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Highly Sensitive Triple-Band Terahertz Perfect Metamaterial Absorber for Sensing Applications in Organic Substance

Mohammad Mahmudul Alam Mia^{1*}, Sayed Shifat Ahmed¹, Md. Ruhul Amin¹ and Md. Evakub Ali¹

¹Electrical and Electronic Engineering, RTM Al-Kabir Technical University, Sylhet-3100, Bangladesh

*E-mail: <u>mahmud_ece_ku@yahoo.com</u>

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Abstract

A highly efficient metamaterial absorber is designed for terahertz (THz) sensing and multiband super absorption, utilizing plasmonic and metamaterial properties to achieve nearly perfect absorption across multiple frequencies. The proposed microstructure design (53 μ m×55 μ m) is composed on a full ground layer and a multiple concentric squared patterned copper ring resonator integrated on an FR-4 substrate exhibits near-perfect absorption at three distinct frequencies (0.717 THz, 1.368 THz, and 3.535 THz), enhancing evanescent waves responses for highly sensitive sensing applications. The modelling and numerical analysis are performed using Finite Difference Time Domain (FDTD) based software (CST Microwave Studio) with a genetic algorithm (GA) employed to optimize the geometric parameters. The proposed metamaterial absorber demonstrates maximum absorption of 99.99% at 0.717 and 3.535 THz and 99.95% at 1.368 THz. The metasurface exhibits stability across varying refractive indices, achieving peak sensitivities of 133, 175, and 479.5 GHz/RIU at respective resonance frequencies. By responding to material-induced resonance frequency shifts, the absorber is explicitly optimized for precise detection of organic substances including biomolecules, virology, tissues, chemicals, and oils making it highly suitable for bioanalysis, industrial quality control, and advanced biomedical diagnostics, and covering a broader application scope than most prior works that typically focus on a single class of materials.



Keywords: Metamaterial; triple band; perfect absorber; refractive index sensing; THz sensing.

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1. Introduction

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Emphasis on terahertz (THz) waves has been complemented by more focused studies before October 2023. The quest for better sensing technologies has led to increased interest in terahertz (THz) waves, which lie between microwave and infrared frequencies [1, 2]. These waves have a set of unique properties, such as non-ionizing radiation, the ability to penetrate through non-metallic substances, and high sensitivity to molecular and structural modifications, making them highly attractive for diverse fields including biomedical imaging, spectroscopy, and security [3]. A significant area of research focuses on developing highly sensitive terahertz devices for biomolecule and organic chemical sensing, where detecting substances is crucial for various biotechnological and industrial applications. Perfect Metamaterial Absorbers (PMAs) are artificially designed periodic structures with anomalous electromagnetic (EM) properties, enabling precise control over wave absorption. By minimizing transmission and reflection while maximizing absorption, PMAs achieve impedance matching with free space at the resonant frequency through geometric optimization. These structures efficiently absorb both electric and magnetic wave radiation, enhancing their performance in THz sensing, imaging, and stealth applications. In the THz regime, PMAs exhibit perfect absorption at specific frequencies, making them ideal for highly sensitive and selective sensing. Their ability to manipulate subwavelength-scale wave propagation enables advanced applications in biomolecule detection, chemical identification, and industrial oil organic characterization. Enhanced absorption can be achieved by modifying shape and material composition, optimizing field localization, and responsiveness to environmental changes. These properties make PMAs valuable for precision spectroscopy, non-invasive diagnostics, and advanced antenna designs, where frequency-selective absorption is crucial for high-performance THz applications [4, 5]. The concept of triple-band metamaterial absorbers has further revolutionized the field by allowing simultaneous detection at multiple frequencies, which is particularly valuable in bioorganic sensing. These devices offer the advantage of detecting different types of molecular interactions across a wide range of THz frequencies, thus improving the specificity and efficiency of sensing systems [6]. The ability to absorb at three distinct resonant frequencies enables the detection of various bioinorganic interactions, such as protein-metal ion binding, DNA-metal complexes, or metal nanoparticle interactions with biological tissues, all of which play crucial roles in biomedical diagnostics, environmental monitoring, and therapeutic applications [7]. THz metamaterial absorbers (MAs) detect biomolecules, tumors, oils, and chemicals by leveraging their unique absorption spectra and frequency-dependent dielectric properties. When

THz waves interact with a target substance, variations in molecular composition, density, and polarity cause shifts in resonance frequency and changes in absorption intensity. Biomolecules and tumors exhibit distinct spectral signatures due to their water content and structural differences, enabling differentiation between normal and pathological tissues. Similarly, oils and organic chemicals possess characteristic absorption peaks influenced by hydrocarbon chains, viscosity, and molecular bonding. MAs, designed to confine and enhance EM field localization, amplify these spectral shifts, improving detection sensitivity. By optimizing geometric design and material properties, MAs maximize absorption at target frequencies, allowing precise identification of substances through resonance peak analysis. THz frequency shifting provides a non-destructive, label-free method for distinguishing organic chemicals based on their unique absorption peaks and frequency shifts [8]. The technique is particularly useful for detecting structural variations, hydrogen bonding effects, and dipole interactions, making it a powerful tool for chemical identification and material characterization. Designing a highly sensitive tripleband terahertz PMA is challenging, requiring near-perfect absorption at multiple frequencies while maintaining sensitivity to organic changes. Optimizing the metamaterial structure ensures a responsive electromagnetic behavior to variations in composition, thickness, and ambient conditions. THz imaging, enhanced with engineered metamaterial absorbers, addresses conventional system limitations by improving signal sensitivity, penetration depth, and imaging contrast. These absorbers manipulate THz waves to enhance penetration and minimize energy loss, making THz imaging more effective for biomedical applications.

Over the past decade, advancements in metasurface based absorbers [9-26] have demonstrated remarkable potential in sensing, imaging, and diagnostic technologies. However, despite these significant achievements, challenges such as fabrication complexity, angle sensitivity, and the need for experimental validation continue to limit their broader applicability. In paper [9], Y. I. Abdulkarim et al. proposed a ZnSe based triple-band absorber that was designed to achieve ~99% absorption at 22.50, 28.98, and 35.14 THz, exhibiting dual-sensing capabilities. However, the design lacks experimental validation and shows performance degradation at incidence angles greater than 60°. Comparatively, L. Ma et al. designed a snowflake-shaped triple-band absorber in [10] reported up to 99.02% absorption at 0.550, 1.249, and 1.867 THz. This design exhibits high refractive index sensitivity but suffers from narrow bandwidths and sharp resonances, limiting its practical applications and fabrication flexibility. A metamaterial absorber with an ultrathin triple-band design achieved a remarkable absorption rate of 99.9% in the X and Ku bands presented in [11] by G. Deng et al. The design was also polarization-insensitive, making it suitable for conformal

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sensitivity and fabrication consistency. A Gear-shaped plasmonic sensor designed for high refractive index sensitivity (1044 nm/RIU) was proposed by A. Sarker et al. [12]. Metamaterial absorbers, as proposed in papers [13, 14, 15] have been utilized for diverse applications, including the detection of glucose, ethanol, biomedical sensing, and petroleum-based oils analysis. These absorbers demonstrate remarkable performance, achieving RI sensitivities up to 56.67 THz/RIU and Figure of Merit (FoM) values of 358.7 RIU⁻¹ [13] as well as high Q-factors of 1.71×10^5 and 62.59respectively in [14] and [15] whereas absorptions of 98.17% and 99.05% at 1.902 and 1.976 THz respectively in paper of A. Teber [16], achieving advantageous in cancer cell detection. Advancements in metasurfaces have shown significant potential for various sensing applications as presented in [16-18]. A Graphene-based metasurface achieve up to 99.7% absorption across 0.1-2.0 THz, offering high sensitivity for terahertz sensing but facing fabrication and tuning challenges as reported by Islam et al. [17]. E. S. Lari et al. also enable biomaterial and liquid sensing, with a maximum sensitivity of 273 nm/RIU for ethanol [18]. A plastic-templated metasurface for SARS-CoV-2 detection demonstrated by R. Ahmed et al. showed high sensitivity (1475 nm/RIU) but struggled with surface non-uniformity and reliability issues [19]. Where S. Banerjee et al. designed polarization-insensitive metamaterials with a narrowband structure (FWHM = 0.02 THz) and a FoM of 106demonstrated enhanced sensing for chloroform gas detection at a precise resonance frequency [20]. In [21], [22] a highsensitivity terahertz metamaterial sensor demonstrated two absorption peaks, in [21] at 1.93 THz and 2.7 THz, demonstrated a Q-factor of 574.46 and sensitivity of 2.37 THz/RIU for the higher frequency peak, while its high FoM of 540 RIU⁻¹ further emphasized its applicability in highprecision sensing. Y. Wang et al. [22] reported a temperature sensitivity of 24.4 GHz/K using a sensor based on InSb and graphene. This metamaterial absorber achieved wide-angle absorption, polarization-insensitive and high absorption rates. Researchers in [23, 24, 25] introduced a triple-band THz metamaterial absorber with three distinct absorption peaks at 0.4072 THz, 0.4232 THz, and 0.455 THz, achieving high absorptivity of 93.4%, 97.7%, and 98%, respectively, in [23]. Later, in [24], a complementary frequency-selective surface with crossed linear and concentric circular slots was proposed by F. Cai and Z. Kou, achieving high absorption at 0.6 THz (99.7%), 1.5 THz (95.4%), and 2.5 THz (99.5%), with tunability enabled by MOS₂ carrier concentration and graphene chemical potential. Where S. Anwar et al. designed an I-shaped resonator design, with a metallic ground layer separated by a dielectric spacer, demonstrated nearly 95% absorption at three resonant frequencies (1.655 THz, 1.985 THz, and 2.86 THz), making it suitable for applications in

applications, although it faces challenges such as angle

sensing, filtering, and stealth technologies [25]. In reference [26], N. R. Sabaruddin et al. presented a broadband terahertz metamaterial absorber with a bi-layer hybrid metal-graphene structure achieving 98.9% absorptance over 0.95-1.95 THz applied for optoelectronic applications. Terahertz Perfect Metamaterial Absorbers (PMAs) offer unique sensing capabilities, particularly for refractive index and gas detection, while recent p-type MOS sensors excel in specific gas sensing applications. PMAs can achieve high sensitivity and figure of merit (FoM) due to their ability to manipulate electromagnetic waves at terahertz frequencies. For example, a study showed sensor based on Pd-NiO nanorods combined with SnO₂ nanowires achieved a response (Ra/Rg) of 14.88 to 500 ppm acetone at 450 °C, with a response time of 11 seconds and a recovery time of 468 seconds. The sensor exhibited good selectivity towards acetone over other gases such as NH₃, CH₄, and VOCs [27]. Another study by Wang et al. reported a W-doped NiO sensor with an ultra-high response of 198.1 to 100 ppm acetone at 250 °C, and a detection limit in the ppb range. The enhanced performance was attributed to increased surface area and hole carrier concentration due to W doping [28].

This research paper presents the design, simulation, and analysis of a highly sensitive triple-band terahertz perfect metamaterial absorber (PMA) specifically tailored for organic sensing applications. The proposed absorber demonstrates perfect absorption at three distinct THz frequencies (0.717 THz, 1.368 THz, 3.535 THz), making it an ideal candidate for detecting various organic interactions with high specificity and sensitivity. The study focuses on optimizing the geometrical parameters of the metamaterial to achieve enhanced absorption and field localization, ensuring a high degree of sensitivity to environmental changes. The symmetrical design of the MA guarantees that its absorption remains insensitive by variations in polarization and incidence angles. Moreover, the proposed absorber is designed to detect various potential applications such as biomedical diagnostics, environmental sensing, and biochemical analysis. The novelty of this research lies in the integration of a triple-band (0.717, 1.368, 3.535 THz) absorption mechanism (99.99%, 99.95%, and 99.99%) with a sensitivity-focused design that caters to organic sensing applications. Through numerical simulations, this paper aims to demonstrate the efficacy of the proposed absorber in realworld sensing scenarios, providing a pathway for future advancements in terahertz-based metamaterial sensors.

2. Design Methodology

Fig. 1 illustrates the comprehensive functionality of a triple-band terahertz metamaterial absorber designed for organic sensing applications. It begins by showcasing a variety of organic and biochemical entities such as viruses, bacteria, DNA, cancer cells, gaseous, and various chemical

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compounds that represent the targets for sensing. These substances interact with the metamaterial absorber as indicated by the converging arrows toward a central Petri dish, symbolizing the platform where these interactions are detected. Below this, a detailed depiction of the metamaterial absorber highlights its intricate, square lattice pattern, which is crucial for its ability to absorb terahertz waves at three specific frequencies, optimizing its sensitivity and specificity for detecting subtle changes in the organic environment. The process culminates in a spectral response graph on the right, which displays the absorber's performance across a terahertz frequency range, with peaks in absorbance showing where nearly perfect absorption occurs, allowing for precise identification and analysis of the materials present. This integrative approach demonstrates how the metamaterial absorber can effectively capture and analyze diverse organic interactions, making it a versatile and powerful tool in fields ranging from environmental monitoring to biomedical diagnostics.

As this study is simulation-based, experimental protocols are not directly applicable. However, to ensure reproducibility and support translation into real-time applications, experimental interfacing of the analyte with the sensing region in a fabricated device involves several critical design elements. First, the sensing area, typically a metamaterial absorber (MA), can be incorporated into a compact sensor array designed for direct interaction with samples such as blood, saliva, or air. Multiple sensing elements can be integrated for multiplexed detection, with flexible substrates enabling use in portable or wearable formats. Second, microfluidic systems can precisely deliver samples to the sensor surface, controlling the flow to ensure effective interaction with the metamaterial structure. Capillary or pump-driven methods can be employed for realtime analysis. Third, THz resonance shifts induced by biomolecular interactions can be captured using THz timedomain spectroscopy (THz-TDS) or miniaturized spectrometers. Coupled with onboard data processing, the system enables real-time detection. Fourth, incorporating wireless communication modules such as Wi-Fi, Bluetooth, or 5G allows for remote monitoring and instant data transfer to healthcare providers or cloud-based platforms. Lastly, periodic calibration using known reference samples ensures the reliability of resonance frequency shifts corresponding to specific biomolecular signatures. Furthermore, to mitigate the influence of ambient humidity on dielectric properties or surface adsorption, hydrophobic coatings may be applied to the metamaterial structure. While these coatings improve environmental stability by repelling moisture, they can hinder analyte access, particularly for hydrophilic species. To balance these effects, ultrathin or selectively permeable coatings are recommended, allowing sufficient analyte interaction while preserving sensor performance.



Fig. 1: Schematic illustration of the proposed metamaterial absorber for organic sensing applications



3. Design Analysis

3.1 Design of Unit Cell Model

The proposed design was developed through multiple stages of evaluation, involving the selection of various substrates, including MgF₂, FR-4, and Quartz. The optimized design achieved dimensions of $53 \times 55 \times 7.8 \ \mu\text{m}^3$ using FR-4 substrate. The top and bottom layers of the structure are entirely covered with copper, with the top layer incorporating a square ring-shaped copper configuration. The design features a series of concentric squares arranged symmetrically and centered within a square boundary on the top surface. This nested arrangement serves as the region where test materials are placed for performance analysis. The optimized results, as depicted in Fig. 3 and Fig. 4, are discussed in detail in the subsequent sections.

3.2 Parameter Optimization

The design of the MTM absorber consists of a periodic unit cell, as illustrated in Fig. 1, which serves as the fundamental building block for the overall structure. To ensure accurate simulation results, periodic boundary conditions were applied along both the x-axis and y-axis, effectively replicating an infinite array of the designed unit cell. Meanwhile, a plane wave was incident along the z-axis, allowing for proper electromagnetic wave interaction with the structure.



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Fig. 3: Genetic Algorithm (GA) flowchart for structure optimization

To achieve optimal absorption performance, the genetic algorithm (GA) optimization technique, integrated within CST Microwave Studio, was employed. This evolutionary algorithm iteratively refines the structural parameters to enhance the absorber's efficiency across the targeted frequency bands. The final set of optimized parameters, obtained through this process, is depicted in Fig. 2 and 5 in graphically. The specific values for these optimized parameters are illustrated in Fig. 6, providing a comprehensive reference for the design configuration. For the genetic algorithm, the optimization process was carried out over 30 iterations, incorporating a 60% mutation rate and maintaining an anchor value of 10%. This cycle repeats until a convergence criterion is met specifically, when the absorptivity of one or more individuals exceeds 96%. At that point, the algorithm returns the best-performing metamaterial absorber structure that satisfies the desired absorptivity threshold, representing the optimized solution. The resonant absorption characteristics of a triple-band metamaterial absorber (MA) are influenced by various factors, including material properties, dimensional variations, and structural configurations. To analyze the spectral response of the proposed nanostructure in the infrared wavelength range, normal incident electromagnetic waves were applied. The optical behavior of the metamaterial is characterized by two fundamental parameters: transmittance, $T(\omega)$, which quantifies the fraction of incident light passing through the structure, and reflectance, $R(\omega)$, which represents the portion of light reflected. These parameters are derived from the scattering parameters (S-parameters), specifically S₁₁ and S₂₁, which describe the reflection and transmission coefficients, respectively. By extracting the S_{11} and S_{21} data from CST software, the transmission (T), reflection (R), and absorption (A) of the nanostructure were calculated using wellestablished equations (1) - (4) [18]. The absorption (A) is determined indirectly by considering the energy conservation principle, where it is obtained as $A(\omega)=1-T(\omega)-R(\omega)$, ensuring that all incident energy is accounted for in terms of reflection, transmission, and absorption within the metamaterial.

$$S_{11} = \frac{\sqrt{P(R)}}{\sqrt{P_i}} \tag{i}$$

$$S_{21} = \frac{\sqrt{P(T)}}{\sqrt{P_i}} \tag{ii}$$

$$R(\omega) = S_{11}^2 \tag{iii}$$

$$T(\omega) = S_{21}^2 \tag{iv}$$

Where, P(R)=Reflected Power, P(T)=Transmitted Power, and P_i =Incident Power.

To comprehensively analyze influences, five sets of simulations were performed using diverse dimensions and materials, as detailed in Fig. 2, offering valuable insights into the absorber's resonant behaviour. Adjusting parameters such as resonator thickness, spacer materials, and substrate types reveals their performances on absorption characteristics. For instance, the dielectric constant of the absorber significantly influences the resonant frequencies by altering the refractive index. Several substrates have been reported in the literature, but in this study, we focus on MgF₂, FR-4, and Quartz materials to investigate the effects of dielectric variations [18]. The selection of materials substantially impacts the observed results. As shown in Fig. 4 (a), both MgF₂ and

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Quartz exhibit absorption values exceeding 86% at two different frequencies: 0.647 and 1.221 THz for MgF₂, and 0.755 and 0.844 THz for Quartz. In comparison, FR-4 demonstrates significantly higher absorption, reaching 99.99% at 0.717 and 3.535 THz, respectively. For the second resonance, FR-4 achieves an absorption value of 99.95% at 1.368 THz, whereas MgF₂ and Quartz show absorption values of almost 75% and 70%, respectively. Changes in the material properties (Table I) lead to variations in the resonant behaviour of the proposed structure. As shown in Fig. 4 (b), altering the metal element (Gold, Copper, Aluminium) significantly affects the performance of the structure and the generation of a triple-band response [29]. Among the tested materials, Copper, with its superior electrical conductivity, demonstrated the best spectral response, achieving an absorbance of 99.99%. Additionally, the FR-4 substrate paired with a copper plate exhibited three distinct absorption peaks at 0.717, 1.368, and 3.535 THz considering thickness $t_1=0.24$ µm. These findings highlight the critical role of material selection in optimizing absorption performance across different frequency bands. Fig. 5 (a-c) illustrates the simulation results, highlighting the effect of resonator lengths (L_1, L_2, L_3) on absorption peaks and emphasizing the critical role of material selection, such as Arlon AD 430, in determining the resonant characteristics of the absorber. Variations in the first resonator length, L_1 (ranging from 5 μ m) to 9 µm), significantly influenced the third resonance frequency.



Metals	Plasma frequency $(\omega_p \times 10^{15} S^{-1})$	Collision frequency (v _c ×10 ¹⁵ S ⁻¹)
Gold	13.8	0.11
Aluminium	22.9	0.92
Copper	13.4	0.14

Similarly, adjustments to the second resonator length, L_2 (16–20 µm), caused noticeable shifts in the second resonance frequency, indicating the sensitivity of the system to dimensional changes. Alterations in the outer resonator length L₃, impacted the first absorption frequency, producing frequency shifts within the 0.6–1 THz range, with optimal absorption 99.99% observed at L₃ = 25.5 µm when L₁ = 7 µm and L₂ = 18 µm. This configuration consistently demonstrated a triple-band response, with distinct absorption



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peaks at 0.717 THz, 1.368 THz, and 3.535 THz in Fig. 5 (c). High absorption values of 99.73% and 99.99% recorded at resonator lengths of $L_1 = 7 \mu m$ ($L_2 = 18 \mu m$, $L_3 = 25.5 \mu m$) in Fig. 5 (a) and $L_2 = 18 \ \mu m$ ($L_1 = 7 \ \mu m$, $L_3 = 25.5 \ \mu m$) in Fig. 5(b), respectively. These results emphasize the significant interplay between resonator dimensions and frequency-dependent absorption performance, providing valuable insights into the design and optimization of metamaterial absorbers for specific applications. Whether in terms of varying thickness in slot, substrate and ground plane in 3D material layers reveal reflection coefficient of antenna vary significantly by increasing value for t_1 (0.16-0.28 μ m), t_2 (7.2-8.4 µm), t_3 (0.33-0.41 µm) but each time it strict in specific frequency that means increasing thickness does not affect the resonance frequency but improve in reflection coefficient, in Fig. 5(d-f) highlighting the precision required in slot and resonator designs in terms of width. Optimal characteristics were observed when the FR-4 thickness and width were adjusted to respectively $t_2=7.8 \mu m$ (Fig. 5e) and $y=55 \mu m$. Finding more adequate results increased width of square ring (W_1, W_2, W_3) causing an influence of reflection coefficient at previous frequencies. An optimal result was gained when $W_1=2.05 \ \mu m$, $W_2=2.5 \ \mu m$, $W_3=1.65 \ \mu m$ at reflection coefficient of (-42.78dB at 0.717 THz, -34.965 dB at 1.368 THz, -42.59 dB at 3.535 THz), (-42.47 dB at 0.717 THz, -54.59 dB at 1.368 THz, -39.53 dB at -39.20 THz) and (-42.47 dB at 0.717 THz, -54.51 dB at 1.368 THz, -39.2 dB at 3.535 THz) respectively. The corresponding S-parameter plot is given in Fig. 5 (g-i) with respect to $t_3 = 0.37 \mu m$. These findings emphasize the intricate relationship between structural dimensions, material selection. and electromagnetic responses in metamaterial absorbers. Fig. 6 illustrates the absorption behavior of four distinct metamaterial absorber designs, each with varying square ring configurations, and their effect on absorption peaks and resonant frequencies across the 0.7-3.6 THz operating range. The analysis reveals that the complexity and size of the square ring structures significantly influence the absorption performance. The simplest configuration, which features a centric small square ring (i), shows a pronounced absorption peak at around 3.51 THz but demonstrates limited tuning capabilities beyond this frequency. The second larger middle square ring configuration achieves a peak at 1.31 THz and displays some absorptive behavior (87.97%), though it does not reach perfect absorption (ii). The outermost rear shape featuring a larger square ring in the third step exhibits maximum absorption, measuring approximately 99.99% peak around 0.717 THz (iii). In contrast, the final configuration (iv), which consists of multiple concentric square rings, exhibits perfect absorption upto 99.99%, indicating superior resonance control and tunability over a broader frequency range. These findings suggest that more intricate square ring configurations improve the metamaterial

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absorber's performance, offering better tuning options and wider frequency coverage, with concentric designs showing the most effective resonance across multiple frequencies. Fig. 6 illustrates the absorption characteristics of the four models.

4. Results investigation

4.1 Parametric Investigations

To better understand the physical absorption mechanism of the proposed metamaterial absorbers, the E-field and H-field distributions of the design were simulated and presented in

Fig. 7 and 8, respectively, at three resonance frequencies (0.717, 1.368, and 3.535 THz). The regions of higher intensity in the figure are indicated by the red and yellow areas on the color scale. For the electric field intensity, shown in Fig. 7 (a, b, c), the highest intensity is concentrated vertically near the outermost boundary in 6 (a), transitions to the intermediate square boundary in 6 (b), and becomes strongly localized around the innermost square boundary in Fig. 7 (c). Similarly, for the magnetic field intensity in Fig. 8 (a, b, c) the highest intensity is initially



Fig. 5: Parametric responses of the metamaterial absorber under geometric variations: (a)–(c) absorbance for varying strip lengths L₁, L₂ and L₃; (d)–(f) reflection coefficient S₁₁ for different substrate thickness t₁, t₂ and t₃; (g)–(i) S₁₁ for varying strip widths W₁, W₂ and W₃.

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distributed along the horizontal outer boundary in Fig. 8 (a), shifts toward the intermediate square boundary in Fig. 8 (b), and finally becomes highly concentrated near the innermost square boundary in Fig. 8 (c). This progression highlights that the intensity of both fields is most pronounced near structural boundaries, with the strongest confinement and localization occurring around the innermost regions. As observed in Fig. 8, the current distribution exhibits a behaviour similar to the previous scenario, with currents localized at distinct locations within the outer and inner sub-branches, respectively. The arrangement in Fig. 9 (a, d) represents the surface current density on the structure at a frequency of 0.717 THz. Each arrow's direction indicates the direction of the current. From Fig. 9 (d), the arrows appear to form a turbulent flow pattern on bottom side of cell, suggesting a spiral current flow within the depicted square metamaterial structures at resonant surface current density strength, with a maximum value of 135,664 A/m. Where on top surface peak current density exhibits at the edge of outer square resonator. The figure displays the surface current distribution on a structure at a frequency of 1.368 THz, as indicated in Fig. 9 (b) more current flow inside the second resonator on the other bottom side (Fig. 9 (e)) current arrows form circular or vortex-like patterns, suggesting rotational current loops around specific points or regions with current density of 76088.1 A/m. In Fig. 9 (c, f) represents the surface current distribution at a frequency of 3.535 THz, where peak current density reaches 93311.8 A/m. The arrows form more localized circular (rotational flows) and denser around certain areas (in center of the square absorber), indicating current loops (regions) of high curl in the surface current vector field for both top and bottom surfaces in Fig. 9 (c, f). At the edges, the surface current density seems to align parallel to the boundary. Lower frequencies excite smoother, larger-scale rotational patterns, while higher frequencies result in finer, more complex structures due to higher-order resonances. The magnitude of the surface current density peaks at the fundamental resonance (0.717 THz) and varies depending on the efficiency of mode excitation at the other frequencies. The surface currents on the top and bottom metallic layers flow in antiparallel directions, moving in opposite to each other.





4.2 Performance Analysis

The primary focus of this study is to evaluate sensitivity, precision, and applicability by detecting refractive index variations, particularly for organic analytes sensing. The effect of analyte depth on the absorption was investigated in Fig. 10 (a). It was observed that modifying the analyte depth caused a resonance shift. These observations were recorded in fig. 10 (a) by increasing the depth of the analyte from 0.25to 0.75 µm in steps of 0.1 µm. Another sensing performance was investigated for the proposed design, in which the refractive index (η) of the surroundings was changed from 1.0 to 2.0 (Fig. 10 (b)) by considering a very small step of 0.1, while the thickness of the analyte was fixed at 0.55 µm. We have used this step as it can be used for applications involving sensing harmful gases. The change of refractive index from 1.0-2.0 exhibits blue shifts in three resonance frequencies and maintained almost constant absorption amplitudes but in higher frequencies absorbances are gradually degraded. In all cases, the peak absorption was greater than 98% in Fig. 10 (a, b). Figures 10 (c)–(e) display sensitivity plots, illustrating a linear relationship between resonance frequency shifts and



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the refractive index unit (RIU). The sensing performance of the proposed triple-band perfect metamaterial absorber is evaluated by varying the refractive index of the surrounding medium. The corresponding absorption spectra are shown in Fig. 10 (c)–(e). It can be observed that the three resonance peak frequencies shift with changes in the refractive index. The slopes of the linear fit lines in Fig. 10 (c-e) represent the sensitivity of the absorber for each peak (peak 1, 2 and 3). The absorber's efficiency is quantified by its sensitivity, which is defined as the ratio of the resonance frequency shift to the variation in refractive index.

sensitivity (S) =
$$\frac{\Delta f}{\Delta n}$$

where Δf is the shift in the resonance frequency and Δn is the shift in the refractive index. The corresponding linear fitting equations for the three resonant frequencies are defined in the respective Fig. 10 (c)-(e) and plotted against the refractive index. From the analysis based on linear fitting graph in Fig. 10 (f), the sensitivities for the three resonance peaks are found to be 133 GHz/RIU, 175 GHz/RIU, and 479.5 GHz/RIU, respectively, as determined from the slopes of the curves. In addition, it has been observed that the R^2 values are close to unity (0.995, 0.9901, and 0.9951), indicating that refractive index change has a significant impact on resonance frequency shifts and the sensor has sufficient precision. The Full Width at Half Maximum (FWHM) for the proposed structure is 0.0551 at 0.717 THz, indicating strong frequency selectivity due to the narrow bandwidth. The FWHM values for the other two peaks are 0.1077 and 0.2449. It is observed that the FWHM bandwidth of the second absorptance peak increases as the background refractive index increases contributing to high spectral resolution and leading to a reduction in the Figure of Merit (FoM) and Quality factor (Q-factor), as shown in Fig. 10. The Figure of Merit (FoM) is an important parameter for comparing the sensing performance of various sensors and is defined as:

 $FoM = \frac{Sensitivity}{FWHM}$

Where Quality factor (Q-factor) is defined as:

$$Q = \frac{Resonance\ frequency}{FWHM}$$

For the first, second, and third peaks, the Q-factors are calculated as 13.0127, 12.7019, and 14.4324, respectively, while the corresponding FoM values are 2,4138, 1.6249, and 1.9579. These results highlight the suitability of the proposed structure for sensing applications. As the refractive index (n) varies from 1 to 2, the sensitivity (S) ranges from 133 GHz/RIU to 479.5 GHz/RIU, the FoM ranges from 1.6249 to 2.4138, and the Q-factor ranges from 12.7019 to 14.4324. The combined linear behavior in resonance frequency and sensitivity validates the high accuracy and consistency of

sensor, making it ideal for applications requiring precise detection of refractive index changes, such as chemical analysis and biosensing. Furthermore, the sensing performance of the designed triple-band absorber surpasses previously published research results, highlighting its effectiveness for sensing applications.

5. Sensing Performance

5.1 Biomolecule & Virology

The frequency shift technique in THz metamaterial absorbers enables precise identification and differentiation of biomolecules, chemicals, and viruses by analyzing changes in resonance frequency is illustrated in Fig. 11. Different biomolecules and chemicals have unique dielectric permittivity (ϵ), which influences how they interact with THz waves. Absorbance spectra of biomolecules in Fig. 11 (a) exhibits distinct frequency-dependent variations due to their structural differences in double-stranded DNA (dsDNA) and single-stranded DNA (ssDNA) mentioned in [30]. Biomolecules, such as DNA, proteins, and viruses, exhibit specific vibrational and rotational modes in the THz range. These intrinsic resonances cause absorption at characteristic frequencies, shifting the meta-absorber's response. For example, in DNA analysis (Fig. 11 (a)) ssDNA and dsDNA have different hydrogen bonding and stacking interactions, leading to subtle resonance shifts. The resonance peak of dsDNA appears at 3.4225 THz with an absorbance of 0.9938, while ssDNA exhibits a slightly lower peak at 3.4015 THz with an absorbance of 0.9914, this 21 GHz fluctuation in frequency indicating structural sensitivity. The strength of this interaction depends on the biomolecule's size, thickness, and binding affinity. From Fig. 11 (b), the absorbance spectra of viruses (FAdV, H9N2, H5N2, H4N6, H5N1) reveal distinct resonant peaks at frequencies f3, allowing differentiation. The simulated results show resonant frequencies of 3.6045 THz for FAdV, 3.608 THz for H9N2, 3.6062 THz for H5N2, and 3.5975 THz for H4N6 and H5N1, indicating clear spectral separation for virus identification. When a biomolecule is adsorbed, it alters the effective refractive index and other self-characteristics [31] near the surface, shifting the resonant frequency. According to Fig. 11 (c) compares the absorbance spectra of IBV (COVID-19) and normal blood, with IBV peaking at 1.37 THz and normal blood at 1.30 THz. A secondary IBV peak appears at 3.545 THz with an absorbance of 0.9996, compared to 0.9964 at 3.447 THz for normal blood. When a molecule is introduced onto the meta-absorber, it modifies the local refractive index, leading to a shift in resonance frequency. Similarly, COVID-19 (IBV) and normal blood have different molecular compositions [32], resulting in distinct frequency shifts, which suggest the feasibility of using THz spectroscopy to detect COVID-19 in blood samples.



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Fig. 11: Sensing performance of metamaterial absorber for (a) biological tissue, (b) virus and (c) IBV

5.2 Tissue Diagnostics



Fig. 12: Response of the proposed metamaterial absorber in terms of absorbance for (a) normal and tumor cells (b) normal and BCC cells

THz imaging is gaining attention in biomedical applications for its ability to interact with water and biomolecular vibrations on ultrafast timescales. This interaction allows it to distinguish tissue states pathological, healthy, burned, or dehydrated by measuring refractive index and absorption coefficient. These measurements provide phase and amplitude data, aiding in the differentiation of biological structures [33]. This frequency shift in THz PMAs occurs due to differentiation between molecular composition and structural alterations between healthy and malignant tissues, affecting their electromagnetic response. As shown in Fig. 12(a), the absorbance peaks of normal and tumor breast tissues exhibit distinct frequency-dependent variations due to differences in their molecular composition [34]. Normal breast tissue displays a resonance peak at 3.3595 THz with an

absorbance of 0.9356, whereas tumor breast tissue shifts slightly lower to 3.3385 THz with frequency transition of 21 GHz. This distinct resonance peaks, with tumor tissue consistently showing a slight downward frequency shift and increased absorbance, indicating denser molecular packing or altered water content. From different optical properties in the double Debye model (Table II) [35], illustrates frequency shifts in Fig. 12(b) for basal cell carcinoma (BCC) skin tissue, both in vivo and ex vivo, further validating the sensitivity of THz spectroscopy to cancerous changes. The ability of THz metamaterial absorbers to capture these spectral shifts highlights their potential for non-invasive cancer diagnostics. By leveraging frequency shifts, in vivo spectra reveal distinct peaks 3.321 THz (normal) to 3.2825 THz (BCC) while ex vivo measurements show peaks at 3.3245 THz (normal) and 3.328 THz (BCC), indicating frequency shifts due to cancerous alterations. The observed spectral variations, particularly the shift in resonance peaks and differences in absorbance intensity, confirm the sensitivity of THz spectroscopy to subtle tissue and structural changes in healthy tissues. These findings reinforce the potential of THz metamaterial absorbers as non-invasive diagnostic tools for early cancer detection, offering reliable differentiation between healthy and cancerous tissues in both conditions.



Materials	High Frequency Permittivity	Static permittivity	Second relaxation permittivity	First relaxation Time	Second relaxation Time $ au_2$ [Ps]	
	$\boldsymbol{\varepsilon}_{\infty}$	ε_s	ε_2	$\tau_1[Ps]$		
Ex vivo (normal skin)	2.58	14.7	4.16	1.45	0.0611	
Ex vivo BCC	2.65	17.6	4.23	1.55	0.0614	
In vivo (normal skin)	3.4	25	5.0	7.0	1.0	
In vivo BCC	4.2	40	6.2	10.0	1.0	

5.3. Oil



When THz waves interact with chemical bonds and molecular vibrations, they cause variations in absorption spectra and resonance frequency shifts, which depend on factors such as dielectric constant, hydrocarbon composition, polarity (e.g., esters in peanut oil, sulphur in carbon disulfide), density, and viscosity. A THz metamaterial absorber, initially designed with a known resonance frequency in a reference environment (air or vacuum), enhances detection by resonating at specific THz frequencies and shifting its absorption peak in response to changes in the surrounding oil medium. The material characteristics of the sensing elements are presented in Table III [36]. Fig. 13 illustrates the terahertz absorbance spectra (within 3–4 THz) of Diesel, Gasoline, Turpentine, Carbon Disulfide, and Peanut Oil, highlighting

Table III: Sensing dielectric properties

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Liquid	High-frequency permittivity ε _∞	Dielectric first relaxation strength E1	Dielectric second relaxation strength E2	First relaxation time $ au_1[Ps]$	Second relaxation time τ 2[PS]
Disel	2.08	2.16		0.053	
Gasoline	1.94	2.36	2.06	3.18	0.05

distinct spectral features. From illustration in Fig. 13 (a), Diesel and Gasoline show a dip near 3.6–3.7 THz, with Gasoline exhibiting higher resonance response at (3.811 THz) compared to Diesel (0.788245 at 3.804 THz), indicating material-specific differences. All three materials in Fig. 13 (b) highlights peak at 3.349 THz (Peanut Oil 0.981198), 3.377 THz (Turpentine, 0.986868), and 3.412 THz (Carbon Disulfide, 0.992391). This comparison data simulated with respect to air medium emphasizes the distinct molecular

properties and dielectric response of these two types in this frequency range, suggesting potential applications in fuel and oil characterization or identification. This non-invasive differentiation underscores the potential of THz perfect metamaterial absorbers (PMAs) as a powerful tool for fuel and oil characterization in industrial quality control and fuel analysis.





Fig. 14: Response of the proposed MA in terms of absorbance for organic industrial chemicals

Different chemical structures exhibit unique THz responses due to differences in molecular dipole moments, bonding and polarizability. When THz waves interact with a material, its permittivity (dielectric response) and refractive index influence how the waves are absorbed or transmitted. This results in distinct spectral peaks and frequency shifts, as a result in Fig. 14 (a) shows the absorbance spectra of four chemicals-Ether, Ethylene glycol, Chlorobenzene, and Quinoline—between 3 and 3.65 THz, each displaying distinct peaks due to variations in the sensing element [37]. Ether exhibits peak at 0.998 near 3.4715 THz, ethylene glycol at 0.995 around 3.433 THz, chlorobenzene at 0.9911 near 3.4085 THz, and quinoline at 0.9871 around 3.377 THz, demonstrating the potential for chemical identification. Reflection coefficient (S_{11}) plotted in Fig. 14 (b) against frequency in the terahertz (THz) range for detecting liquid of chloroform. Both exhibit resonance near 3.54 THz, with annotated points marking key values. For air, the resonance occurs at 3.53887 THz with -42.4035 dB, while for chloroform, it is within -38.072 dB. The slight shift in resonance highlights the medium influences in resonant properties.

6. Comparative Analysis

The proposed absorber was evaluated in comparison to previous designs documented in recent literature, considering parameters such as operating frequency, FWHM, quality factor (Q-factor), number of absorption bands, absorbance, and sensitivity. As summarized in Table IV, the proposed design outperforms earlier designs by achieving triband terahertz absorption with significantly improved sensitivity.

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4	Table IV: Comparison table									
5 - 6 7 _	Ref.	Operation range (THz)	Number of bands	Material substrate	Q-Factor	FWHM	Absorbance (%)	Polarization Angle	Sensitivity (GHz/RIU)	Applications (Sensing/Det ection)
8 9 10	[10]	≈0.5–1.9	3	Copper & Polytetrafluoroethylene (PTEE)	26.01 17.83 58.04	0.2124, 0.7005, 0.5804	97.43 79.22 99.02	0-60	137.70 306.25 473.86	Liquid
11	[15]	≈2.55-2.65	1	Quartz, Silicon	62.59	_	99.8		733	Liquid
12 ⁻ 13	[16]	≈1.90–1.98	2	Aluminium	240.15, 181.61	_	98.17, 99.05	0-90	794, 971	Biological Samples
14	[20]	_	1	Gallium Arsenide	145.25	0.02	99.65	0-90	2120	Chloroform
15- 16	[21]	1–3	2	Dielectric	574.46	0.142, 0047	Near 100	-	2370	Tuberculosis Bacteria
17- 18	[22]	1.0-3.5	1	Quartz	30	0.08	99.9	0-90	21.9 GHz/K	—
20 21_	[23]	0.4–0.46	3	Polyimide	—	_	93.4, 97.7, 98	0-60	—	—
22 22 23_	[24]	0.2–3.2	3	MoS_2	_	_	99.7, 95.4, 99.5	0-90	_	_
24 25	[25]	1.655–2.86	3	Polyimide	1.03, 9.925, 58.3	0.15, 0.20, 0.049	95, 93, 96	0-60	100, 150, 1200	Gas
26	[26]	0.95-1.95	2	SiO_2	—	(98.9	0-90	—	—
27 28 29 30	Prop. work	0.7–3.6	3	FR-4	13.0127, 12.7019, 14.4324	0.0551, 0.1077, 0.2449	99.99, 99.95, 99.99	0-90	133, 175, 479.5	Organic Substance (Biomolecule, Virology, Tissue, Chemical, Oil)
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7. Future Outlook

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In the next phase of the research, metasurfaces are planned to be fabricated using nanoimprint lithography (NIL) or electron-beam lithography (e-beam lithography), both capable of achieving the high-resolution patterning required for absorber structures. The design will be refined based on simulation results to ensure optimal resonance characteristics for targeted sensing applications. Material selection and structural parameters for the meta-absorber will be guided by these simulations. The absorber patterns will then be transferred onto an FR-4 substrate using the chosen lithography technique, followed by the deposition of a thin metallic layer, such as copper, to complete the meta-absorber fabrication. To enhance detection sensitivity, a biological interface layer will be applied to the metasurface to support biomolecule adsorption. This interface layer will be optimized for stability and functionality under practical conditions. To further enhance the applicability of the proposed design, future studies will experimentally investigate the influence of environmental factors specifically humidity and temperature on the sensor's reliability and stability. Such investigations would provide valuable insights into the sensor's robustness under real-world operating conditions and support the development of protective

strategies such as encapsulation or environmental compensation algorithms.

8. Conclusion

In summary, this paper contributes to the ongoing development of metamaterial-based terahertz absorbers by proposing a novel triple-band PMA with enhanced absorptivity of (99.99%) and a wide polarization angle (0-90°), together contributing to increased robustness for organic sensing applications. By integrating advanced design techniques with the unique properties of metamaterials, our sensor achieves a broader frequency range (0.7-3.6 THz) than most references, unlocking new possibilities for highly sensitive and multifunctional sensing applications. The sensor's high sensitivity (479.5 THz/RIU) and precision in detecting refractive index variations with demonstrate its potential for advanced sensing applications, including harmful gas monitoring and bio-analyte detection. Such sensitivity is particularly crucial for detecting trace-level biomolecules and chemicals. This frequency shift-based mechanism enhances the capability of THz metamaterial absorbers (MAs). By leveraging spectral shifts and absorption variations, MAs enable precise identification of biomolecules, chemicals, and other substances by analysing

variations in absorption intensity and resonance peak positions. The ability to operate at multiple resonance frequencies improves selectivity and sensitivity, making MAs powerful tools for non-invasive diagnostics, chemical analysis, and industrial quality control applications. These findings underscore the significance of this research in developing next-generation THz sensors with superior performance. The findings of this research have the potential to impact a wide range of fields, from medical diagnostics and environmental monitoring to industrial process control and biochemical analysis, establishing a benchmark in terahertz sensing technologies and offering a promising pathway for next-generation THz sensors with reliable sensing systems.

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