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SPR Enhanced Detection of Isopropanol Vapor Using Au/MIP-Coated Optical Fiber Sensor

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Abstract—Isopropanol (IPA) is a common volatile organic compounds (VOCs) linked to lung cancer. This study presents an experimental validation of a highly sensitive and selective method for detecting IPA vapor. The method employs a molecularly imprinted polymer (MIP) functionalized on a thin gold (Au) film, which is coated over a small section of no-core fiber (NCF). The sensitivity of the MIP-coated sensor with surface plasmon resonance (SPR) facilitated by the thin gold layer is experimentally compared with the MIP-coated bare NCF. The fabricated sensors were tested with various VOCs, including acetone, methanol, ethanol, and IPA, to evaluate their selectivity. The sensors demonstrated selective detection of IPA at parts per million (ppm) levels at room temperature. Our results show that the Au/MIP sensor exhibits seven times higher sensitivity (0.014 nm/ppm) compared to the bare fiber coated only with the MIP layer (0.002 nm/ppm) along with a LOD of 82.41 ppm. Control experiments suggest that the combined effect of the MIP and the gold film significantly enhances the performance of the optical fiber sensor. These findings highlight the potential of this sensor for non-invasive exhaled breath measurement of VOC biomarkers.

Index Terms—Optical fiber sensor; Surface plasmon resonance; molecularly imprinted polymer; volatile organic compounds; biomarker detection.

I. INTRODUCTION

The World Health Organization (WHO) identifies lung cancer as the most common cancer type and the primary cause of cancer-related deaths worldwide [1]. Each year, the number of lung cancer cases rises, resulting in approximately 1.59 million deaths annually, making it the leading cause of cancer mortality for both men and women [2]. Despite the existence of the several treatment modalities, the prognosis of the disease remains unsatisfactory. This is primarily due to a significant proportion of patients being diagnosed at an advanced stage, thereby limiting the effectiveness of available interventions. [3]. Consequently, in China, the five-year survival rate for lung cancer is merely 19.7% [4]. Thus, achieving early diagnosis is crucial for reducing the mortality rate. Among several available clinical approaches, computed tomography (CT) and chest radiography fails to identify the early-stage lung cancers [1]. While histopathological analysis of biopsies is precise, it is invasive and can result in complications, including death. Hence, there is an urgent need for a non-invasive, cost-effective, safe and

extremely sensitive tool to ensure early detection in lung cancer diagnosis.

Diagnosis of various diseases through breath analysis is considered another viable alternative to current diagnostic techniques. Breath monitoring has been in practice since Hippocrates defines the role of breath odor in order to identify health conditions, including kidney failure, liver diseases, lung disease and uncontrolled diabetes [5]. The volatile organic compounds (VOCs) present in exhaled breath can be utilized as disease biomarkers to identify disease and their stages [6]. In identifying lung cancer, various VOCs including toluene, formaldehyde, 2-butanone and isopropanol, are considered as major VOC biomarkers [7]. To determine VOC concentrations in exhaled breath, significant effort has been devoted by researchers to develop analytical approaches based on chromatography or portable sensors. Gas chromatography - mass spectrometry (GC-MS) is popular for its reliability, semi-quantitative capability, and offline approach to VOCs monitoring. This method offers a highest certainty in determining VOC concentrations compared to the proton transfer reaction-mass spectrometry (PTR-MS), which is considered as the most sensitive tool among other analytical tool used for VOCs detection [8]. The GC-MS technique employs ion-pair extraction of breath samples and quantification through mass spectrometry, allowing for the detection of VOC concentrations as low as parts per trillion (ppt). Although the characterization and obtained result are accurate and promising, it suffers from significant limitations including being time-consuming, expensive, off-site testing, and need of skilled technicians [9]. To tackle this issue, numerous researchers have proposed various user-friendly interfaces for sensing systems. These interfaces are designed to detect VOC biomarkers in exhaled breath by leveraging catalysts [10], resistance [11], electrochemical [12], and optical sensors [8]. Depositing different VOC-specific sensing materials is a widely used method to enhance sensing performance. Among several approaches, optical fiber integrated with a molecularly imprinted polymer (MIP) layer is considered the most suitable method for selective detection of target analytes [13].

Molecular imprinting is a technique for creating polymer matrices with tailored binding sites to detect specific target molecules, or templates. The process involves polymerizing a mixture of the target template, monomer, and cross-linker, then extracting the template with ethanol or

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methanol. This creates small size cavities in the polymer matrix that match the template's shape, size, and affinity, serving as recognition sites. This technique shows great potential for enhancing vapor sensor systems with high sensitivity and selectivity [13].

While several studies have reported SPR-based optical fiber sensors, our work presents distinct advancements. Specifically, it focuses on the detection of IPA vapor, a potential biomarker for lung cancer, using an optical fiber platform. We systematically demonstrate how the SPR enhances sensitivity and how the incorporation of a MIP layer improves selectivity. Furthermore, we show that dip coating can be effectively employed to optimize the MIP layer thickness, with a clear trend observed across multiple coating cycles. This article aims to fabricate a highly sensitive and target-selective optical fiber sensor for the detection of VOC biomarkers associated with lung cancer, utilizing a MIP-functionalized plasmonic fiber sensor. In this study, the impact of surface plasmon resonance (SPR) on sensor sensitivity is investigated by depositing a thin gold layer to the optical fiber, followed by MIP coating. A comparison between the Au/MIP-coated sensor and the MIP-coated sensor is presented. The proposed optical fiber sensor comprises a no-core fiber (NCF) region that exploits an evanescent field sensing mechanism. The NCF is coated with a thin film of gold, followed by 6 layers of MIP to leverage the plasmonic phenomenon for target-specific detection. The variation in the absorption spectra of the MIP layer in the presence of VOC molecules is recorded using a spectrometer. The fabricated sensor is characterized for various VOC gases, i.e., acetone, ethanol, methanol, and IPA, with concentrations ranging from 50 to 450 ppm. The fabricated sensor exhibits extremely high sensitivity compared to several other VOC sensors published in recent years [14], [15], [16], [17], [18].

II. SENSOR DESIGN AND NUMERICAL MODELLING

1. Sensor structure

This article focuses on the discussing the step-index distribution sensor, which involves splicing a NCF between two single mode fibers (SMFs), forming a single mode – no core – single mode (SM – NC – SM) structure. The NCF is a pure silica fiber with an undoped core and no cladding, popular for its high precision. A schematic representation of the fabricated Au/MIP sensor is depicted in Fig. 1. The SM – NC – SM structure is fabricated by splicing a 3.5 cm segment of sensing head (Au/MIP) between two SMFs. The diameter of the NCF is 125 μm while the SMF has core and cladding diameters of 8 μm and 125 μm , respectively.

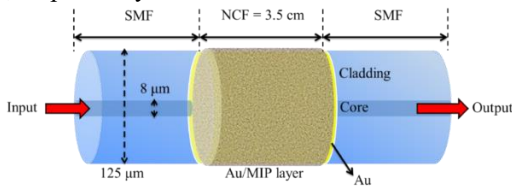


Fig. 1. Schematic diagram of the Au/MIP coated NCF sensor

When the launched light is coupled from the SMF into the NCF, the fundamental mode (LP_{01}) excites a series of higher-order modes (LP_{0m}), resulting in multimode interference

(MMI). This MMI causes periodic light focusing in the NCF, which is known as the self-image effect [19] as shown in Fig. 2. At the self-imaging distance, the output signal shows high coupling efficiency, resulting in increased sensor sensitivity. Hence, the sensor was designed with a sensing length of 3.5 cm to maximize sensitivity from the self-image effect due to MMI.

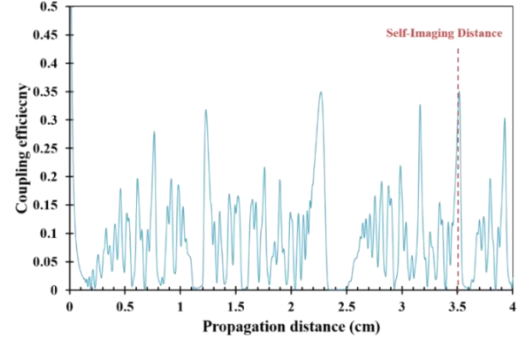


Fig. 2. Coupling efficiency in the sensing region showing self-imaging distance at 3.5 cm.

The working of the fabricated sensor relies on the evanescent field sensing mechanism. Changes in the surrounding environment affect multimodal interference, which is detected through the evanescent fields at the sensor interface [20]. With the ~~no-core fiber~~ NCF, light is less confined to the fiber core and extends more to the interface, where the evanescent field takes place. The enhanced intensity of the evanescent waves at this interface improves light interaction with the surrounding environment, thereby increasing the sensitivity of the sensor

2. Numerical optimization of thickness of gold film (t_{Au})

In addition, a 60 nm thin gold layer was deposited along the length of the NCF to help improve the sensitivity. As light propagates through the gold-coated NCF, it induces the surface plasmon resonance (SPR) phenomenon at the Au/MIP interface [21]. These surface plasmons are extremely sensitive towards any changes in the refractive index of the coated MIP, such as those caused by the binding of target IPA molecule.

The optimization of thickness of the gold film (t_{Au}) is crucial for achieving maximum energy transfer from the core mode to surface plasmon polariton (SPP) modes of the gold film, and consequently enhances the sensitivity of the device [21]. For this optimization, an NCF with a diameter of 125 μm made of fused silica glass is used. In this work, the Sellmeier equation is used to determine the refractive index (n_s) of the optical fiber as shown below [22]:

$$n_s = \sqrt{1 + \frac{a_1 \lambda^2}{\lambda^2 - b_1^2} + \frac{a_2 \lambda^2}{\lambda^2 - b_2^2} + \frac{a_3 \lambda^2}{\lambda^2 - b_3^2}} \quad (1)$$

where a_1 , a_2 , a_3 , b_1 , b_2 , and b_3 represent the Sellmeier coefficients with values obtained from a previously reported article [22]. The material dispersion of the gold is determined using the Lorentz-Drude model, offering a precise permittivity value that closely matches with experimental values, and can be calculated as [22]:

$$\epsilon_m = 1 - \frac{\Omega_p^2}{\omega(\omega - i\Gamma_0)} + \sum_{j=1}^k \frac{f_j \omega_p^2}{(\omega_j^2 - \omega^2) + j\omega\Gamma_j} \quad (2)$$

where, ϵ_m exhibits the dielectric constant and ω_p represent the plasma frequency, while k denotes the count of oscillators characterized by frequency ω_p and strength f_j . $\Omega_p = \sqrt{f_0 \omega_p}$. A numerical modelling and simulation were performed to

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optimize the thickness of gold film utilizing Finite Element Method (FEM). Fine meshing was applied to the NCF and the surrounding medium (air with a refractive index of 1), with extremely fine meshing at the thin gold film as shown in Fig. 3(a). With the specified mesh, we consider a fundamental optical mode propagating through the fiber and interacting with the gold film at the metal-dielectric interface, as shown in Fig. 3(b).

To optimize the thickness of the gold, we varied it to $t_{Au} = 30$ nm, $t_{Au} = 60$ nm, and $t_{Au} = 90$ nm. Electric field profiles (E_y) corresponding to selected areas at the sensing interface with different gold thicknesses are illustrated in Fig. 3(c). It is evident that the E_y for the 60 nm thick layer is more prominent, reaching a higher peak at the sensing interface compared to the 30 nm and 90 nm thick layers. The heightened electric field profile for the 60 nm thick layer indicates greater energy transfer from the dielectric core mode to the surface plasmon polariton (SPP) modes of the 60 nm film. Thus, the gold with 60 nm thickness can be considered more sensitive to the surrounding medium compared to the 30 nm and 90 nm gold layer.

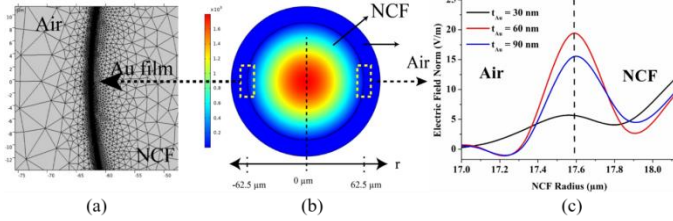


Fig. 3 (a) Schematic meshing at the sensing interface. (b) Fundamental optical mode field propagating through NCF. (c) Electric field profile at the sensing interface with different gold thicknesses.

III. MATERIALS AND METHODS

1. Chemical

2,2'-azobis-isobutyronitrile (AIBN), Ethylene glycol dimethacrylate (EGDMA), and 3-(trimethoxysilyl) propyl methacrylate (3TMPMA) were purchased from Sigma Aldrich, Thailand. Sodium hydroxide (NaOH), Hydrochloric acid, toluene (C_7H_8), and 99.5% isopropanol (C_3H_8O) were purchased from Merck, Thailand. Methacrylic acid (MAA) was obtained from TCI, Japan. All chemicals were of pure analytical grade and utilized without any purifications.

2. Synthesis of MIP

The synthesis of MIP solution is carried out using a non-covalent method. IPA acts as the target template in this process, while MAA, EGDMA, and AIBN serving-serve as the monomer, cross-linker, and initiator, respectively. The prepolymeric solution containing the IPA template is prepared by mixing IPA, MAA, EGDMA, and AIBN (IPA: MAA: EGDMA: AIBN = 21 μ L: 45 μ L: 188 μ L: 20 μ L) in a small vessel. The amount of cross-linker in the mixture plays a crucial role in polymerization. When the cross-linker content exceeds 60%, the surface becomes hard and cracked, whereas if it is less than 60%, the surface becomes non-smooth and semi-liquid. Subsequently, the mixture is dispersed uniformly using sonicator and degassed with nitrogen for 5 minutes to obtain a

transparent and homogeneous solution. The polymerization process, conducted in the presence of a cross-linker, creates a porous matrix with specific template sites. After polymerization, the template is extracted from the polymer matrix. The target IPA analyte can then selectively rebinding to the polymer at the sites originally formed by the template, known as the imprints. The schematic diagram of synthesis of MIP and selective binding of IPA with MIP is depicted in Fig. 4. Similarly, the non-imprinted polymeric (NIP) solution is also synthesized in the absence of IPA.

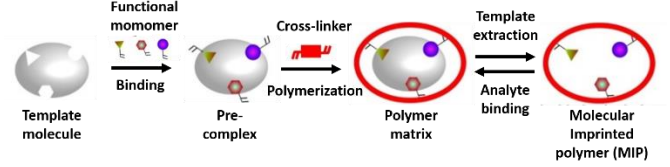


Fig. 4. Schematic diagram of MIP synthesis

IV. SENSOR FABRICATION

The fabrication of the SM – NC – SM sensing configuration for selective detection of IPA involves multiple steps, including deposition of gold film and MIP, followed by template extraction, and splicing. The detailed procedure is discussed in the following subsection.

1. Gold film deposition

To investigate the influence of surface plasmon resonance (SPR), two optical fiber sensors were prepared: one with MIP coated on a thin gold layer and another with MIP coated directly onto the bare fiber. The SPR effect is induced by coating a thin gold layer onto the optical fiber using a sputtering machine (Zhengzhou CY Scientific Instrument, CY-MSP180G-DG, China). In this study, a 5 nm thick layer of platinum was applied prior to the gold layer. This platinum layer acts as an adhesive to improve the bonding between the gold layer and the surface of the optical fiber. The gold film was deposited for 40 seconds at a current of 135 mA, resulting in a 60 nm thick gold film. Field emission scanning electron microscopy (FSEM) images of the gold-coated silica optical fiber are shown in Fig. 5 (a). The surface morphology and thickness are shown in Fig. 5 (b) and Fig. 5 (c), respectively. The presence of a gold film (51.9% by weight) is confirmed through elemental analysis using Energy Dispersive X-ray (EDX).

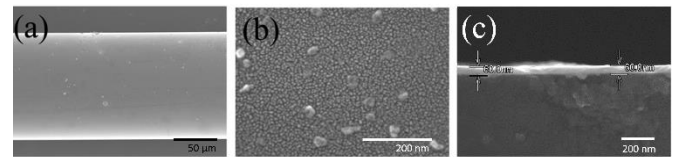


Fig. 5. FSEM images of (a) optical fiber coated with thin gold film. (b) Surface morphology of gold film. (c) Cross-section of gold-coated optical fiber showing the thickness of the gold layer.

2. MIP deposition

In addition to achieving the SPR effect to improve the sensitivity of the sensor, a thin gold layer offers the advantage of allowing MIP to be deposited on the gold-coated surface without the need for surface modification or functionalization [23]. For the deposition of MIP on the bare NCF, it is necessary

to vinylize the surface to introduce a vinyl group, thereby enhancing the adhesion of MIP on NCF. To functionalize the NCF for MIP deposition, the fiber was cleaned by immersing it in 0.1% HCl for 30 minutes and then in NaOH for 1 hour to remove excess positive and negative ions. After cleaning, the NCF was washed with DI water multiple times and dried under nitrogen. The vinylization step was performed by immersing the fiber in a solution containing 10% of 3TMPMA in toluene for 1 hour. After functionalization, the fiber was placed in an oven at 70 °C for 2 hours. To optimize the thickness of the MIP, a bare NCF was coated with 3, 6, 9, and 12 layers of MIP using a dip coating method, as depicted in Fig. 6(a). The dip coating was performed at a speed of 100 mm/min with a wait time of 15 seconds using a dip-coater (Biolin Scientific, AAM100161, Finland). After the first layer of dip coating, the MIP solution coated on the fiber was polymerized under UV irradiation at $\lambda = 365$ nm for 20 minutes. To achieve 6, 9, and 12 uniform layers of MIP, the dipping process, along with polymerization, was repeated 6, 9, and 12 times, respectively. The variation in thickness corresponding to the number of deposited layers is shown in Fig. 6(b), with SEM images of the cross-section presented as insets. From the obtained data, it is evident that the thickness increases exponentially with the number of layers. The exponential growth in thickness observed during the deposition of the MIP is driven by various factors including the multiplicative nature of layering, diffusion and penetration, electrostatic attraction, surface saturation, cooperative binding, and self-assembly processes. In the case of a 3-layer coating of MIP, no polymer was observed on the optical fiber.

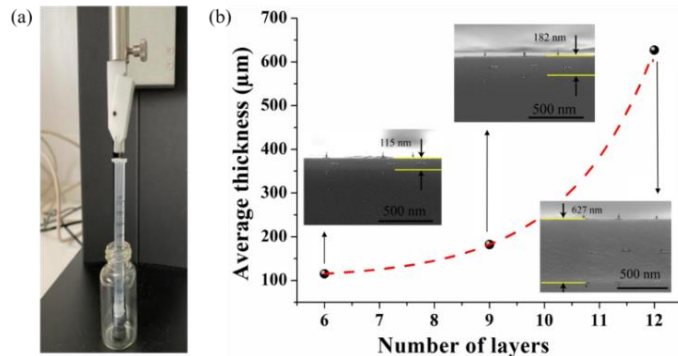


Fig. 6. (a) MIP deposition using dip coater. (b) Variation in thickness of MIP corresponding to various layers. Insets are SEM cross-sectional images showing the thickness.

3. Fabrication of SM – NC – SM optical fiber sensor

After successfully depositing 6 layers of MIP, the IPA template was then extracted from the MIP matrix by sonicating the MIP-coated fiber in ethanol for 1 minute. Subsequently, the MIP-coated fiber was spliced between two SMFs using a fiber splicer (Sumitomo Electric, Z2C, Osaka, Japan) to ensure high coupling efficiency into the sensing region and spectrometer. The fabrication of SM – NC – SM structure is illustrated in Fig. 7(a), while Fig. 7(b) displays an actual fabricated sensor with Au/MIP sensing region in the middle. The sensing region, represented by the bright red light resulting from the high intensity of the evanescent field at the interface, is 3.5 cm long. To ensure the complete evaporation of the washing solvent from the MIP matrix, the sensor was left at room temperature for 48 hours before characterization.

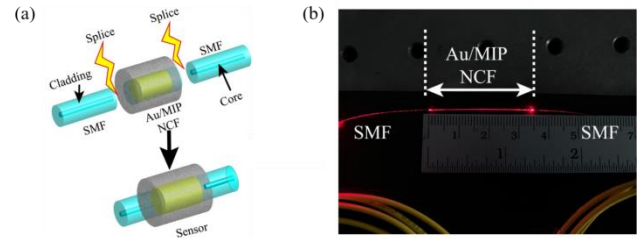


Fig. 7. (a) Schematic image of SM-NC-SM structure fabrication. (b) Actual fabricated sensor with the sensing length of 3.5 cm.

IV. RESULT AND DISCUSSION:

1. Fourier-transform infrared analysis

Fourier-transform infrared spectroscopy (FTIR) serves as a valuable analytical tool for identifying polymerization. Fig. 8(a) illustrates the FTIR (Thermo Scientific Nicolet Apex, USA) spectrum for the pure MMA and MIP. The peak appeared at 2963 cm^{-1} corresponds to the stretching vibration of C–H in MAA. The subsequent peak appeared at 1689 cm^{-1} represent presence of C=O group, whereas the peaks observed at 1631, 1375, and 1200 cm^{-1} represent the C=C, O–H, and C–O functional groups due to MAA, respectively. The FTIR spectra of MIP persist for various groups, including the C–H group, appeared at 2958, 2957, and 2957 cm^{-1} . The presence of a cross-linker, EGDMA, is indicated by the C–O peak at 1143 cm^{-1} in MIP. Furthermore, the bending vibration of O–H appeared at 1375 cm^{-1} confirms the existence of carboxylic acid groups in MIP. Successful polymerization of MIP is evidenced by the reduction in intensity observed for C=C peak at 1631 cm^{-1} , as shown in inset graph. The absence of the peak at 1631 cm^{-1} strongly suggests that polymerization has occurred between the monomers and cross-linkers. The procedure of polymerization is evident through the reduced transmittance intensity of C=C stretching and C=O bending (553 cm^{-1}) in the MIP compared to the intensity of the C=C in the MAA monomer.

2. Morphological Study of the MIP

Field emission scanning electron microscopy (FESEM, HITACHI, SU8030, Japan) and atomic force microscopy (AFM) constitute essential and invaluable analytical methodologies to obtain detailed information on the surface morphology, as shown in Fig. 8(b) to Fig. 8(d). Roughness of the polymers surface is shown in Fig. 8(e). The thickness of the MIP layer from the cross-sectional area is depicted in Fig. 8(b). This cross-sectional image shows significant separation between the gold (~60 nm) and MIP layers with thicknesses around 60 nm and 100 nm, respectively. To validate the material composition, an EDX analysis was performed on the same sample. The Au/MIP coated NCF indicates a significant increase in carbon (C) content to 63.9% by weight, suggesting the presence of the MIP, which is predominantly composed of carbon-based polymers. The decrease in gold content to 16.5% further supports the deposition of the MIP layer onto the gold-coated fiber surface. Additionally, the presence of Si at 19.6% indicates the silica substrate, which is NCF. SEM images showing the surface morphology of the MIP layer before and after IPA template removal are illustrated in Fig. 8(c) and Fig.

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8(d), respectively. A smoother and less porous surface is evident on the MIP layer before template removal because the template molecules remain in the polymer matrix, resulting in no specific binding sites for IPA on the MIP surface. After successful removal of the IPA templates, an increase in the wrinkled structure and surface roughness is observed, this can be attributed to the increase in the surface area due to the accommodation of the IPA template. The uniform MIP layer facilitates effective template extraction and rapid binding kinetics, leading to the good performance of the MIP-coated sensor.

An AFM analysis was conducted to obtain a detailed view of the surface roughness as, shown in Fig. 8(e). The analyzed surface area is $1 \times 1 \mu\text{m}^2$ on the optical fiber coated with Au/MIP. The 3D image reveals an average roughness (S_a) of 5.47 nm following the formation of the binding sites for IPA molecules.

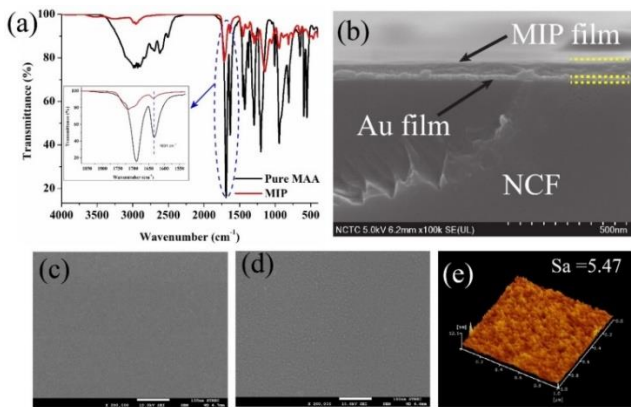


Fig. 8. (a). FTIR analysis for the Au/MIP substrate; FESEM images of (b). Cross-sectional image of Au/MIP coated sensor showing thickness of gold and MIP layers (c). MIP surface before extracting the template. (d). MIP surface after extracting the template, (e). AFM images of MIP layer after template removal.

3. Optical Analysis

3.1. Gas chamber and VOC vapor preparation

The experimental procedure involves generating vapors of acetone, ethanol, isopropanol, and methanol within the VOC chamber. This work includes the fabrication of a testing chamber to perform static measurements of VOC concentrations. The testing chamber has a volume of 10368 cm^3 ($36 \text{ cm} \times 24 \text{ cm} \times 12 \text{ cm}$), allowing for assessments of VOC concentrations ranging from 150 to 450 ppm. Constructed with a 3 mm thick acrylic body, the chamber was chosen for its minimal absorption of VOCs and its resilience against degradation from all exhaled breath VOCs. To facilitate VOC injection, a 2 mm diameter hole was precisely made at the top of the gas chamber using a laser-cutting machine. To determine the volume of VOCs required to achieve various concentrations in ppm, the fundamental dilution equation was used:

$$C_1 V_1 = C_2 V_2 \quad (3)$$

This equation establishes the relationship between the initial concentration (C_1), and volume (V_1) of VOCs and their desired final concentration (C_2) and chamber volume (V_2).

All the VOC vapors were prepared using 99.9% analytical

grade liquid VOCs (Merck, Germany) by placing 10 ml of liquid VOC in a sealed glass vial. To ensure the conversion from liquid to vapor, the vial was placed on a hotplate at 60°C for 1 minute. The selected volume for each VOCs is listed in Table1.

TABLE I
AMOUNT OF INJECTED VOCs VAPORS FOR EACH CONCENTRATION

Concentration (ppm)	Volume (ml)
150	1.5
250	2.6
350	3.6
450	4.7

3.2. Optical Setup

The fabricated sensor was then tested with various VOCs, including acetone, ethanol, and methanol, with concentrations ranging between 150 and 450 ppm. The schematic diagram of an optical setup to test the fabricated sensor is shown in Fig. 9, with the inset displaying the actual setup. The optical setup consisted of the Au/MIP-coated sensor placed inside the gas chamber with a volume of 10368 cm^3 , halogen light source (Ocean Optics, HL-2000, Largo, FL, USA), and spectrometer (Thorlabs, CCS200/M, Newton, NJ, USA). The light was launched from the broadband light source and coupled into the Au/MIP-coated optical fiber sensor. The evanescent field at the sensor interface, enhanced by the SPR, interacts with VOC molecules, causing a change in the effective index and absorption spectra. This change in absorption spectra was then recorded by the spectrometer, which is connected to a computer for further signal processing. The sensing principle is based on the tuning of the plasmonic phenomena, in terms of resonance wavelength [24]. Surface plasmons are excited in the gold-coated NCF through the interaction between the incident light and the collective oscillations of free electrons at the metal-dielectric interface. This phenomenon induces strong electromagnetic field confinement, enhancing light-matter interaction and consequently improving sensitivity. When VOC vapors were injected into the gas chamber, they interacted with the MIP-coated sensing probe, resulting in significant shifts in the absorption spectra. To ensure sensor stability, the experiments were repeated three times to assess both repeatability and stability. After each measurement, the sensor chamber was purged with nitrogen gas for at least 1 minute to remove residual VOC vapors on the MIP matrix of the sensor. The transmission spectrum was monitored to ensure it returned to the original baseline before introducing the next VOC concentration [20].

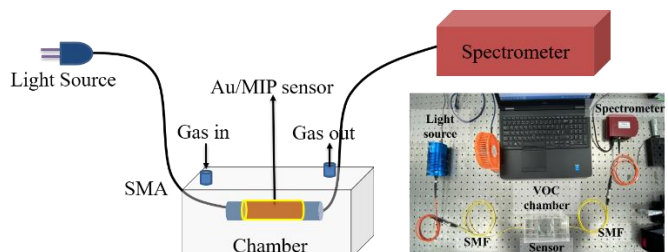


Fig. 9. Schematic diagram of experimental setup

3.3. Sensitivity

The thickness of the MIP layer is crucial for sensor performance, ensuring sufficient binding sites and proper diffusion kinetics. Optimization showed that 6 MIP layers provided high linearity ($r^2 = 0.97$) across IPA concentrations (150-450 ppm). Thicker layers (9 and 12) had lower regression values (0.83 and 0.72) and reduced sensitivities due to fewer binding sites. All experiments were performed with 6 MIP layers coated on Au film. The effective refractive index of the sensor changes according to different concentrations of VOC vapors, resulting in shifts in the transmission spectra (T). The output signal from the light source coupled into the fabricated optical fiber sensor, with air as the medium, was measured and used as the reference output signal (I_0). This helps minimize the influence of the light source and material absorption from the optical fiber. The output spectrum at various vapor concentrations is denoted as I_c . Therefore, the transmittance spectrum (T) can be defined by the following relation:

$$T = \frac{I_c}{I_0} \quad (4)$$

The transmission spectra for the Au/MIP and Au/NIP-coated NCF, obtained by varying IPA concentrations in the chamber from 150 to 450 ppm are shown in Fig. 10(a) and Fig. 10(b), respectively. In an SPR-based sensing platform, the resonance wavelength shifts are changes in the refractive index at the gold-dielectric interface. The presence of an MIP receptor layer on the gold film leads to a shift in the resonance wavelength due to IPA molecule penetration into the MIP layer and subsequent refractive index variation at the interface between the MIP layer and the gold film. Peak shifts of the resonance wavelength corresponding to different vapor VOC concentrations for Au/MIP and Au/NIP are shown in Fig. 10(c). These shifts demonstrate a positive correlation with increasing IPA concentration in the chamber, indicating a decrease in the refractive index value of the MIP layer upon IPA interaction with the MIP receptor. Sensor repeatability was evaluated by performing three repeated measurements at each isopropanol concentration level, with standard deviations shown as error bars. The response time was assessed by measuring the wavelength shift at 1, 3, and 5 minutes of exposure. A stable response with the highest linearity ($R^2 = 0.97$) was observed at 3 minutes, which was used for all subsequent measurements. With a strong relationship between resonance wavelength and VOC concentrations as confirmed by regression ($r^2 = 0.97$), linear sensitivity can be determined by calculating the ratio of the change in wavelength to the change in concentration:

$$\text{Sensitivity} = \frac{\Delta \text{wavelength}}{\Delta \text{concentration}} \quad (5)$$

The results indicate minimal or negligible evidence of resonance wavelength shift in the Au/NIP-coated sensor when compared to the Au/MIP-coated sensor. This observation suggests that the target specific binding sites formed by imprinting IPA molecules play a predominant role in the interaction between target molecules and the polymer in Au/MIP sensor, and hence shows excellent sensitivity of 0.014 nm/ppm. In the case of Au/NIP, a slight variation in the shift can be attributed to the variation in the refractive index of NIP in the presence of VOC vapors. The maximum sensitivity of the

Au/NIP-coated sensor is determined to be 0.006 nm/ppm, which is less than twice the sensitivity of the Au/MIP-coated sensor, along with a low linearity of 0.78. The sensor shows a linear response up to 450 ppm, beyond which the graph does not reach saturation. However, IPA concentrations in lung cancer patients' exhaled breath are typically in the low ppm range, and the sensor's performance at these clinically relevant concentrations is the main focus of the study.

3.4. Selectivity test

To test the selectivity of the device, other major VOC biomarkers, including methanol, acetone, and ethanol, were included as interferent gases due to their presence in exhaled breath and chemical similarity to isopropanol. Selectivity testing against these compounds is essential to ensure reliable performance in breath analysis. The selectivity of the sensor was evaluated three times in the presence of each VOC, across a concentration range of 150 to 450 ppm. The response of the sensor to each VOC is shown in Fig. 10(d). The linear regression coefficient (R^2) for isopropanol was 0.97, with a sensitivity of 0.014 nm/ppm, while weak linear relationships were observed for methanol ($R^2 = 0.43$), acetone ($R^2 = 0.09$), and ethanol ($R^2 = 0.76$), making the calculated sensitivity for these gases unreliable. This further confirms the selectivity of the sensor towards isopropanol. Nevertheless, it shows a consistent trend and excellent linearity with IPA molecules. Given the absence of significant resonance wavelength shifts for any VOCs besides IPA, it can be inferred that there is no specific adsorption of the considered substances occurring on the Au/MIP-coated sensor. The MIPs are capable of forming selective binding cavities that match the size, shape, and functional group of target molecules [25]. By designing the polymer matrix with precision, MIP-based sensors can be customized to selectively bind a wide range of analytes (in this case, IPA), making them highly adaptable for various sensing applications.

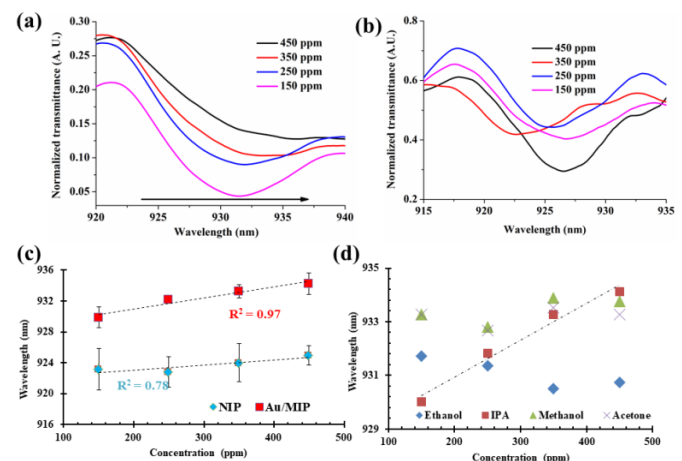


Fig. 10. Transmission spectra of (a) Au/MIP and (b) Au/NIP sensors with different concentrations of IPA. (c) Resonance wavelength of the Au/MIP and Au/NIP coated sensor corresponding to IPA concentrations. (d) Selectivity performance of the fabricated sensor under the exposure of various VOCs.

TABLE II

COMPARISON OF THE SENSING RESPONSE OF THE FABRICATED AU/MIP SENSOR WITH OTHER TYPES OF VOC SENSORS

Sensing materials	Target VOC	Sensitivity	LOD (ppm)	Ref.
Pt NPs/GO	Ammonia (0-120 ppm)	10.2 pm/ppm	NA	[16]
PDMS/PMMA composite	Ammonia (5-500 ppm)	4.18 pm/ppm	4.8 pm	[15]
MoS ₂ flakes	IPA (0-100 ppm)	0.0058 nm/ppm	1.72	[26]
Cholesteric liquid crystal	Acetone (0-16962 ppm)	0.0021 nm/ppm	NA	[17]
ZnSnO ₃ /TiO ₂	Ethanol (0-360 ppm)	3.85 pm/ppm	34.36	[14]
Au/MIP	IPA (150-450 ppm)	0.014 nm/ppm	82.41	This work

Utilizing Au/MIP technology, our sensor offers an alternative method for VOC detection, particularly for IPA. Compared to other VOC sensors with sensitivities ranging from 0.0021 nm/ppm to 10.2 pm/ppm, a sensitivity of 0.014 nm/ppm is achieved. This suggests that even subtle changes in isopropanol concentration can be effectively detected. While acknowledging the valuable contributions of other sensing materials, promising potential for accurate and sensitive detection of isopropanol is demonstrated. Although the demonstrated sensor operates at relatively high IPA concentrations, it establishes a foundation for further development of highly sensitive sensors targeting clinically relevant breath IPA levels. The fabricated sensor also exhibited a good limit of detection (LOD) of 82.41 ppm, calculated as reported in our previous article [27].

V. APPLICATION OF OPTICAL FIBER VOC SENSOR

VOC sensors are essential for industrial safety, air quality monitoring, and disease diagnosis, particularly lung cancer detection. With a high mortality rate, lung cancer, mainly caused by tobacco smoke, demands rapid diagnostic tools. Existing devices struggle with bulkiness, sensor drift, and limited sensitivity, highlighting the need for more accurate VOC sensors. The fabricated optical fiber sensor, with a compact size of 3.5 cm, exhibits high sensitivity and good selectivity toward target VOCs. A major advantage of this device is its suitability for breath monitoring due to the inherent properties of optical fibers. Compared to electronic noses and GC-MS, optical fiber-based VOC sensors offer several benefits, including smaller size, higher sensitivity, room temperature operation, faster response times, and greater stability. These sensors are more stable and can operate across a wider range of environmental conditions. Using various VOC molecules as templates for target-specific MIPs in optical fibers allows multiplexing and simultaneous detection of multiple VOCs. Integrating these sensors with IoT interfaces and ML algorithms enables real-time breath monitoring and enhances their utility in medical applications.

VI. CONCLUSION

This work proposed the numerical optimization and experimental validation of a highly sensitive IPA sensor coated with an Au/MIP layer. IPA is known as a common VOC associated with lung cancers. Operating on wavelength interrogation and at room temperature, the sensor monitored wavelength shifts corresponding to various VOC concentrations to analyze sensing performance, device selectivity, and response time. Two types of sensors are compared in this work: one bare fiber coated with an MIP layer and the other a plasmonic fiber coated with an Au/MIP layer. The Au/MIP coated sensor exhibits seven-times higher sensitivity of 0.014 nm/ppm compared to the bare fiber coated with MIP only (0.002 nm/ppm) and more than two times than the Au/NIP coated fiber (0.006 nm/ppm). In addition to good sensitivity, the sensor also demonstrates excellent selectivity when tested with other VOC gases such as methanol, acetone, and ethanol. Overall, the sensitivity performance is promising and applicable for real-time VOC biomarker monitoring.

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