

# Silicon on Sapphire Chip Based Photonic Crystal Waveguides for Detection of Chemical Warfare Simulants And Volatile Organic Compound

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**Abstract:** We experimentally demonstrate the first holey and slotted photonic crystal waveguides in silicon-on-sapphire at mid-infrared wavelength of 3.43 $\mu$ m. Chemical warfare simulant triethylphosphate was detected in gas phase at 10ppm concentration via optical absorbance signature.

**OCIS codes:** (300.6340) Spectroscopy, Infrared; (130.6010) Sensors; (130.5296); Photonic crystal waveguides

Infrared (IR) absorption spectroscopy is widely accepted as the ideal technique for chemical sensing due to its capability to distinguish analytes of interest based on unique molecular vibration signatures [1],[2]. Slow light in photonic crystal waveguides (PCWs) [3] and slotted photonic crystal waveguides (SPCW) [4],[5] has been used to reduce the optical absorption path length and achieve high detection sensitivity in on-chip optical absorption spectroscopy for the selective detection of volatile organic compounds (VOCs) [3], [4] and greenhouse gases [5] based on unique analyte absorption signatures in the near-infrared (near-IR). In contrast to the near-IR, the mid-infrared (mid-IR) wavelengths offer at least two orders of magnitude larger absorption cross-sections than the near-IR. We previously compared absorbance of different waveguide devices in the near-IR [6] with strip waveguides in the mid-IR [7] and showed the higher sensitivity to the detection of VOC xylene in water. PCW devices enable higher absorbance of light by analyte due to the unique slow light effect afforded by this platform and hence higher absorbance sensitivity in the mid-IR.

In this paper, we experimentally investigate three PCW based structures that take benefits of the slow light effect to enhance light matter interaction. The first structure is a regular PCW with no defect holes along the propagation direction within the PCW. The second one is a holey PCW (HPCW) wherein smaller diameter holes than the bulk PC are etched along the propagation direction within the PCW at the antinodes of the PCW propagating mode. The third is a SPCW wherein a rectangular slot is etched uniformly at the center of the PCW from the input to the output.

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 free-space based sensors,  $L$  must be large to achieve high sensitivity since  $\gamma=1$ . 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 [8]. 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  $n_g$ . 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 ( $n_g \sim 100$ ), and (d) slotted PCWs ( $f \sim 10$  and  $n_g \sim 100$  for a combined factor of  $\sim 1000$ ). In mid-infrared, fundamental vibration signatures of organic compounds are stronger by two to three orders of magnitude in general than their corresponding overtones in the near-infrared. Hence, due to an increase in  $\alpha$  in Eq. 1, together with the device enhancements from Eq. 2, mid-infrared spectroscopy can be expected to have a larger sensitivity in absorption spectroscopy than in the near-infrared.

In mid-infrared, due to strong absorption loss from silicon dioxide, silicon on sapphire (SOS) substrate is considered as an alternative material which has a transparent window up to 5.5 $\mu$ m and high refractive index contrast between the core and the cladding. The wavelength adopted is at 3.43  $\mu$ m which has a stronger absorption peak for xylene and triethylphosphate. Device fabrication and measurement setup are described in our previous work [9]. We

developed an experimental method to enable our single wavelength probe laser working at the high  $n_g$  region to fully utilize the slow light effect [10]. The fabricated devices are shown in Figs. 1(a)-(c) for regular PCW, HPCW and SPCW respectively. The corresponding electric field profiles are shown in Figs. 1(d)-(f) and intensity enhancement are shown in Figs. 1(g)-(i) respectively. It is clear that SPCW has the biggest enhancement factor compared with the other two while HPCW is also 4 times stronger than regular PCW. The sensitivity of the three devices is first characterized by adding tetrachloroethylene ( $C_2Cl_4$ ) on the device. 3D FDTD simulation and experimental results are plotted in Figs. 2(a)-(c) and Figs. 2(d)-(f) respectively. Both theoretical and experimental results show SPCW device is the most sensitive followed by HPCW and then regular PCW due to the progressively larger mode overlap with analytes, for the same slowdown factors. However, due to large propagation loss of SPCW device, it is hard to make a SPCW around 1mm length, we hence made a trade-off between the sensitivity and length and then decide to use HPCW device for gas sensing. Time scanning of power change of 800 $\mu$ m long HPCW is plotted in Figs. 2(g) and (h) when 10ppm and 50ppm of TEP gas in nitrogen is introduced. In comparison, a significant change in absorbance with TEP was observed in a slot waveguide at a much higher concentration of 28pph (parts per hundred) in Fig. 2(i). No change in 9mm long strip waveguide absorbance due to TEP was observed at 28pph.

In summary, we demonstrated three PCW based devices for the first time in mid-IR in SOS. The chemical warfare simulant TEP was identified by absorption signatures in an 800 $\mu$ m long HPCW. Higher mid-IR sensitivity of PCW devices versus strip and slot waveguides was demonstrated. Experimental detection of xylene is in progress.

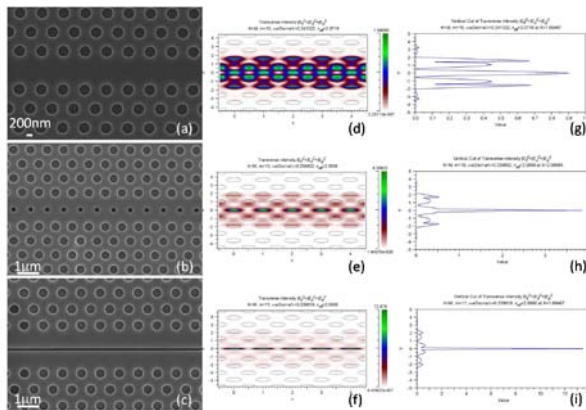


Fig. 1. SEM images of fabricated devices on SoS substrate (a) traditional PCW, (b) Holey PCW, and (c) Slotted PCW. Electric field intensity profile of the propagating slow light mode at the Brillouin zone boundary (d) traditional PCW, (e) Holey PCW, and (f) Slotted PCW. Cross-section of the electric field intensity profile at the center of PCW (g) traditional PCW, (h) Holey PCW, and (i) Slotted PCW.

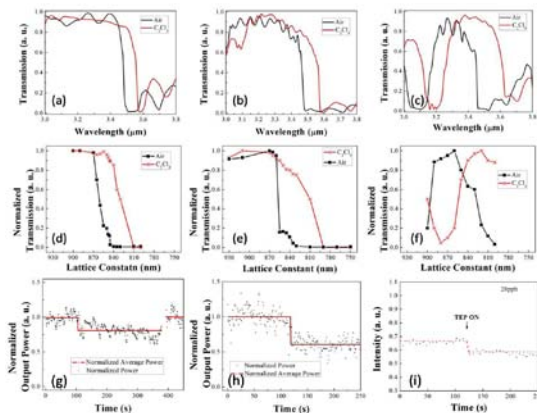


Fig. 2. Simulated transmission with air-clad and  $C_2Cl_4$ -clad conditions for (a) traditional PCW, (b) Holey PCW, and (c) Slotted PCW. Measured normalized transmitted intensity through air-clad and  $C_2Cl_4$ -clad conditions for (d) traditional PCW, (e) Holey PCW, and (f) Slotted PCW. TEP sensing measurement (g) 10ppm concentration, and (h) 50ppm concentration using 800 $\mu$ m long HPCW. (i) 28pph concentration using slot waveguide.

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## Acknowledgements

The authors thank NSF for partially supporting this work (SBIR Grant #IIP-1127251). S.C., P.W and R.C acknowledge the Army SBIR Contract #W911SR-12-C-0046 for partially supporting this work.