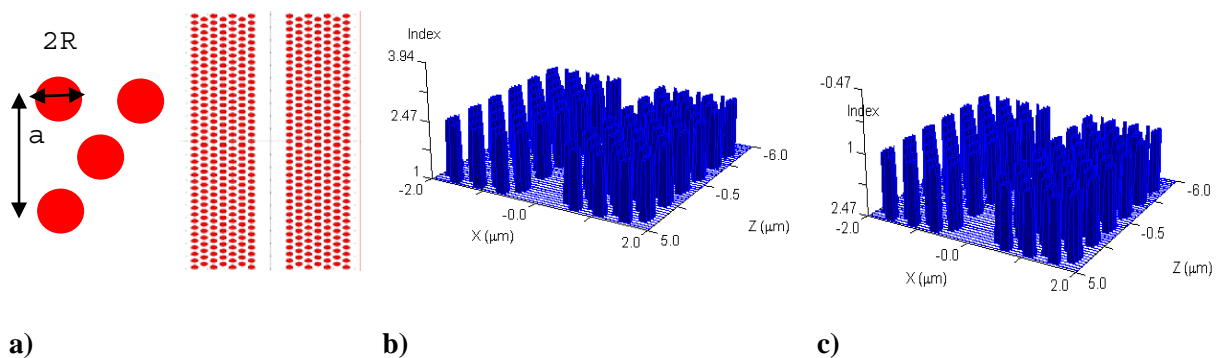


Figure 2. a) Photonic Crystal Waveguide configuration, b) index profile of an air core PCW and c) the index profile of an air holes PCW.

Figure 2 shows the PCW simulated using a 2D FDTD modeling 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. At first, simulations are performed to optimize the lattice constant and the rods radius R (figure 2). Indeed the interesting property of PCW is the sudden drop in transmission when 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, $a = 130, 260, 390$ 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 (figure 2). Both structures presented in figure 2b and 2c were studied and the results are presented in the following.

3.1. Air core PCW

Figure 3 shows the main working points of such a device when the core refractive index is varying. Two PCW structures b) and c) allow sensing in the visible range and in the red where sources are easy to find and cheap. The structure a) allows sensing in the extreme UV range.

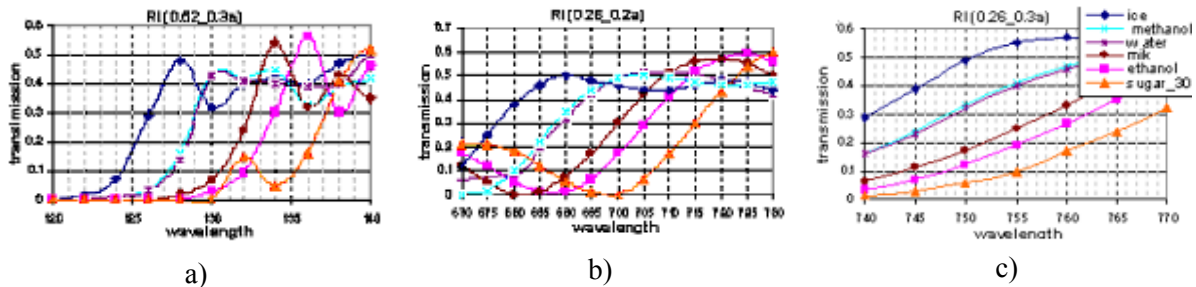


Figure 3. Simulated transmission spectra of the air core PCW for various liquids for a) $a = 0.52$, $r = 0.3a$, b) $a = 0.26$, $r = 0.2a$ and c) $a = 0.26$, $r = 0.3a$.

Figure 4 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 figure 3 at a transmission level of 0.3. It shows that the most sensitive region of the spectrum is the region around 700 nm.

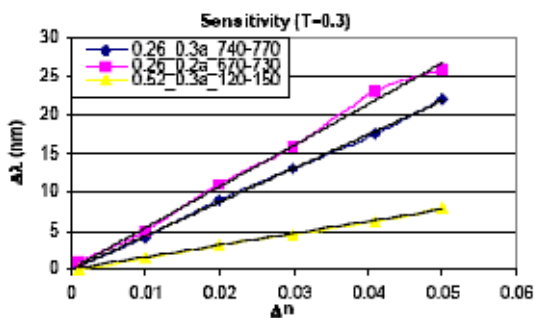


Figure 4. Sensitivity of an air core TiO_2 PCW for different lattice size and radius.

3.2. Air holes PCW

Figure 5 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, to get all the working points of PCW made of TiO_2 , we performed the same study as for the air core PCW. This time the refractive indexes chosen were larger (figure 6) than in the previous case showing that the sensitivity is lower for this PCW configuration.

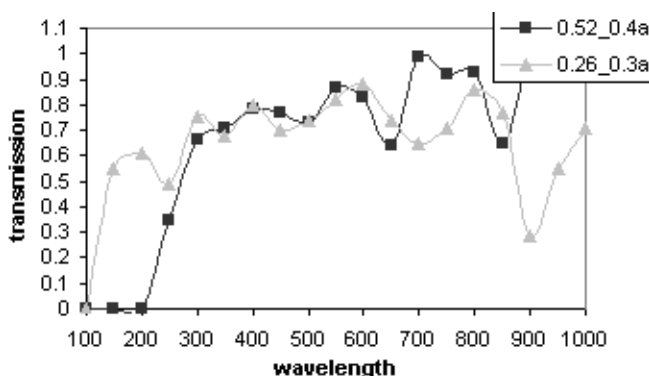


Figure 5. Calculated transmission spectra for TE-like polarization vs. wavelength from a TiO_2 PCW in water with $a = 0.52$ and $R = 0.4a$ and $a = 0.26$ and $R = 0.3a$.

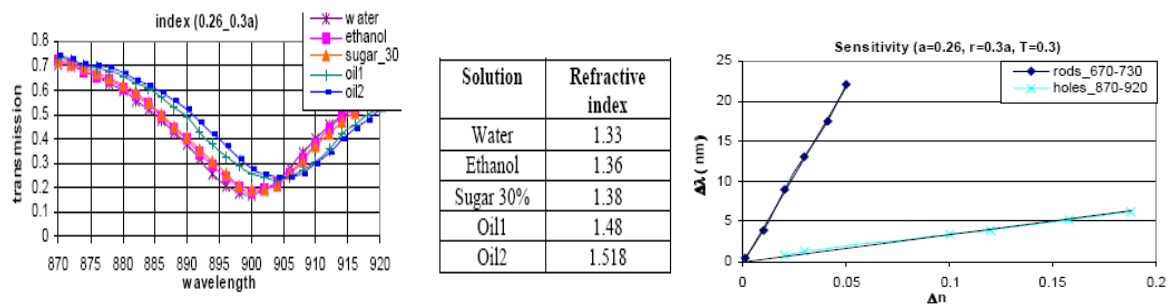


Figure 6. a) Calculated transmission spectra for TE-like polarization vs wavelength from a TiO₂ PCW for different covers with the different refractive indexes used; b) Sensitivity comparison between air holes and air core TiO₂ PCW with a = 0.26 and R = 0.3a at a transmission value of 0.3.

4. Conclusion

We have presented a photonic crystal waveguide used for RI measurements fabricated using ALD TiO₂. We have shown that it is a good candidate for sensing applications from the UV to the near infrared. By comparing an air holes structure to an air core structure we found out that by far the more sensitive one is the air core configuration with sensitivity as high as 0.002 nm⁻¹. Such structure presents also sensitivity higher than air holes biosensors made of silicon that exhibits a sensitivity of 0.0157 nm⁻¹ [7].

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