On-chip sensing of volatile organic compounds in water by hybrid polymer and silicon photonic-crystal slot-waveguide devices

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ABSTRACT

Lab-on-chip integrated infrared spectroscopy and sensing with hybrid polymer and silicon photonic crystal slot waveguides is demonstrated for the specific and selective identification of volatile organic compounds, xylene and toluene, in water. A 300 micron long photonic crystal slot waveguide was demonstrated that enabled the detection of 100ppb xylene in water by near-infrared absorption signatures, with five times higher sensitivity on an order of magnitude smaller length scale. The on-chip absorption spectroscopy, determined by Beer-Lambert absorption law, is enabled by the combined effects of slow light and high electric field intensity enhancement in photonic crystal slot waveguides.

Keywords: photonic crystal waveguide, photonic crystal slot waveguide, on-chip absorption, infrared absorption spectroscopy.

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1. INTRODUCTION

Infrared (IR) absorption measurements are the simplest label free techniques for detection and identification of substances based on their unique spectral signatures. It is widely used in applications in organic [1] and inorganic chemistry, studies of polymer degradation in forensic analysis [2], water content or moisture characterization in agricultural and food products [3], fuel quality control [4], hydrocarbon processing [5] and refining and petroleum characterization [6]. On-chip infrared absorption spectroscopy provides an opportunity to make a new generation of sensors that recognize substances based on their unique molecular absorption signatures. However, in order to provide the same or similar sensitivity as bench-top sensors, it is necessary to have the same effective absorption path length. We previously demonstrated that photonic crystal slot waveguides provide the combined benefits of slow light and high electric field enhancement in a narrow low index slot which increase the effective absorption path length on miniature length scales that can be shrunk to dimensions of a chip which can thus be fabricated by planar lithography [7-8]. Furthermore, since the dispersive properties of photonic crystal slot waveguides are determined by Maxwell's electromagnetic wave equations which are independent of frequency, designs are therefore valid across a wide wavelength range as long as the material of the waveguide is transparent. Since silicon is transparent in the wavelength range 1.2-6μm, the silicon platform can be used for the fabrication of chip-integrated near-infrared absorption spectroscopy sensors.

The slow light bandwidth is however small ~10nm over which the group index is greater than 20, hence multiple photonic crystal slot waveguides each covering a portion of the infrared spectrum need to be fabricated on the chip to create a complete absorption spectroscopy device. Furthermore, the group index changes continuously as a function of wavelength from the transmission band edge of the photonic crystal slot waveguide. Since it is necessary to ensure that the slow light bandwidth of the photonic crystal slot waveguide coincides with the absorption peak of the material to be detected, small errors in device fabrication can cause the slow light bandwidth to deviate leading to reduction in slow light effect and hence a reduction in sensitivity.

In this paper, we present designs of photonic crystal slot waveguide devices with a nearly constant group index over a range of wavelength that results in a fabrication tolerant design to ensure the sensitivity of the device at the absorption

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maxima of the substance to be detected. Designs are presented here for the detection of two volatile organic compounds, xylene and trichloroethylene (TCE) in water by near infrared on-chip absorption spectroscopy. Near-infrared absorption signatures of xylene and TCE are located at 1697nm and 1646nm respectively.

2. PRINCIPLE OF OPERATION

The principle of infrared absorption spectroscopy is based on the Beer-Lambert law. According to this law, transmitted intensity I is given by:

$$I = I_0 \exp(-\gamma\alpha L) \;\ldots\ldots..(1)$$

where I_0 is the incident intensity, a is the absorption coefficient of the medium, L is the interaction length and γ is the medium-specific absorption factor determined by dispersion enhanced light-matter interaction. In conventional free-space systems, $\gamma = 1$; thus L must be large to achieve a suitable sensitivity of measured I/I_0.

For lab-on-chip systems, L must be small, hence g must be large. Mortensen et al showed [9] using perturbation theory that

$$\gamma = f \times \frac{c/n}{v_g} \;\ldots\ldots\; (2)$$

where c is the velocity of light in free space, vg is the group velocity in medium of effective index n and f is the filling factor denoting relative fraction of optical field residing in the analyte medium. Equation 2 shows that slow light propagation (small v_g) significantly enhances absorption. Furthermore, greater the electric field overlap with analyte, greater the effective absorption by the medium. Both conditions of small v_g and high f are fulfilled in a photonic crystal slot waveguide.

Photonic crystal (PC) waveguides have demonstrated group velocity slow-down factors ~100 [10]. 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 [11]. 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 [7-8].

3. DEVICE DESIGN

The photonic crystal waveguide (PCW) is a hexagonal structure with a Wx line defect waveguide with uniform lattice constant a, where Wx denotes that width of the PCW is x times $\sqrt{3}a$. Silicon slab thickness and air hole diameter are $h=0.5a$ and $d=0.55a$. A slot is patterned at the center of the photonic crystal waveguide of width $w=0.2a$. Various designs for photonic crystal slot waveguides with different constant group indices are made as shown in Fig. 1.

As described previously, poly dimethyl siloxane (PDMS) is spin coated as the top cladding. Since PDMS is hydrophobic, use of PDMS ensures that absorption signatures of xylene are obtained without interference from strong near-infrared absorption of water. The PDMS cladding thickness is chosen appropriately to avoid interaction between the guided optical mode in the slot and the water ambient. All designs are performed with the flat band slow light region centered on the absorption peak of xylene at 1697nm. As observed in Fig. 1, devices are designed for group indices 25, 31, 38 and 46.5 respectively. The flat band slow light bandwidth in each case is indicated in the figures. It is noted that as the group index increases, the bandwidth of the slow light region decreases. To ease fabrication, radius of all holes is kept constant.

As shown in Fig. 2, final design parameters are chosen so that n_g ~30 and varies by less than 10% within a bandwidth of 5.3nm around the center wavelength of 1697nm. Our fabrication in the past has shown that repeatability can be achieved within ±2nm of the designed wavelength. Hence, a fabrication tolerant design has been made to guarantee the absorption efficiency at the wavelength of the specific chemical absorption maximum.

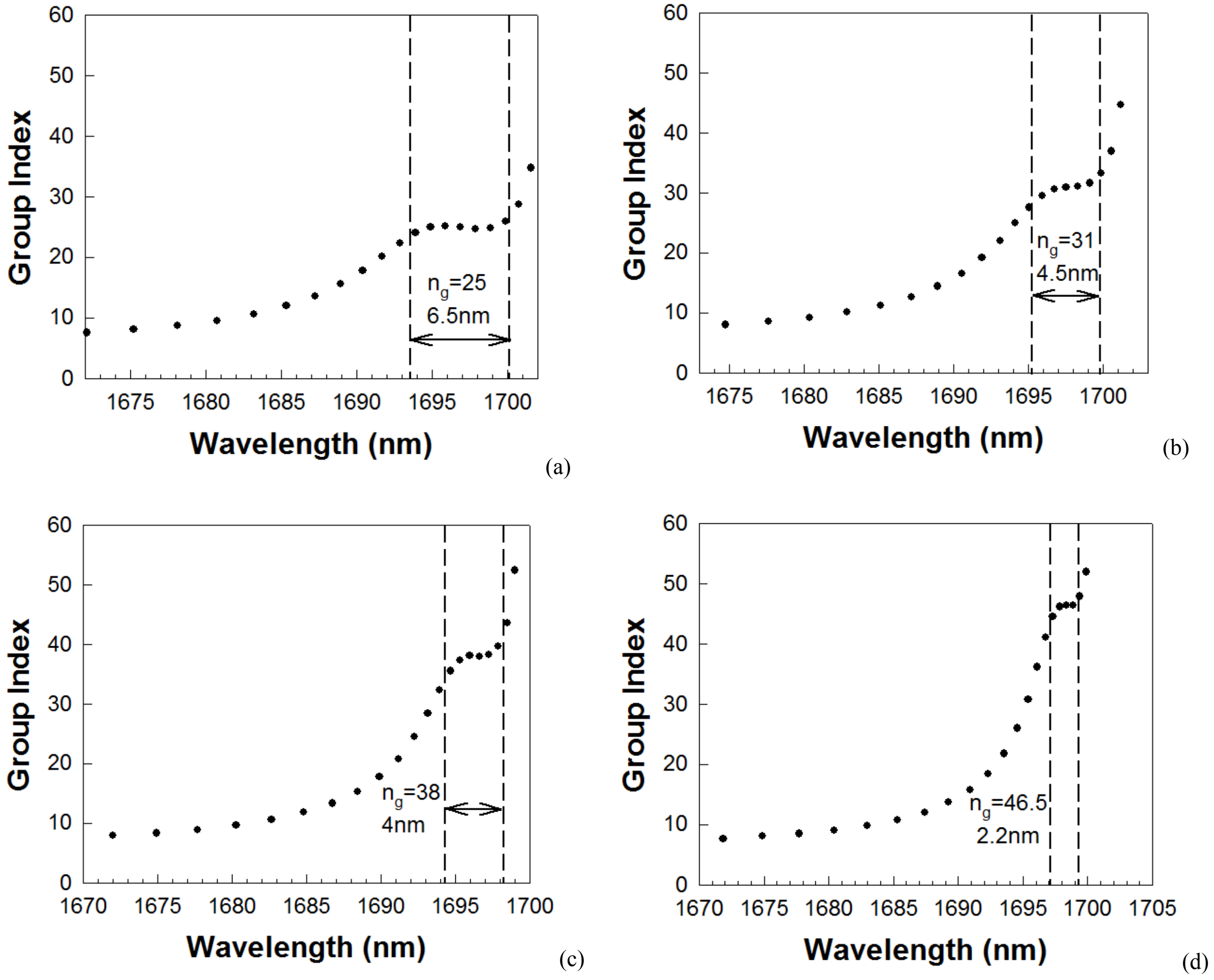


Fig. 1: Designs for flat group index profiles versus bandwidth showing that the bandwidth related inversely with flat band group index.

In addition to the flat band slow light design, it is also necessary to ensure that light can be coupled efficiently from the ridge waveguide to the photonic crystal slot waveguide at the slow light wavelengths. A group index taper is therefore designed where the group index is varied gradually from the ridge waveguide to the photonic crystal slot waveguide. Fig. 3 shows the group index taper designed at the wavelength of 1697nm. n_g ~30 has been chosen conservatively in Fig. 2 since our past research has shown that good coupling efficiency can be achieved up to n_g ~38. We have chosen n_g ~30 so that a wide flat band slow light bandwidth of 5.3nm is observed. [12]

Two volatile organic compounds with no overlap in their absorption spectrum are chosen to show the multiplexed and mutually exclusive nature of detection. As shown in Fig. 4, xylene has an absorption spectrum maximum at 1697nm. Trichloroethylene (TCE) has an absorption maximum at 6075cm^{-1} (1646nm). The two chemicals each have zero absorption at the other's respective absorption maximum. The same design as demonstrated above at 1697nm is repeated at 1646nm. The only difference between the two photonic crystal slot waveguides is the lattice constant *a*. For the device at 1697nm for xylene detection, *a*=436nm. For the device at 1646nm for TCE detection, *a*=422.5nm

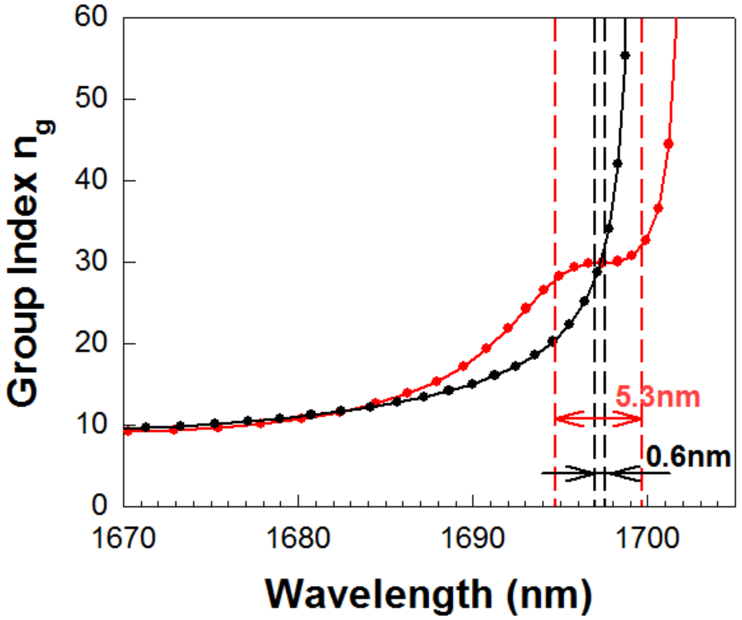


Fig. 2: Group Index profile of the photonic crystal slot waveguide (a) black curve as designed in Phase 1 with the bandwidth shown by the black dashed lines and (b) current design shown by the red curve with flat band profile over a bandwidth of 5.3nm between red dashed lines.

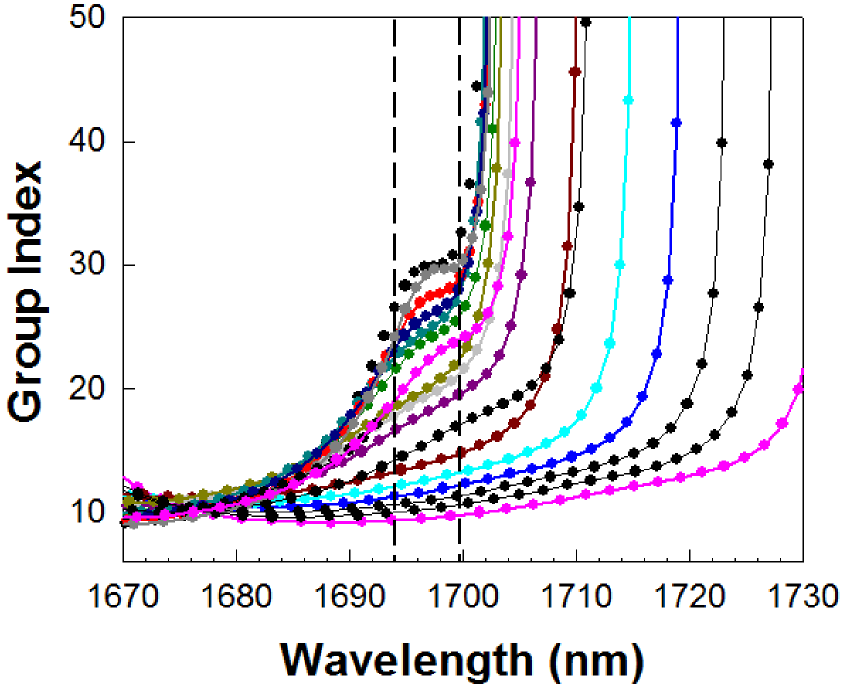
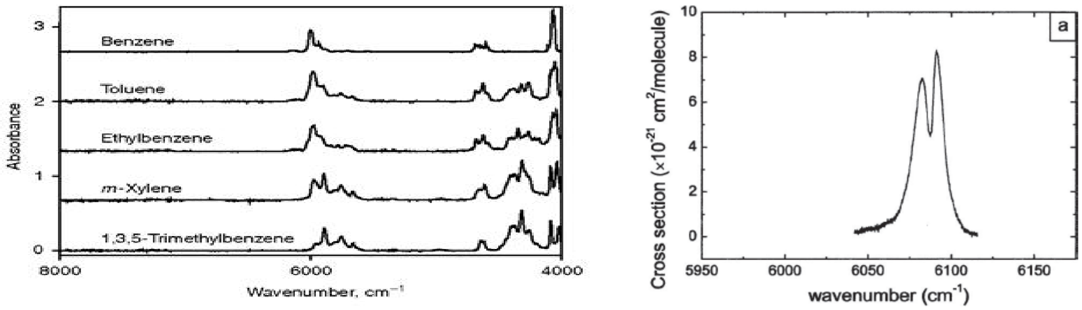
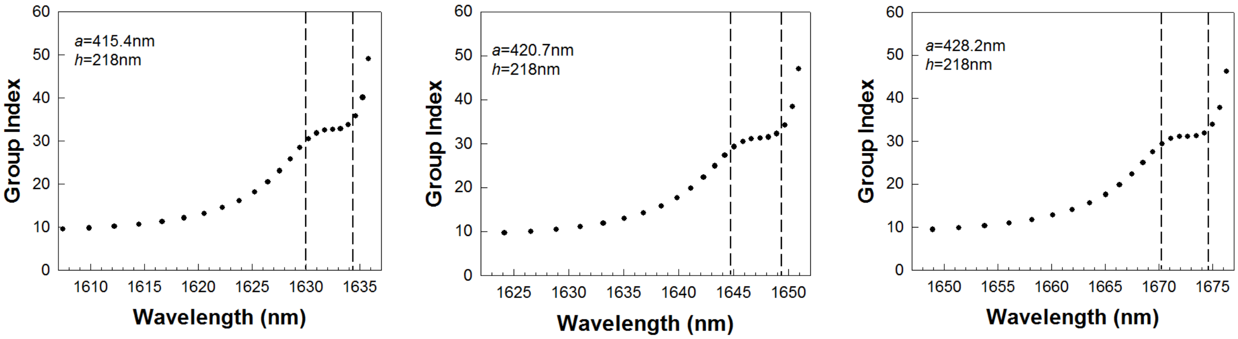


Fig. 3: Group Index taper design showing the gradual change in group index from low values (shown by pink curve) to the final design value shown by the black scatter plot.



(a) (b)

Fig. 4: Absorption spectrum of (a) m-xylene and (b) trichloroethylene.

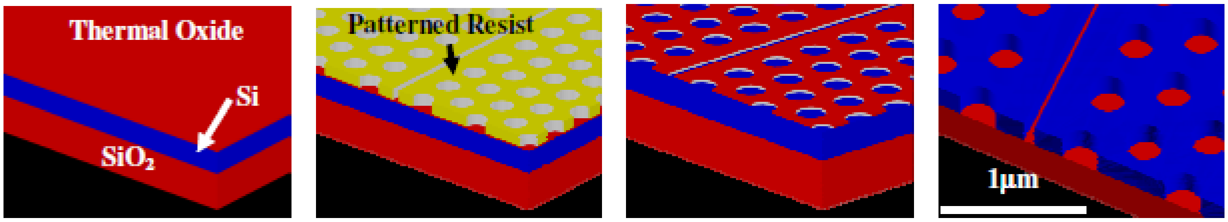


(a) (b) (c)

Fig. 5: Flat band slow light simulations of photonic crystal slot waveguides to probe the wavelengths of 1632nm, 1646nm, 1674nm respectively.

4. DEVICE FABRICATION

Devices were fabricated on silicon-on-insulator (SOI) wafer with 230nm top silicon layer and 3μm buried oxide**.** 45nm thermal oxide was grown on top of silicon as etch mask for pattern transfer. PC slot waveguides, tapers, 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 6.



(a) (b) (c) (d)

Fig. 6: Fabrication steps of a PC slot waveguide (a) Growth of thermal oxide (b) E-beam Resist (ZEP-520A) patterning (c) Transfer of resist pattern to thermal oxide by RIE using CHF_3 followed by resist strip (d) Transfer of pattern from thermal oxide to Si by RIE in HBr and Cl_2. [**Legend:** **Silicon (blue)**, **Silicon Dioxide, SiO_2 (red)**]

PDMS top cladding was prepared by spinning a 10:1 mixture of Sylgard Elastomer 184 from Dow Corning, NY (refractive index *n*=1.46) and curing agent, followed by oven-baking for 3 hrs at 90^{o}C. The device processing prior to PDMS deposition is exactly the same as in a previous demonstration with the photonic crystal slot waveguide [7-8]. We thus have a robust platform for various kinds of on-chip optical spectroscopy that can be tailored for each individual sensing environment.

5. EXPERIMENTAL SETUP

The devices are currently being tested on a Newport six-axis auto-aligning station. Input light from a broadband source was TE-polarized and butt-coupled to / from the device with polarization maintaining single mode tapered lensed fiber with mode field diameter ~3μm. Light is guided in and out of the photonic crystal slot waveguide by ridge waveguides with PC group index taper to enable high coupling efficiency into the slow light guided mode [12]. Devices were fabricated on silicon-on-insulator (SOI) wafer using established methods [12].

6. SUMMARY

In summary, we have designed flat band slow light structure where the group index is constant over a wide range of wavelength. We have shown that such design ensures fabrication tolerance so that the sensitivity of the device is not affected.

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