

# Ultra-Sensitive Mid-IR Gas Sensing: Engineering High Group Index Air-Core Modes in Vertical Photonic Crystal Waveguide Arrays

Kang-Chieh Fan<sup>1</sup>, Jason Midkiff<sup>1</sup>, Sourabh Jain<sup>1</sup>, May H. Hlaing<sup>2</sup> and Ray T. Chen<sup>1,2</sup>

<sup>1</sup>Department of Electrical and Computer Engineering, The University of Texas at Austin, 10100 Burnet Rd. Austin, TX, 78758, USA.

<sup>2</sup>Omega Optics Inc., 8500 Shoal Creek Blvd., Bldg. 4, Suite 200, Austin, TX, 78757, USA.

Author e-mail address: james.fan@utexas.edu, chenrt@austin.utexas.edu

**Abstract:** An air-core mode with an even mode and high group index in the VPCW structure has been confirmed. Optimizing the selection of the appropriate air-core mode improves the Mid-IR detection capabilities of the targeted analytes. © 2024 The Author(s)

## 1. Introduction

In the realm of gas sensing, the accurate measurement and quantification of greenhouse gases are crucial. For industrial and environmental on-site sensing applications, a compact, highly sensitive, and cost-effective smart device is much more preferable. The advancement and design of photonic crystals (PhCs) over more than two decades have led us into a novel area termed 'periodic electromagnetic media.' This technology enables the manipulation of light propagation by altering the symmetry of the structure and inserting a defect to steer light in a specific direction. This technique represents a groundbreaking approach in the field of implementing light absorption spectroscopy on-chip [1,2]

## 2. The Method

In this study, we present a VPCW on a silicon platform, characterized as a two-dimensional hexagonal lattice with air holes and a central hollow core. The hollow core array (Fig.1), leveraging cavity-enhancing mechanisms, acts as sampling gas cells, which efficiently trap light, facilitating interactions with molecules in small volumes.

In slow-light studies, the group velocity of the wave packet is critical and is defined as,  $v_g = d\omega/dk = c/n_g$ . Where  $c$  is the speed of light in the vacuum, and  $n_g$  is the group index. As the group index increases, it signifies the presence of a slow light effect, meaning the light is more effectively trapped in the defect area. This allows for extended time of interaction between the light and gas analytes, thereby enhancing the sensitivity of detection.

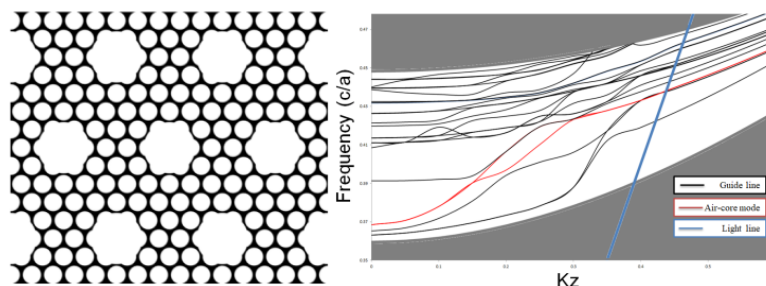


Fig. 1. Left: Schematic of vertical photonic crystal with hollow core array. Right: Band structure results by using MPB simulation.

## 3. Results and Discussions

In order to study the extraordinary slow light behavior in a VPCW, we studied a dispersion diagram of the vertical photonic crystal, performing plane wave expansion (PWE) simulation using two analytical software (1) the MIT Photonic Bands (MPB)[3] and (2) Finite Difference Eigenmode (FDE) by Ansys MODE to extract the band structures and the mode profile at the specific band. As shown in Fig. 1, the optimized structure has a complete gap at  $kz = 0$  with a silicon/air dielectric contrast of 3.4:1. The band diagram generated from this study displays a complex array of guided modes. These modes can be categorized based on how the light exits, such as surface states or air-core modes. The observed intensity patterns (Fig.1 Right) show a notable contrast between two groups of bands: those above the air's light line and the one band that lies below it. The bands above the air's light line predominantly localize in the air core, whereas the band below it concentrates around the air core's surface. This phenomenon exemplifies a surface state. It exhibits evanescence within the crystal, being in the band gap, and also within the air core due to its position below the air light line.

The spatial profiles and frequency dependencies of the modes can be determined using the FDE solver through the solution of the Maxwell equation. Fig.2 shows twelve (12) modes that can be propagated by VPCW, of which 11 are surface-state modes, and the last one is the air-core mode. It is noteworthy that the computational results indicate that this air-core mode is an even mode, allowing a Gaussian beam to easily couple high energy into this mode and maintain its form of propagation as an air-core mode.

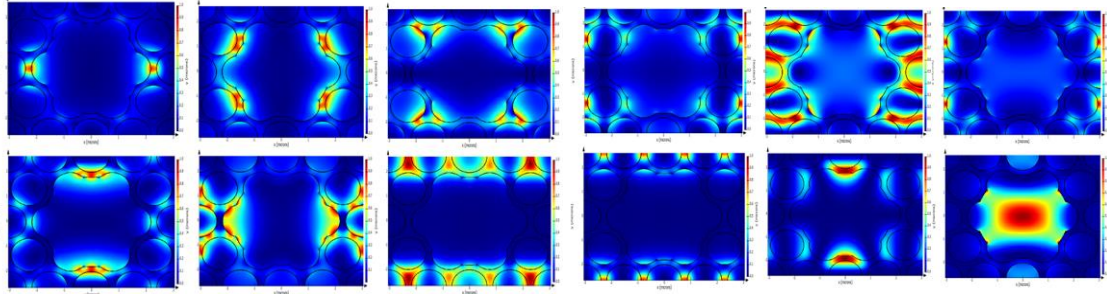


Fig. 2. Different 12 modes plots of surface-normal VPCW, with the last one identified as an air-core guided mode.

Next, we are interested in the consistency between the two software programs. Fig. 3a and Fig. 3b show the Electric field X/Y calculated by FDE, while Fig. 3c and Fig. 3d present the Electric field X/Y computed using MPB. It is evident that both software programs yield consistent results for the electric field calculations of the air-core mode. Finally, FDE can be used to calculate the central wavelength for different analytes, resulting in the Group index ( $n_g$ ). As observed in Table 1, under these structural conditions, the group index can reach up to a maximum of 1424. This outcome obviously indicates that this air-core mode exhibits a high slow-light effect, effectively confining light within the VPCW structure.

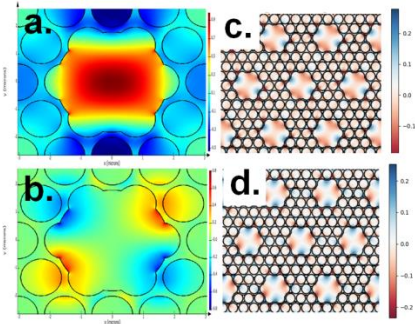


Fig. 3a. 3b. Electric field in x,y direction calculated by FDE. 3c. 3d. Electric field x/y computed by MPB.

Table 1. The group index for difference analytes computed by FDE

Analytes	Center wavelength	Group Index
CH <sub>4</sub>	3.31um	1424
CO <sub>2</sub>	4.25um	866
N <sub>2</sub> O	4.47um	698

#### 4. Conclusions

This paper presents the calculation and validation of a high coupling efficiency in the air-core mode with a high group index within the VPCW structure. We demonstrate theoretically simulated results through two different simulation methods: MPB and FDE. Consequently, we have successfully engineered a photonic crystal waveguide using these software tools. The waveguide is structured as a two-dimensional hexagonal lattice with defect air holes, specifically designed to exploit an air-core mode with an ultra-high group index. This design effectively confines and guides light within its central air core, allowing it to function as a spectrometer.

#### References

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