

# Comparative sensitivity analysis of integrated optical waveguides for near-infrared volatile organic compounds with 1ppb detection

Wei-Cheng Lai<sup>a</sup>, Yi Zou<sup>\*,a</sup>, Swapnajit Chakravarty<sup>\*,b</sup>, Liang Zhu<sup>a</sup>, Ray T. Chen<sup>\*,a,b</sup>

<sup>a</sup>Dept. of Electrical and Computer Engineering, University of Texas, 10100 Burnet Road Bldg. 160, Austin, TX, USA 78758;

<sup>b</sup>Omega Optics Inc., 8500 Shoal Creek Blvd., Bldg. 4, Suite 200,, Austin, TX, USA 78757

## ABSTRACT

We compared different on-chip silicon waveguide based absorption sensors for the detection of xylene in water in near-infrared with detection limit down to 1ppb. Strip waveguide, slot waveguide and PC-based chip integrated optical absorption spectroscopy devices are compared in near-infrared. PCW utilizes slow light effect to enhance absorbance and is most sensitive while slot waveguide strengthens light-matter interaction in a narrow low index slot by a factor up to 10 and performs better than a strip waveguide. The results provide a route for enhanced sensitivity via absorption spectroscopy while retaining device miniaturization.

**Keywords:** spectroscopy, photonic crystal waveguide, waveguides, infrared.

\*yzou@utexas.edu, swapnajit.chakravarty@omegaoptics.com, raychen@uts.cc.utexas.edu;  
phone 1 512 471-4349; fax 1 512-471-8575;

## 1. INTRODUCTION

Infrared (IR) absorption spectroscopy is widely accepted as the ideal technique for chemical sensing due to the unique capability to distinguish analytes of interest based on unique molecular vibration signatures [1,2]. It has an overwhelming advantage over other methods that depend on sensing changes in refractive index. In our previous work, PC slot waveguide structures successfully detected and identified VOCs in liquid and gaseous phases for xylene in water and methane in nitrogen respectively [3, 4]. Results showed that the enhancement due to slow light effect in photonic crystal waveguide (PCW) greatly reduces the total interaction length with chemical analytes. The length of PC slot waveguide for sensing xylene in water is only 300 $\mu$ m, which showed that the miniature PCW structure is an ideal platform for chip integrated optical absorption spectroscopy. Miniaturization enables the potential for multiplexed detection for the simultaneous identification and quantification of multiple organic compounds of interest. We also detected xylene and trichloroethylene in water simultaneously by multiplexing PCW with different lattice constants [5].

In this paper, we experimentally compare absorbance of different types of silicon waveguide devices in the near-infrared including PC waveguide, slot waveguide and strip waveguide. The results show PC waveguide has the best performance among these three devices while slot waveguide is superior to strip waveguide. The results are consistent with theoretical prediction.

## 2. DEVICE WORKING PRINCIPLE

The principle of operation of optical absorption spectroscopy is governed by the Beer–Lambert law. According to this law, the transmitted intensity  $I$  is given by

$$I = I_0 \times \exp(-\gamma\alpha L) \quad (1)$$

where  $I_0$  is the incident intensity,  $\alpha$  is the absorption coefficient of the medium,  $L$  is the interaction length, and  $\gamma$  is the medium-specific absorption factor determined by dispersion-enhanced light–matter interaction. For various applications,  $L$  must be large to achieve high sensitivity since  $\gamma=1$ . In addition, from perturbation theory

$$\gamma \propto f \times \frac{c/n}{n_g} \quad (2)$$

where  $c$  is the speed of light in free space,  $v_g$  is the group velocity in the medium, and  $n$  is the refractive index of the medium [6]. The term  $f$  is the filling factor denoting the relative fraction of optical field residing in the analyte medium. Group velocity  $v_g$  is inversely proportional to the group index  $n_g$ .

Photonic crystal waveguides (PCWs) have demonstrated group velocity slow-down factors  $\sim 100$  [7]. Slot waveguides have also demonstrated significant increase in the electric field intensity in a narrow low index slot in a high index ridge waveguide, by at least a factor of 10 [8]. Slow light in PC waveguides coupled with electric field intensity enhancement in a slot in the PC waveguide, can therefore reduce  $v_g$  and enhance  $f$ , thereby theoretically shrinking the required absorption path length by a factor of 1000, an order of magnitude greater than ring resonator devices [9].

Hence, theoretically, the optical absorbance by a waveguide on a same chip increases in order as follows in silicon: (a) strip waveguides, ( $n_g \sim 3$ ), (b) slotted strip waveguides ( $n_g \sim 3, f \sim 10$ ) since the intensity of light in a low-index slot is significantly enhanced compared to strip waveguides, (c) PCWs ( $n_g \sim 100$ ) [7], and (d) slotted PCWs ( $f \sim 10$  and  $n_g \sim 100$  for a combined factor of  $\sim 1000$ ).

During the past two decades, PC devices have attracted significant interest due to their unique dispersive properties that allow control and manipulation of light-matter interactions on length scales of the wavelength of light [10]. Various miniature applications have been demonstrated with PC microcavities and PC slot waveguides for light emission [11], cavity quantum electrodynamics [12] and electro-optical modulation [13]. PC devices have shown significant promise in sensing applications due to high sensitivity to refractive index changes of the ambient [14]. Change in refractive index of a medium caused by an analyte is however not sufficiently analyte-specific and is therefore not a unique signature of the analyte. In contrast, absorption spectrum of an analyte is based on analyte-specific molecular vibrations, and thus identifies the analyte uniquely. In this paper, we demonstrate a PC waveguide that enables near-infrared spectroscopy of xylene in water, xylene being chosen as a representative volatile organic compound (VOC) contaminant in water with environmental and human health significance.

### 3. DEVICE DESIGN

All the devices are on SOI platform which has 250nm silicon nanomembrane on top of 3 $\mu$ m buried oxide and 500  $\mu$ m handle silicon substrate. In Fig. 1(a), the structure we design is based on W1 line defect waveguide with lattice constant  $a$ , where W1 denotes the width of PCW is  $\sqrt{3}a$ . The air hole diameter is  $d=0.53a$  and silicon slab thickness is  $h=0.63a$ . The PCWs are designed so that the slow light guidance bandwidth of PCW overlaps with the absorbance peaks at 1674nm. In our structure, the device has lattice constant  $a=405$ nm. Hence it will have a bandedge around 1675nm. Fig. 1(b) shows the designed slot waveguide working at 1674nm with SU8 top cladding. The device has 240nm rail width and 120nm slot width on SOI platform that result to 1.88 effective index. A single mode strip waveguide with 500nm width and 250nm height dimension is also shown in Fig. 1(c).

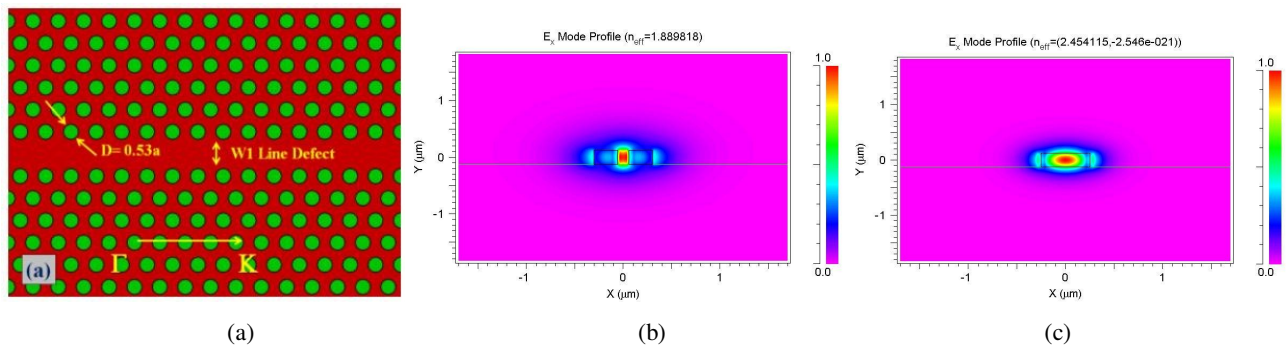


Fig. 1. (a) photonic crystal structure, (b) slot waveguide, and (c) strip waveguide.

## 4. DEVICE FABRICATION

Devices were fabricated on silicon-on-insulator (SOI) wafer with 250nm top silicon layer and 3 $\mu$ m buried oxide. PC waveguides, tapers, slot waveguides and strip waveguides are patterned in one step with e-beam lithography followed by reactive ion etching. Scanning electron micrograph (SEM) of fabricated structure is shown in Fig 2. SU8 top cladding was prepared by spinning, followed by baking for 3 mins at 95°C. The device processing prior to SU8 deposition is exactly the same as in a previous demonstration of biomarker detection with the photonic crystal microcavity device [15]. Similar to previous demonstration of PC slot waveguide in xylene detection, SU8 is hydrophobic; hence the absorption spectrum of VOCs can be obtained independent of any interference from the strong absorbance signatures of water. In contrast to our previous method using PDMS as the VOC absorbing layer [4], we found that SU8 has low optical absorption loss in the wavelength range of interest between 1620-1700nm resulting in high signal-to-noise ratio

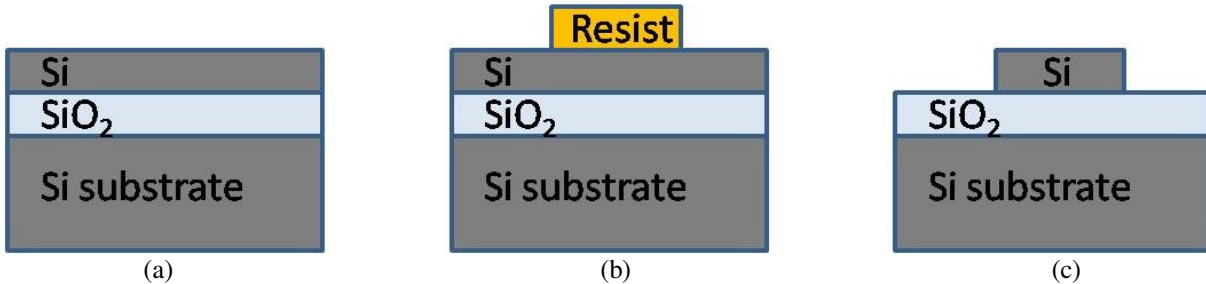


Figure 2: Fabrication steps of a PC slot waveguide (a) Start with Piranha cleaned SOI wafer (b) E-beam Resist (ZEP-520A) patterning (c) Transfer of resist pattern to Si by RIE in HBr and Cl<sub>2</sub>.

Scanning electron micrograph (SEM) images are shown in Fig. 3 for fabricated devices. Absorption signature of xylene in near-infrared extends from 1665nm to 1745nm with absorption peaks at 1674nm, 1697nm and 1720nm respectively. Here we focus our PCW design targets 1674nm wavelength since 1697nm and 1720nm are not at the best working wavelength of our optical spectral analysis (OSA).

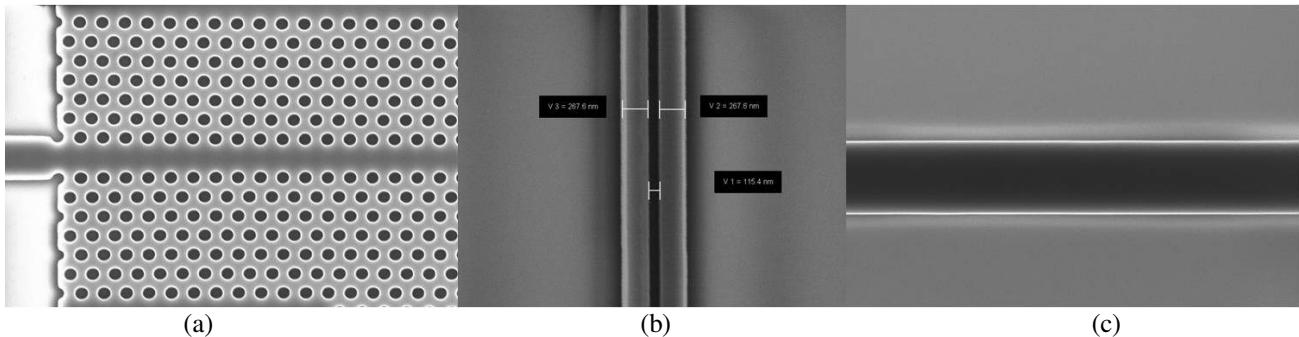


Fig. 3. SEM images of fabricated devices on SOI substrate (a) W1 type PCW, (b) slot waveguide, and (c) single mode strip waveguide.

## 5. EXPERIMENTAL RESULTS

Light is coupled in and out through grating coupler and PCW to detect the chemical analytes. The transmission of the device designed for xylene is shown in Fig. 4(a). It shows the band edge is located at 1676nm for device with  $a=405$ nm for xylene detection as in Fig. 4(a). Transmission spectra show that the slow light region near the transmission band edge overlaps with the absorbance peaks of xylene. The testing xylene sample is added on top of SU8 cladding, we wait for 10 mins and then measure the transmission and do the absorbance calculation. Fig. 4 (b) shows the xylene absorbance when 10<sup>-3</sup> % (v/v) concentration is added. A strong absorbance peak is located around 1674nm while the adjacent wavelength has negligible absorbance which confirms the absorbance is from xylene. Fig. 4(c) shows the absorbances

measured at 1674nm for xylene as a function of the increasing concentration of the analytes. From the absorbance, the detection limit for device for xylene is  $10^{-7}$  % (v/v) in water (~1ppb).

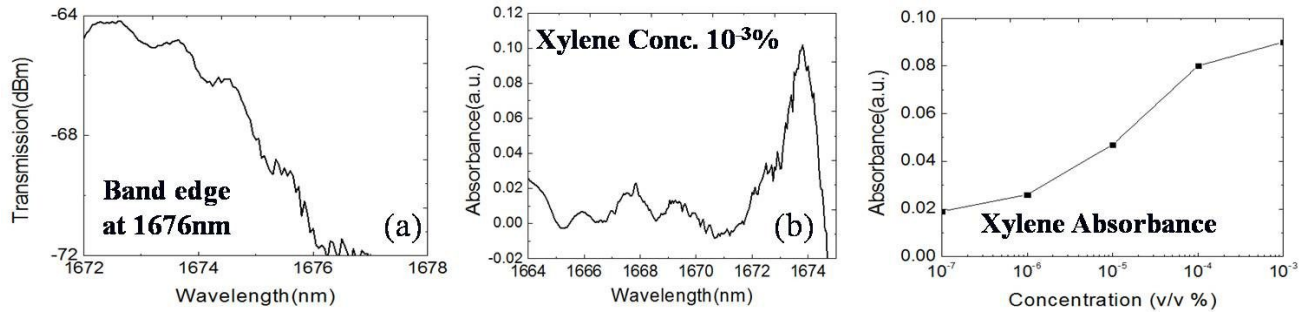


Fig. 4. (a) Experimental transmission of device for xylene which has band edge around 1676nm, (b) Absorbance around 1674nm (c) Absorbance of xylene at different concentrations.

We also measured xylene with different concentration by using slot waveguide and strip waveguide following the same procedure as we did by using PCW device. The absorbance of these three devices are plotted as a comparison shown in Fig. 5. As we can clearly see that the PCW has the best performance among these three types of devices. The slot waveguide also shown very good respond when different concentrations is added, the absorbance is a little weaker than PCW but significantly better than single mode strip waveguide.

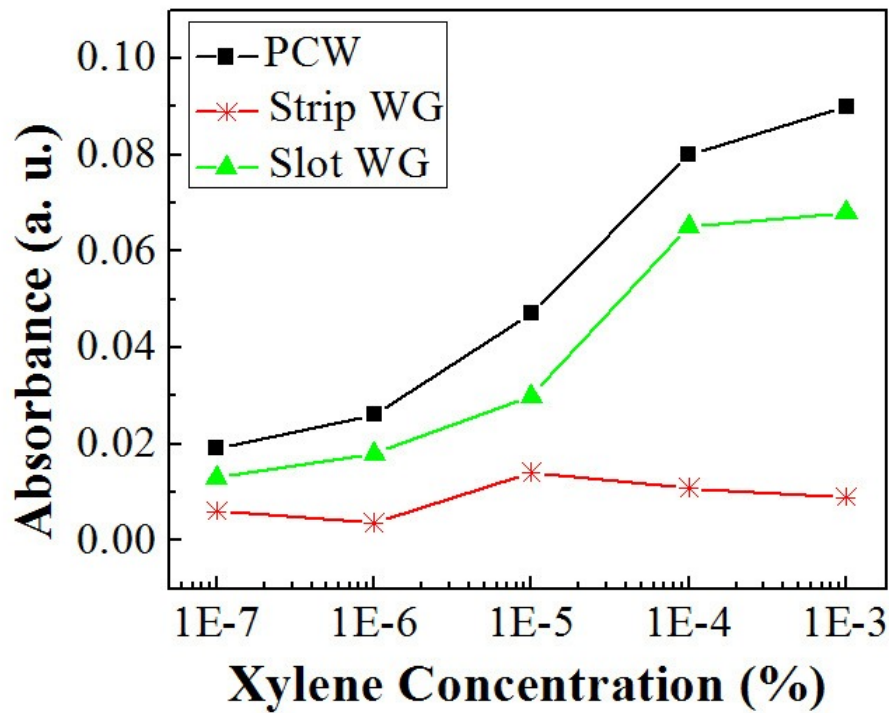


Fig. 5. Absorbance comparison of xylene measured at 1674 nm with strip waveguide (red), slot waveguide (green), and PCW (black) for NIR

## 6. SUMMARY

In summary, we demonstrated a 300  $\mu\text{m}$  long on-chip silicon based absorption spectroscopy sensor for the detection of xylene in water in near-infrared with detection limit down to 1ppb. Strip waveguide, slot waveguide and PC-based chip integrated optical absorption spectroscopy devices are compared in near-infrared. The results provide a method for further improving the sensitivity while ensuring device miniaturization.

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