

# On-Chip Mid-IR Spectroscopy with Slow Light Enhanced Silicon-on-Sapphire Waveguide

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**Abstract:** An engineered slow-light enhanced 2D-PCW on the silicon-on-sapphire platform is proposed as a Mid-IR on-chip spectrometer. Theoretical calculation exhibits strong-mode confinement in the air-guided holey-slotted defect-waveguide with high-group-index of 69 around the carbon-monoxide absorption wavelength.

## 1. Introduction

The utilization of slow light in photonic waveguides has been employed to minimize the optical absorption path length, resulting in enhanced detection sensitivity in on-chip scale optical absorption spectroscopy for various gas analytes, including greenhouse gases. The majority of reports demonstrating chemical and biological sensing using on-chip optical waveguides have been observed in the near-infrared (near-IR) telecom wavelengths, approximately around 1550 nm. However, there has been a recent surge in interest in integrated mid-infrared photonics. This increased attention is primarily attributed to the significant potential it holds for innovative applications in optical interconnects and sensing. The distinctive absorption signatures of analytes in the mid-infrared (mid-IR) are particularly significant because most compounds and gases exhibit absorption cross-sections that are 10-1000 orders of magnitude larger than those in the near-IR [1]. Considering silicon's optical transparency within the 1.1  $\mu\text{m}$  to 8  $\mu\text{m}$  range, high index contrast Photonic Crystal Waveguides (PCWs) implemented in silicon-on-insulator (SOI) are widely favored due to their compatibility with Complementary Metal-Oxide-Semiconductor (CMOS) technology. However, the transparency range of such structures is limited to 1.1  $\mu\text{m}$  to 3.7  $\mu\text{m}$  due to the presence of oxide cladding. An alternative approach involves employing free-standing silicon membranes, allowing for the utilization of the entire spectrum from 1.1  $\mu\text{m}$  to 8  $\mu\text{m}$ . Nonetheless, the fabrication of such membranes is challenging, and concerns about their durability arise. Within the realm of existing CMOS-compatible platforms, silicon-on-sapphire (SoS) emerges as a promising option. Sapphire ( $\text{Al}_2\text{O}_3$ ) cladding offers a substantial refractive index contrast with the silicon core. In the SoS platform, PCW structures can be constructed without the risk of bending and buckling that may occur in free-standing silicon membranes. SoS can offer transparency coverage from 1.1  $\mu\text{m}$  to 5.5  $\mu\text{m}$ , making it an ideal platform for on-chip optical absorption spectroscopy with heightened sensitivity. This spectral coverage is crucial, particularly in the Mid-Infrared (Mid-IR) band spanning 2.8-5.5  $\mu\text{m}$ , where absorption lines correspond to stretching motions of specific molecular groups containing bonds such as C=O, C-H, C $\equiv$ C, and C $\equiv$ N, as found in molecules like  $\text{CO}_2$ ,  $\text{CH}_3$ , CO, and  $\text{N}_2\text{O}$ .

Our group has demonstrated various spectroscopy methods and on-chip components on the SoS platform and demonstrated several key biomarkers. Our team has demonstrated diverse spectroscopy techniques and on-chip elements on the SoS platform, illustrating various key biomarkers. Previously, we reported better sensitivity using 1D and 2D PCWs compared to strip and slot waveguides [2,3], employing near-infrared infrared absorption spectroscopy on the chip. Additionally, we presented the use of slot waveguides in the mid-infrared range within the SoS framework. We have also featured the first demonstration of PCW characteristics in SoS at a mid-infrared wavelength of 3.43  $\mu\text{m}$ , utilizing a fixed wavelength [4]. In this work, we theoretically investigate defect-guided dispersive photonic crystal waveguides to enhance the slow-light factor. Our focus centers on the 4.71  $\mu\text{m}$  wavelength, corresponding to the absorption cross-sections wavelength of carbon monoxide (CO). By strategically exploiting the refractive index perturbations within a specially designed holey-slotted defect region, surrounded by a two-dimensional PCW deliberately engineered within the bandgap region, we achieve remarkable light confinement in the air defect core. This intricate arrangement is beyond the diffraction limit, allowing for highly controlled light propagation. The high group index of 69 intensifies this confinement, suggesting a reduced group velocity and a more concentrated distribution of energy. This feature proves highly beneficial for enhancing the interaction between light and analytes, offering significant potential for the realization of on-chip spectroscopy applications.

## 2. Device Design and Working

The device design process initiates by considering a silicon device layer with a height of 1  $\mu\text{m}$  on the sapphire cladding. The PCW is constructed as a W1.5 PCW, where the central defect width of the PCW is  $1.5\sqrt{3}a$  along the  $\Gamma$ -K direction in a hexagonal lattice of air holes in silicon, with 'a' representing the PC lattice constant. The

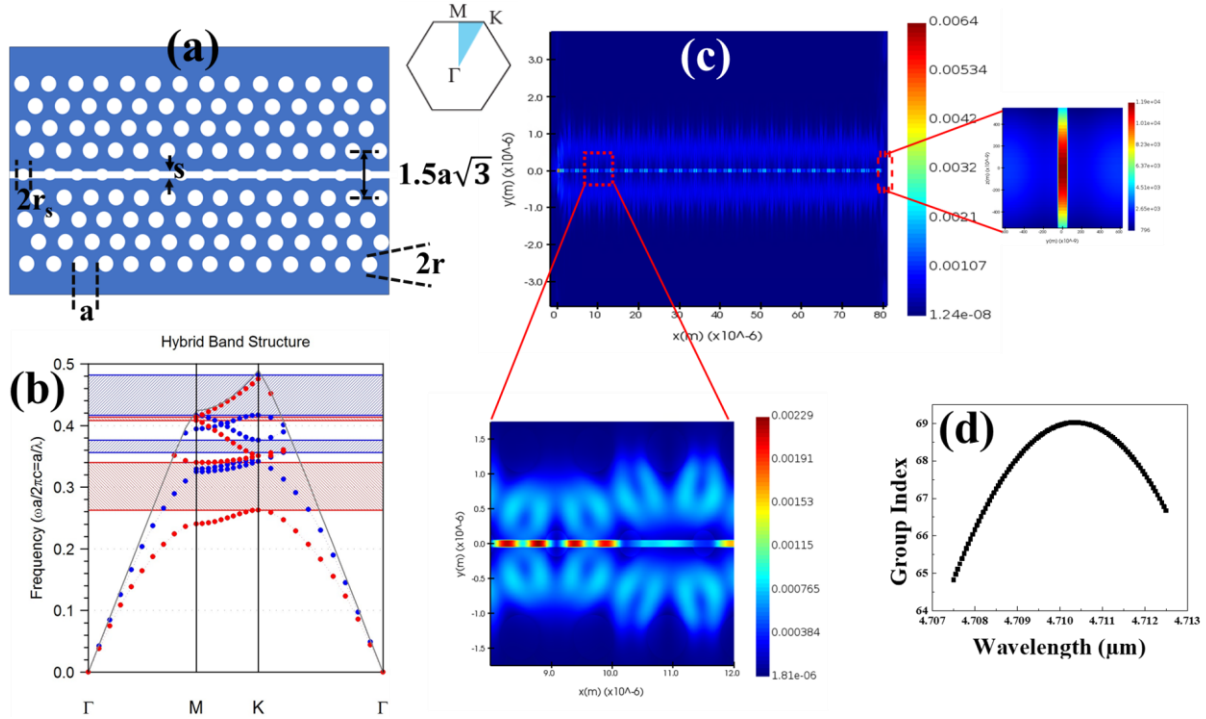


Figure 1: (a) Illustration of the W1.5 PCW with central hole-slotted defect region designed on an SoS wafer. (b) The computed band diagram for hexagonal arranged air holes in silicon slab with bottom sapphire cladding. (c) The electric field (EF) distribution of the defect-guided mode is presented in the inset. In the right inset, there is an illustration of the corrected EF distribution at the output, and the bottom inset displays a high-resolution EF distribution within the red dashed box. (d) Simulated group index at resonating wavelength of  $\lambda=4.71 \mu\text{m}$ .

investigated PC microcavity features a slotted central defect overlapped with smaller periodic holes in the defect region of the photonic crystal. The air holes have a radius ( $r$ ) of  $0.25 \times a$ . At the PCW center, a nano-slot with a width ( $s$ ) of  $0.03 \times a$  is optimized, along with smaller defect holes with a radius ( $r_s$ ) of  $0.58r$ . The design and optimization of slotted and holey waveguides employed in this study have been thoroughly explained in a previous publication [4]. The photonic band-gap calculation involves accounting for sapphire and air cladding both above and below the central Si core region. Fig. 1(b) illustrates the separation of modes based on the central plane of the Si slab, defining even (in red) and odd parity (in blue) within the light cone of the 1.7 refractive index of sapphire. This figure distinctly outlines the bandgap region, crucial for designing a defect region that achieves a flat band to facilitate slow mode in the waveguide. Given our emphasis on enhancing light-analyte interaction, we introduced and optimized the central defect waveguide using the band structure from the plane wave expansion method and optimized through particle swarm analysis via the FDTD method. In Fig. 1(c), a low-resolution top-view image of the electric field distribution of the propagating mode is depicted, with higher mesh accuracy highlighted in the integrated part of the image, as shown in the two insets of Fig. 1(c). The horseshoe-shaped evanescent field of the propagating mode in the holey-slot region (as shown in the bottom inset) is intriguing to note. This pattern serves as evidence of robust reflection by the surrounding photonic crystal, contributing significantly to the effective light confinement in the air region. The resultant mode, characterized by a notable group index of 69, is graphically represented in Fig. 1(d). The suggested research holds the promise to utilize the molecular fingerprint region of various chemicals, enabling their identification and quantification using chip-scale mid-IR spectroscopy. The authors acknowledge and thank DOE for supporting this work under contract number DE-SC0023917.

### 3. References

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