

# Design and Simulation of A Square-Core Photonic Crystal Fiber-Based Chemical Sensor to Identify Ethanol, Benzene, and Water in the Terahertz Regime

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## Abstract

Our study introduced a new approach involving a Segmented cladding and a Square-core (SC) design. The fiber exhibits notable relative sensitivity (RS), registering 97.46% for Ethanol, 98.32% for Benzene, and 95.73% for Water. The sensor showcases shallow CLs of  $2.09 \times 10^{-08}$  dB/m,  $2.08 \times 10^{-08}$  dB/m, and  $2.09 \times 10^{-08}$  dB/m.

**Keywords:** Photonic crystal fiber, relative sensitivity, Segmented cladding, Confinement loss, Square Core.

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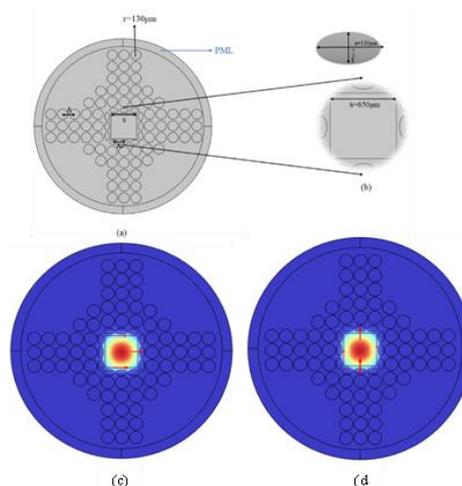
## Introduction

Recently, a wide range of sectors, including genetics [1-2] and organic areas [3-4] communication, have found great benefits from using THz waves. Biomedical studies have strengthened the THz band's frequency range of 0.1 to 10 THz, and the PCF device has been connected to it as a suitable element for various cancer treatments. Furthermore, because the THz spectrum contains no harmful radioactivity, it is more ideal than the X-ray spectrum.

In their PCF-based research work, Sen et al. obtained 78.56%, 79.76%, and 77.51% sensitivity for benzene, but this sensitivity is low for ethanol and water [5]. Hossain et al. (2023) recently attained a sensitivity for ethanol, benzene, and water, which is 92.55%, 94.65%, and 90.30% [6]. As a result, the background material is employed as silica in the study mentioned above to achieve CL, RS, and other optical guiding features. Therefore, we have an excellent opportunity to suggest SC-PCF to obtain low confinement loss and very RS for THz waveguide chemical detection.

## Methodology

Figure 1(a) illustrates the configuration of a Segmented cladding and an SC structure of side ( $s = 650\mu\text{m}$ ) within a PCF designed for chemical sensing in the THz frequency range.



**Figure 1:** (a) Geometry of PCF Sensor (b) cross-section square core PCF and Mode profile of proposed PCF for (c) X-polarization and (d) Y-polarization.

Two types of air holes are featured: circular air holes with a radius of ( $r = 130\mu\text{m}$ ) and a pitch of ( $\Lambda = 40\mu\text{m}$ ), and elliptical air holes with a semi-major axis of ( $a = 110\mu\text{m}$ ), semi-minor axis of ( $b = 55\mu\text{m}$ ), and a pitch of ( $\Lambda_1 = 30\mu\text{m}$ ). The simulation of the fiber was conducted using the COMSOL Multiphysics software, employing the FEM and incorporating PML boundary conditions with a thickness of  $140\mu\text{m}$ .

### Numerical Analysis

A perfectly matched layer (PML) is used as the boundary condition in this numerical investigation, and the widely used full vector FEM is fully utilized. With this FEM method, different optical properties are examined. The most critical optical aspect in determining the chemistry of a PCF structure is its relative sensitivity. Here, the following equation expression calculates the RS.

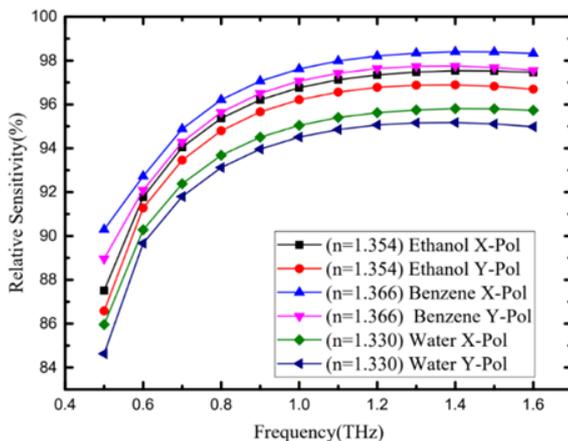
$$RS = \frac{n_a}{n_{eff}} \times E \quad (1)$$

An essential optical parameter for evaluating a PCF-based sensor is confinement loss (CL). This refers to the propagation loss caused by light leakage, which directly impacts the light-confining ability of a PCF. A lower confinement loss signifies a stronger light-confining capability, a critical requirement for any PCF-based sensor [7]. The confinement loss is influenced by the imaginary part of the effective mode index and can be expressed as:

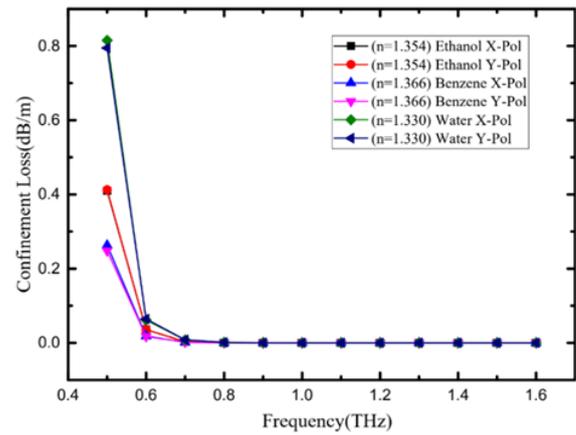
$$\text{Confinement loss (CL)} = 8.686K_0 I_m [n_{eff}] \quad (2)$$

### Results and Discussions

It can be shown that the relative sensitivity of ethanol, benzene, and water peaks at 1.50 THz and starts to decline at 1.60 THz. When measured at 1.60THz, the highest relative sensitivity of the proposed SC-PCF is 97.46%, 98.32%, and 95.73% for water, ethanol, and benzene.



**Figure 2:** RS vs frequency of three chemical compounds for both polarizations at optimal parameters.



**Figure 3:** CL vs. frequency of three chemicals aimed at both polarizations.

Figure 3. reveals a decrease in confinement loss with increasing frequency. Notably, it is observed that confinement losses exhibit consistent responses within the frequency range of 0.5 to 1.60 THz. Precisely, at 1.60 THz, the confinement losses for specified chemicals such as Ethanol ( $n = 1.354$ ), Benzene ( $n = 1.366$ ), and Water ( $n = 1.330$ ) are consistently measured at  $2.09 \times 10^{-08} \text{dB/m}$ ,  $2.09 \times 10^{-08} \text{dB/m}$  and  $2.08 \times 10^{-08} \text{dB/m}$  respectively.

**Table 1:** The comparison between our proposed SC-PCF fiber and the previously published PCF fiber.

Ref. No	Region (THz)	Sensitivity (%)	Confinement loss(dB/m)
[1]	F=1THz	79.76	$6.02 \times 10^{-08}$
[2]	F=1THz	94.65	$6.01 \times 10^{-08}$
Square-Core PCF	F=1.60THz	98.32	$2.09 \times 10^{-08}$

### Conclusion

This article presents a SC-PCF for THz waveguide chemical detection. For any numerical research, the perfectly matched layers and the finite element method (FEM) are used. Simulation research is used to assess the efficacy of our suggested SC-PCF fiber. The backdrop component of this suggested SC-PCF sensor is Teflon. Our comprehensive square-core-PCF fiber reveals, following the numerical results, the high relative sensitivity of 97.46%, 98.32%, and 95.73%.

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