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Barbie

(24/MSCPHY/43)

ABSTRACT

For the label-free and non-invasive detection of Tuberculosis (TB) cells, this work presents a detailed computational study of a highly sensitive Terahertz (THz) metamaterial (MM) based biosensor. The proposed structure are simulated and analyzed using CST Studio Suite. The finite element method (FEM) along with a frequency-domain electromagnetic (EM) solver are used to evaluate its performance characteristics. The proposed unit cell is consists of a ground plane made up of gold, an inexpensive dielectric substrate which is made up of paper material, and a top resonator which consists of two brick-shaped structure along with three closed circular ring structures placed between them. This resonator structure is made up of Vanadium dioxide (VO_2). The absorptivity curves are also evaluated by varying several geometrical parameters, such as the substrate thickness, the separation between the two bricks, and the radii of the rings etc. The optimized design achieves 99.88 % absorption at a resonance frequency of 3.3777 THz.

The sensing mechanism of the proposed sensor relies on the strong localization of electric and magnetic fields within the analyte layer at resonance. Consequently, small variations in the optical properties of the analyte sample, especially changes in the refractive index, can be accurately detected. A noticeable redshift in the resonant frequency is observed with the increase in the refractive index of the analyte, indicating a high sensitivity of the sensor to variations in the surrounding dielectric environment and enabling effective detection of TB cells. The proposed sensor exhibits clear resonance frequency variations in response to changes in the analyte, achieving a maximum sensitivity of 700 GHz/RIU for TB1. In addition, the highest quality factor (Q-factor) and figure of merit (FOM) values obtained are 16.2633 for TB4 and 3.4516 RIU^{-1} for TB1, respectively. These results indicate that the developed design has strong potential to be utilized as an effective computational platform for future development, fabrication, and experimental assessment of THz biosensors.

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LIST OF ABBREVIATIONS

Abbreviation	Full Form
TB	Tuberculosis
THz	Terahertz
MM	Metamaterial
FEM	Finite element method
EM	Electromagnetic
VO_2	Vanadium dioxide
RHM	Right- handed materials
LHM	Left - handed materials
DPS	Double positive materials
ENG	Epsilon negative materials
MNG	Mu negative materials
DNG	Double negative materials
SRR_S	Split – ring resonators
$CSRR_S$	Complementary split ring resonators
FOM	Figure of merit
Q-factor	Quality factor
RI	Refractive index
A	Absorption Capability
GHz	Gigahertz
S	Sensitivity
FWHM	Full width at half maximum
CST	Computer Simulation Technology
3D	Three dimensional

CHAPTER-1

INTRODUCTION

1.1 Classification of materials

The propagation behavior of electromagnetic waves in a material is strongly influenced by two important parameters: electric permittivity (ε) and magnetic permeability (μ). In conventional materials, where both of these parameters possess positive values, the electromagnetic wave follows the right-hand rule. In such media, the wave vector $\vec{k}$, which represents the direction of wave propagation, and the poynting vector $\vec{p}$, which indicates the direction of energy flow between the source (A) and receiver (B), point in the same direction. Materials exhibiting this behavior are commonly referred to as right-handed materials (RHM).

However, under certain conditions, both permittivity and permeability can attain negative values. In this case, the propagation characteristics of the electromagnetic wave become entirely different from those observed in conventional materials. The direction of energy flow and the direction of wave propagation become opposite to each other, meaning that the poynting vector $\vec{p}$ and wave vector $\vec{k}$, are oriented in reverse directions, as illustrated in fig.1. Materials showing this unusual electromagnetic behavior are known as left-handed materials (LHM), and they form the basis for many unique metamaterial properties such as negative refraction and reverse wave propagation [1-4].

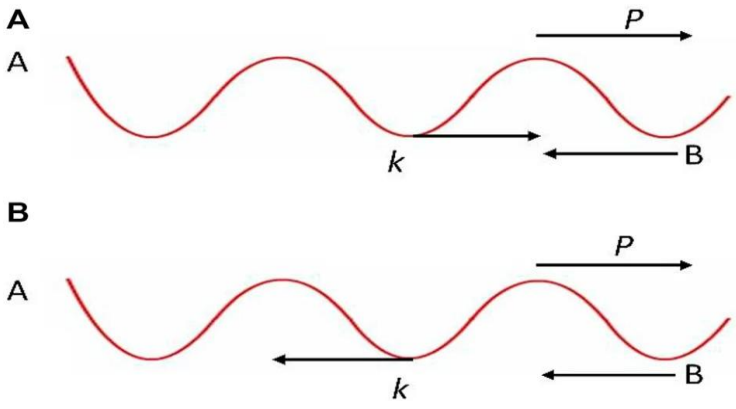


Fig.1 Wave propagation in **(A)** RHM and **(B)** LHM

Therefore, the propagation behavior of electromagnetic waves within a medium is mainly determined by the values of permittivity (ε) and permeability (μ). Based on the different combinations of these two parameters, materials can generally be classified into four distinct categories, as illustrated in fig.2.

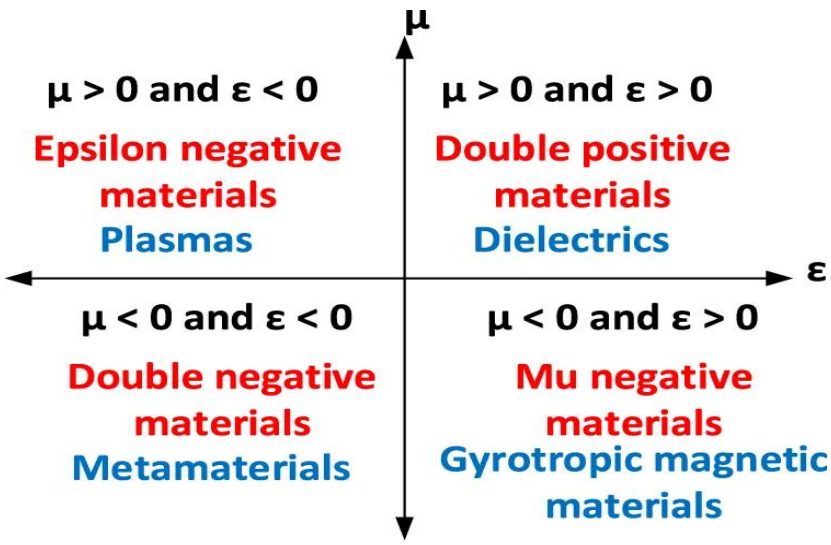


Fig.2 Classification of materials

24 Materials can be broadly classified into four categories based on the signs of their electric permittivity (ε) and magnetic permeability (μ). The first category is known as **double positive (DPS) materials**, in which both permittivity and permeability have positive values. Most naturally occurring dielectric materials belong to this group and exhibit normal electromagnetic wave propagation behavior.

The second category consists of **epsilon negative (ENG) materials**, where the permittivity becomes negative while the permeability remains positive. Certain plasma materials show this type of electromagnetic response within specific frequency ranges. Due to their negative permittivity characteristics, these materials interact with electromagnetic waves differently from conventional dielectrics.

The third category includes **mu negative (MNG) materials**, which possess positive permittivity and negative permeability. Materials with gyrotropic magnetic properties commonly exhibit this behaviour and have unique magnetic responses when exposed to electromagnetic fields.

23 The fourth category is referred to as **double negative (DNG) materials**, where both permittivity and permeability are negative simultaneously. These materials do not naturally exist but are artificially engineered using various metamaterial structures. One of the most unusual characteristics of these materials is that electromagnetic (EM) waves

propagate in the reverse direction after entering the medium which results in negative refraction.

1.2 Concept of Metamaterial

Metamaterials are specially engineered materials that are designed to control and manipulate electromagnetic waves in ways that are not normally possible with naturally available materials. Unlike conventional materials, the behavior of metamaterials is largely governed by their structural design, size, geometry and arrangement of unit cells. These unique features allow metamaterials to exhibit unusual characteristics such as negative refractive index [5,6], near-perfect absorption [7,8], wave bending, cloaking effects [9], and polarization conversion [10,11].

The word metamaterial is came up from word meta which means beyond. This name reflects the extraordinary properties of these materials that are not found in conventional materials. The metamaterials was first introduced by Victor Veselago in 1968. He proposed that materials having both negative permittivity, permeability could show a negative refractive index. After major developments in fabrication technologies, microelectronics, and nanotechnology the practical implementation of such structures became achievable.

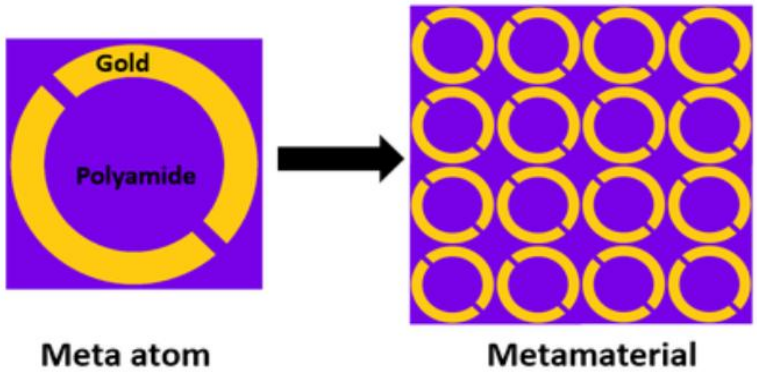


Fig.3 Meta atom as a building block of metamaterial

Metamaterials are generally formed by arranging artificially designed elements ,in a periodic manner, called as unit cells or meta-atoms [12-15]. These unit cells are usually much smaller than the wavelength of the incident electromagnetic wave, which results in phenomenon of effective homogeneous medium [16]. Different types of resonator geometries such as split-ring resonators (SRRs) [17], complementary split-ring resonators

(CSRRs), circular rings, wire structures, and various patterned metallic elements are commonly used in metamaterial design. According to the specific application requirements, researchers modifying the structure and geometry of these metamaterial across various frequency ranges like in microwave, terahertz, infrared and optical [5].

1.3 Some Unusual Properties of Metamaterials

Metamaterials exhibit various unique properties that are generally not found in naturally occuring materials. These exceptional characteristics arise due to their structures rather than their chemical composition. By carefully designing the geometry, arrangement, and dimensions of the resonating elements, metamaterials can interact with electromagnetic waves in various unusual ways. Some of the major unusual properties of metamaterials are listed in this section.

1. Negative Refractive Index

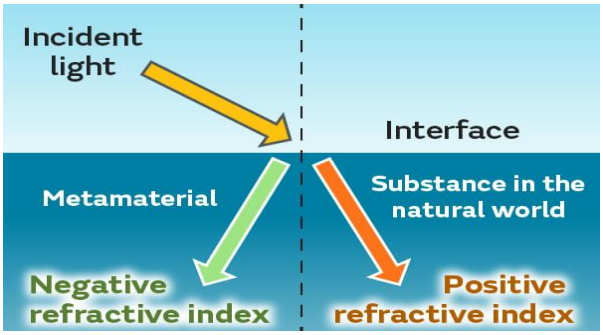


Fig.4 Conceptual Diagram of the Negative Refractive Index in Metamaterials

One of the most common features of metamaterials is their ability to produce a negative refractive index. In ordinary materials, electromagnetic waves bend in the usual direction when moving from one medium to another but in metamaterials which have both negative electric permittivity (ε) and magnetic permeability (μ) cause electromagnetic waves to refract in the opposite direction.

$$n = \sqrt{\varepsilon\mu} \qquad (1)$$

This unusual behavior of metamaterial is known as negative refraction.

2. Near-Perfect Electromagnetic Absorption

Metamaterials can be designed to absorb incident electromagnetic waves almost completely which can be done by carefully optimizing the resonator geometry and impedance matching conditions, which results into minimise reflection and transmission also allowing the incoming energy to be trapped inside the structure.

3. Electromagnetic Cloaking Capability

Another extraordinary property of metamaterials is their potential to achieve electromagnetic cloaking. In such structures, electromagnetic waves can be guided around an object in a controlled manner, reducing scattering and making the object partially invisible to detection systems. This phenomenon is mainly based on transformation optics and gradient-index metamaterial designs.

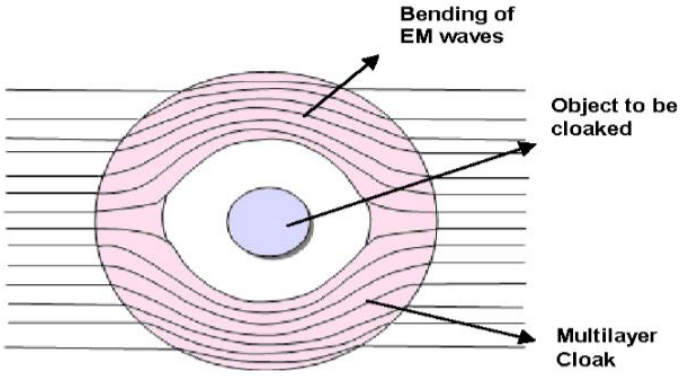


Fig.5 Phenomenon of invisibility cloaking

4. Super-Lensing and Subwavelength Imaging

Traditional optical lenses are restricted by the diffraction limit, which limits the resolution of imaging systems. Metamaterials can overcome this limitation by amplifying evanescent waves and focusing electromagnetic energy at dimensions smaller than the wavelength. As a result, metamaterial-based super-lenses can generate extremely high-resolution images.

5. Strong Localization of Electromagnetic Fields

Metamaterials are capable of producing highly concentrated electric and magnetic fields around their resonating structures. Due to resonance effects, electromagnetic energy becomes confined within a very small region, leading to enhanced wave–matter interaction.

This strong field localization improves the performance of biosensors, chemical sensors, nonlinear optical devices, and energy harvesting systems.

6. **Reverse Doppler Effect**

   Metamaterials may also demonstrate the reverse Doppler effect, which behaves opposite to the conventional Doppler phenomenon. Normally, when a source approaches an observer, the observed frequency increases. However, in metamaterials with negative refractive index, the frequency shift occurs in the reverse manner.

   This effect has importance in communication systems, wave physics, and signal processing technologies.

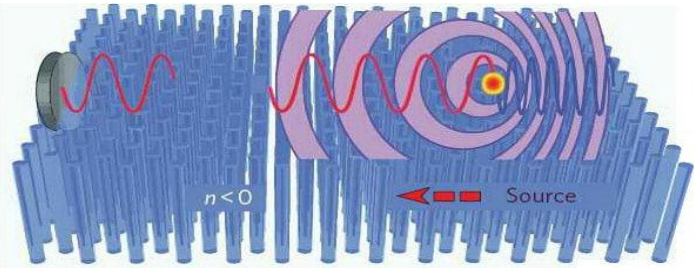


Fig. 6 Showing phenomenon of inverse doppler effect

1.4 Absorption Mechanism

These structures show absorption behaviour because of several significant factors, like negative values of electric permittivity (ε) and magnetic permeability (μ), effective impedance matching to free space, reduction of the metal plasma frequency, and excitation of strong electric and magnetic responses. The geometry of the absorber can be carefully designed and optimized to control and improve the overall absorption performance. The interaction between the electromagnetic waves and the structure can be effectively studied by altering the shape, size and arrangement of the resonating elements. The three main absorption mechanisms are discussed in more detail in the following subsections.

1.4.1 Magnetic and Electrical Responses

The absorption behavior is mainly governed by the combined effects of electric and magnetic resonances generated within the structure. Magnetic resonance is produced through loop-shaped or closed-ring geometries, while electric resonance is commonly produced by introducing gaps or splits in the resonating elements. By carefully optimizing

the geometry and arrangement of these structures, both the electric and magnetic responses can be effectively controlled and changed according to the desired operating frequency requirement. Among the various resonator configurations, the split ring resonator (SRR) is one of the most commonly used designs in metamaterial absorbers. SRR-based structures are widely preferred because they support both magnetic and electric resonances which enables strong electromagnetic absorption characteristics.

The interaction between these absorber structures generate additional absorption resonances, while the arrangement of closely positioned concentric split-ring resonators (SRRs) generate broad absorption bandwidth characteristics.

1.4.2 Impedance Matching

Another important mechanism responsible for electromagnetic (EM) wave absorption is impedance matching. When electromagnetic waves propagate from one medium into another, causing a portion of the incident energy to be reflected while the remaining energy is transmitted through the material then this phenomenon occurs. The amount of reflection becomes minimum when the characteristic impedance of the absorbing structure closely matches the impedance of the incident medium, as shown in fig.7. Therefore, achieving proper impedance matching is considered one of the most critical and challenging point in the design of perfect absorbers.

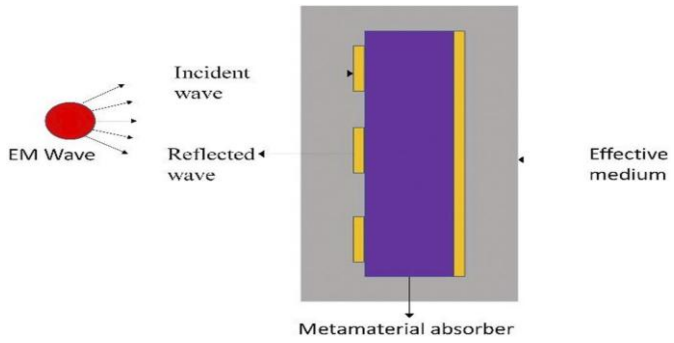


Fig.7 Showing mechanism of impedance matching in a metamaterial absorber

1.4.3 Reduction in Plasma Frequency

The plasma frequency of a material is the frequency at which the free electron cloud in the material naturally oscillates and it can be written as:

$$w_p = \sqrt{\frac{Ne^2}{m\varepsilon_o}}\, w_p \qquad (2)$$

where,

- w_p is plasma frequency
- N is density of the free electron gas
- m is effective mass
- e is charge of an electron

Equation 2 clearly indicates that the plasma frequency w_p is dependent on the concentration of free electron carriers present within the metal as the plasma frequency and carrier concentration are directly proportional. By increasing or decreasing the doping concentration, the electrical properties of the material can be modified accordingly. In metamaterial absorbers, negative permittivity can be achieved by lowering the plasma frequency in relation to the desired operating frequency range. The primary objective behind reducing the plasma frequency is to enable metamaterial absorbers to function effectively across different frequency regions. Hence, it becomes essential to carefully tune the plasma frequency so that it matches the intended operating frequency regime of the absorber [18-20].

1.5 Applications of Metamaterial

Metamaterials have a wide range of possible uses, such as optical filtering, biomedical sensing [21], aerospace systems, sensors, and structural monitoring.

They are also explored for telecommunications [22-24], optics [25-27], sensing and image processing [28-31] and energy harvesting [32, 33]. Research is further looking at improving ultrasonic sensing, earthquake-resistant structures, and even creating super-lenses or limited forms of invisibility using gradient-index designs. Acoustic and seismic metamaterials continue to be active research topics.

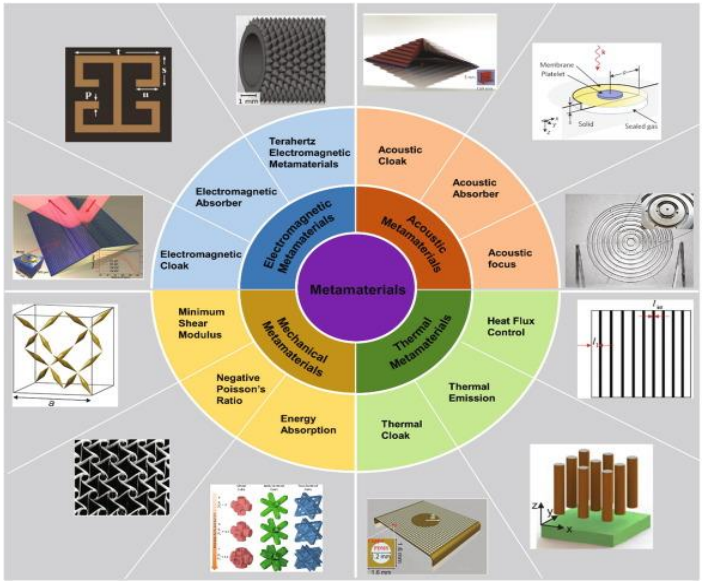


Fig. 8 Various applications of Metamaterial

Research on metamaterials spans many interconnected fields, including electrical engineering, electromagnetics, optics, solid-state physics, microwave and antenna design, optoelectronics, materials science, nanotechnology, and semiconductor engineering. New advances also indicate potential for metamaterials in optical computing, where certain operations might be carried out more efficiently than with traditional computing methods.

1.6 Identified Research Gaps and Challenges

Although metamaterials have demonstrated outstanding capabilities in controlling electromagnetic waves for applications such as sensing, imaging, communication, and absorption systems, several limitations and unresolved issues still exist. These challenges impact their practical implementation, large-scale manufacturing and long-term performance. Thus, researchers are still searching for new design approaches, materials, and optimization techniques to improve the efficiency and applicability of metamaterial-based devices. Below we discuss some of the major research gaps and challenges associated with metamaterials.

1.6.1 Research Gaps

• **Fabrication and Scalability**: The complex fabrication techniques makes the large-scale production of metamaterial sensors more difficult and expensive.

• **Broadband Operation:** Most metamaterial sensors operates efficiently only within a narrow frequency range and have limiting wideband applications.

• **Integration with Other Technologies:** Hybrid sensing systems which combines metamaterials with conventional sensor technologies are still limited.

• **Material Losses:** High metallic and dielectric losses occurs in plasmonic metamaterials which results in reducing sensing efficiency and resonance quality.

• **Flexibility and Miniaturization:** It is reducing sensor size while maintaining high performance and structural stability still a challenge.

• **Lack of Standardization:** The absence of common performance evaluation methods makes comparison between different sensor designs difficult.

• **Sensitivity in Complex Environments:** The sensor performance often degrades in heterogeneous environments such as biological samples etc.

• **Quantitative Sensing Limitations:** Achieving accurate quantitative measurements by including analyte concentration detection remains difficult.

1.6.2 Challenges

• **High Fabrication Cost:** By using advanced microfabrication and nanofabrication methods results in increase of the overall production cost of sensors.

• **Limited Material Availability:** Using suitable low-loss materials for high-performance metamaterial sensor design are still limited.

• **Complex Electromagnetic Simulations:** For accurate modelling in electromagnetic interactions occurs in metamaterial structures requires high computational resources.

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• **Environmental Sensitivity:** Various external factors such as humidity, temperature, and electromagnetic interference can affect sensor performance thus become a challenge.

• **Integration with Electronics:** If combining metamaterial sensors with existing electronic and signal-processing systems then this become very difficult.

• **Low Stability under Practical Conditions:** Long-term operational stability and reliability under real-world conditions are still insufficiently explored.

• **Trade-Off between sensitivity and quality Factor:** Improving sensitivity often negatively affects bandwidth or resonance quality.

• **Commercialization Difficulties:** Large-scale industrial implementation of metamaterial sensors remains limited due to manufacturing and cost-related challenges.

CHAPTER -2

RESEARCH OBJECTIVE

I. The current work aims to design a highly sensitive Terahertz (THz) metamaterial based biosensor for the detection of Mycobacterium Tuberculosis (TB). The work focuses on shift in resonance due to even small changes in refractive index when TB analytes interact with the metamaterial.

II. To optimize all structural parameters of the metamaterial unit cell to achieve maximum absorption and minimum Reflection Coefficient.

III. To achieve high sensitivity by providing strong electromagnetic field confinement and measurable resonance shifts for different TB analyte refractive indices.

IV. To evaluate key performance metrics such as:
- FWHM
- Q-Factor
- FOM

V. To compare the sensor's performance with previously reported data.

CHAPTER-3

LITERATURE REVIEW

Over the few years metamaterial based absorbers and THz biosensors have become really promising for a lot of different uses like sensing, medical diagnosis, imaging technologies and advanced communication systems. Metamaterial-based absorbers and THz biosensors are getting better and better. To make these devices work better researchers have tried out different shapes for the resonators different materials for the substrates and different structural designs to improve things like how well they absorb how sensitive they are, how wide a range of frequencies they can handle and other important factors.

They have also tried to make sure the impedance matches well and that the electromagnetic field is strong and focused and that the device can work at frequencies. This helps the device sense things better. Absorb more effectively. The next part will talk about some studies that have been done on metamaterial absorbers and THz biosensing applications. It will focus on how these devices were designed what the researchers found out and what they contributed to the field.

In the area of TB diagnosis, Ragavan and their team proposed a model for identifying *Mycobacterium tuberculosis*. This developed system results in excellent classification capability which achieves an accuracy of 99.12 %, along with a sensitivity of 98.74 % and a specificity of 98 % [34]. These results show that this new approach is very promising, for detecting tuberculosis reliably.

In another study, Singh et al. designed a biosensor for the detection of TB cells. The proposed sensor applied a split-square resonator structure with a gap at the end. This was constructed using a dielectric substrate layer made up of polyimide and placed between an aluminium ground layer and a metallic resonator at the top. The designed structure demonstrated notable sensing performance, providing sensitivities of 666 GHz/RIU, 500 GHz/RIU, 333 GHz/RIU, and 250 GHz/RIU for TB1, TB2, TB3, and TB4 samples, respectively [35]. These results show that metamaterial biosensors are really good at finding tuberculosis using terahertz waves.

Recently people have been very interested in metamaterials because they are great at sensing things. This makes them useful for detecting cancer and for biomedical sensing. Saadeldin and his team made a sensitive biosensor in 2019. They used a structure and added a Teflon layer between two gold layers to make it work better. This sensor achieved an absorptivity of 0.99 at a resonance frequency of 2.24 THz. Metamaterial biosensors like this one are very effective for detecting tuberculosis and other diseases. Metamaterials are being used more and more for these kinds of applications because they are so good, at sensing things. Also, the device shows a maximum sensitivity of 300 GHz/RIU, a figure of merit (FOM) of 2.94 RIU^{-1}, and a quality factor (Q-factor) of 22.05 which indicate the strong sensing performance [36].

Later, Patel and his team (2022) introduced a graphene-based metamaterial biosensor which was designed to detect various cancerous cells. The structure consisted of a split-ring resonator on a glass substrate, where graphene was incorporated to improve the sensing response. The sensor achieves a sensitivity of 207.14 GHz/RIU along with a Q-factor and FOM of 13.11 and 3.86 RIU^{-1} respectively which highlights its potential for various sensing applications [37].

Guo and his team proposed a kind of biosensor in 2023. This biosensor uses a geometry called an open square ring resonator and it is made with copper. They used lead glass as the dielectric spacer layer.. The proposed structure promising sensing characteristics

which achieves a Q-factor of 79.26, a sensitivity of 91.50 GHz/RIU, and figure of merit (FOM) of 11.97 RIU^{-1} [38].

Qu and his team made a kind of sensor in 2023. This sensor is made with a material and has four identical square rings on a lead base. The sensor works well with a high Q-factor of 55.3. It is also very sensitive with 78.6 GHz/RIU. Has a good figure of merit of 9.81 RIU^{-1} [39].

In 2023 Zhang and his team made another kind of sensor. This sensor can detect two frequencies and works with any kind of light polarization. It has a ring shape, with two openings and is made of gold. The ring is placed on a spacer made of Polytetrafluoroethylene, which is a kind of plastic. The proposed sensor achieves a average refractive index (RI) sensitivities of 163 and 488 GHz/RIU for the two resonance bands. figure of merit (FOM) values were reported as 5.09 and 9.04 RIU^{-1}, while the obtained Q-factors were reported as 22.8 and 40.7, respectively [40].

Later, Aliouar et al. [2025] developed a terahertz metamaterial biosensor employing gold as the metallic layer and polyimide as the substrate material. The proposed structure consisted of a rectangular resonating element placed at the center and surrounded by a ring-shaped geometry. The sensor exhibited excellent absorption performance of 99.97 % at a resonance frequency of 2.96 THz. Furthermore, the device achieved a maximum average sensitivity of 600 GHz/RIU, along with a FOM of 60 RIU^{-1} and a high Q-factor of 296.90 [41].

In another investigation, Tammam et al. [2025] developed a flexible THz metamaterial sensor aimed at hemoglobin (Hb) monitoring and the early identification of cancer. The proposed sensor achieved a high absorptivity of 98 % at a resonance frequency of 1.1 THz, along with an average sensitivity of 556.3 GHz/RIU and a quality factor of 13.2 for cancer detection applications [42].

Zhang et al. [43] introduced an terahertz (THz) metamaterial biosensor which was used to coupled resonator structures for the classification of glioma cell. The proposed sensor report a theoretical sensitivity of 496.0 GHz/RIU and was experimentally capable of differentiating between mutant and wild-type glioma cells.

Further improvements in sensing accuracy, stability, and reliability are still needed before terahertz biosensors can be widely used in real biomedical diagnostic applications.

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CHAPTER-4

SIMULATION SOFTWARE

In our work we analyzed the proposed structure using a special software called CST Studio Suite. This software uses a method called finite element method (FEM) to solve problems in the frequency domain. This method is good for studying how electromagnetic waves interact with materials in the THz region. The Frequency-Domain Solver in the software helped us study how the designed structure behaves at frequencies absorbs energy and distributes electric fields. This approach helps us examine and optimize performance parameters.

This numerical approach gives information of key performance parameters like resonance frequency, sensitivity, quality factor, and detection accuracy. Therefore, the simulation setup helps improve the performance and stability of the THz metamaterial biosensor for biomedical sensing applications.

4.1 CST STUDIO SUITE

CST Studio Suite is a widely used software for the design and analysis of high frequency and microwave devices. It helps researchers understand the behavior of electromagnetic waves and simulate structures working in the microwave, millimeter wave, and terahertz (THz) regions. The software applies numerical techniques to obtain accurate results for complex electromagnetic studies.

The software provides a 3D simulation platform where different structures such as antennas, resonators, waveguides, metamaterials, and biosensors can be designed and analyzed. It allows the study of several electromagnetic properties, including resonance frequency, absorption, transmission and reflection coefficients, and electric field distribution. In this work, the simulated S parameters were used to determine absorptivity. The shift in resonance frequency at different refractive index values was further used to evaluate the sensitivity of the proposed biosensor.

For metamaterial biosensor applications, CST Microwave Studio is useful for studying the interaction between electromagnetic waves and different material structures. It also supports material models like the Drude model, which is commonly used for tunable materials such as Vanadium dioxide. Due to its accuracy, flexibility, and visualization capability, CST Microwave Studio is widely applied in terahertz and electromagnetic research.



Fig. 9 Computer Simulation Technology Logo

4.2 Numerical Approach used in CST Studio Suite

The simulation software used advanced algorithms for the numerical analysis of the proposed biosensor designs and to check their overall performance. These tools use mathematical techniques to perform a detailed evaluation of the their characteristics and behavior. The main method used for this analysis is explained in the section.

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Finite Element Method (FEM)

The Full Vector Finite Element Method (FEM) is a numerical technique which is used in CST Studio Suite for designing and analysing the metamaterial biosensors. In this method, the whole simulation area is divided into many small parts therefore are known as finite elements or meshes. Maxwell's electromagnetic equations are solved in these small sections to study structures with complex geometry and different material properties accurately. The method calculates all components of the electric and magnetic fields, including Ex, Ey, Ez, Hx, Hy, and Hz. After solving each element, the complete electromagnetic response of the sensor is obtained by combining all the results.

For THz metamaterial biosensors, FEM is useful for studying how electromagnetic waves interact with the resonator structure. It helps in analyzing important parameters such as resonance frequency, electric and magnetic field distribution, absorption, transmission, reflection, and sensing performance.

Also they uses adaptive meshing to improve the accuracy. The mesh becomes finer in regions only where strong field variation occurs. This improves the precision of the simulation while reducing unnecessary computational effort. The thing about FEM is that it really works well for making biosensor designs better. FEM is great for getting sensitivity from biosensors. It also helps to improve the quality of biosensors.. It makes the sensing characteristics of biosensors better. So FEM is very useful for optimizing biosensor designs to get the results, from biosensors. FEM helps to make biosensors more effective.

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CHAPTER-5

NUMERICAL ANALYSIS

5.1 Introduction

This chapter presents the numerical and computational analysis of the proposed THz metamaterial biosensor which is designed for the detection of tuberculosis using CST Studio Suite. The performance of the sensor and its electromagnetic behavior are studied using the finite element method (FEM). This method helps in accurately examining the resonance response, field distribution, and interaction between the sensor structure and the target sample. During the simulation study to observe the sensing response of the biosensor different refractive index values are used. The proposed design is further judged through important performance parameters such as absorption, sensitivity, Q factor, and figure of merit (FOM). These parameters help in understanding the sensing accuracy, selectivity, and also the overall efficiency of the biosensor for future THz biomedical sensing applications.

5.2 Mathematical modelling

1. Absorption capability:

The absorption performance is a factor in how well it absorbs electromagnetic radiation at a specific frequency. This connection helps improve sensing efficiency. The absorption performance directly impacts its ability to efficiently absorb radiation. When absorption is high the interaction between the waves and the material is stronger leading to sensing results. The materials design plays a role in achieving high absorption performance. It helps in absorbing electromagnetic radiation at the resonant frequency. The absorptivity of the structure is determined from the transmission and reflection coefficients, where near-perfect absorption is achieved when both transmission and reflection are minimized at the resonance frequency.

The absorption capability (A) of the proposed metamaterial structure was determined using the following expression:

$$A(\omega) = 1 - R(\omega) - T(\omega) \qquad (3)$$

In this equation, R(ω) and T(ω) represent the reflection and transmission coefficients, respectively. By analyzing these coefficients, the absorption behaviour of the designed metamaterial biosensor can be effectively examined. The reflection coefficient is calculated as $R(\omega)=|S_{11}|^2$ whereas the transmission coefficient is given by $T(\omega)=|S_{21}|^2$

Here, S_{11} corresponds to the reflection amplitude coefficient, while S_{21} denotes the transmission amplitude coefficient of the proposed structure.

As the ground plane of the proposed unit cell is composed of gold, a highly conductive material, the transmission of EM waves through the metamaterial (MM) structure becomes nearly negligible, while the reflected waves are also considerably minimized. Consequently, the majority of the incident THz radiation is effectively absorbed by the structure, preventing the THz waves from propagating through the absorber. Therefore, the transmission coefficient can be approximated as $S_{21}=0$. Under this condition, the absorption capability (A) of the proposed structure can be expressed as:

$$A = 1 - |S_{11}|^2 \qquad (4)$$

2. Drude Model for VO_2:

The electromagnetic response of VO_2 is modeled using the Drude model, which describes the interaction of free charge carriers with incident THz waves. This model helps in studying how the dielectric properties and conductivity of the material change with frequency under different conditions. The numerical results give a clear understanding of the sensor behavior. They also show that the proposed THz metamaterial biosensor can be effectively used for sensitive tuberculosis detection.

The complex permittivity of VO_2 can be expressed as:

$$\varepsilon(\omega) = \epsilon_\infty - \frac{\omega_P^2}{(\omega^2 + i\gamma\omega)} \quad (5)$$

In this expression, ϵ_∞ denotes the dielectric constant at high frequency and is set to 12, ω_p corresponds to the plasma frequency, γ represents the collision frequency assumed to be 5.75×10^{13} rad/s, and ω *is* the angular frequency of the incoming THz radiation [44].

The plasma frequency (ω_p) is directly influenced by the electrical conductivity (σ) of the material. As the conductivity changes, the plasma frequency also varies accordingly. Their relationship can be expressed as:

$$\omega_p^2(\sigma) = \frac{\sigma}{\sigma_o}\,\omega_p^2(\sigma_o) \quad (6)$$

where σ_o represents the reference conductivity, while $\omega_p(\sigma_o)$ denotes the plasma frequency corresponding to that reference conductivity. This equation indicates that the square of the plasma frequency is proportional to the conductivity of the material.

3. Sensitivity:

21 Sensitivity describes the capability of the sensor to detect the minor changes in the refractive index of the analyte. In our study, sensitivity is analyzed by checking the variation in resonance frequency when the refractive index of the sensing medium changes. A larger shift in the resonance frequency results into enhanced sensing efficiency and improved detection accuracy.

12 The sensitivity is determined as the ratio of change in the resonance frequency shift and the corresponding change in refractive index, which is commonly measured in unit GHz/RIU.

$$S = \frac{\Delta f}{\Delta n} \quad (7)$$

where S represents the sensitivity, Δf denotes the shift in the resonance frequency, and Δn denotes the variation in the refractive index.

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4. Quality-factor:

The quality factor (Q-factor) parameter describes the sharpness and strength of the resonance response. A larger Q-factor means it corresponds to a narrow resonance bandwidth and it improved the confinement of electromagnetic energy within the resonator. This results in higher sensing precision and better capability to detect the small variations.

4

The Q-factor is determined as the ratio of the resonance frequency to the full width at half maximum (FWHM) of the resonance peak.

$$Q - factor = \frac{f_o}{FWHM} \quad (8)$$

where fo represents the resonance frequency corresponding to a particular value of the refractive index.

5. Figure of Merit (FOM):

Figure of Merit (FOM) is used to measure the sensing performance and detection capability. A larger FOM value signifies that the sensor can identify very small changes in refractive index which then improved the accuracy and stability of the biosensor.

FOM is also defined as the ratio of sensitivity and the value of FWHM.

$$FOM = \frac{S}{FWHM} \quad (9)$$

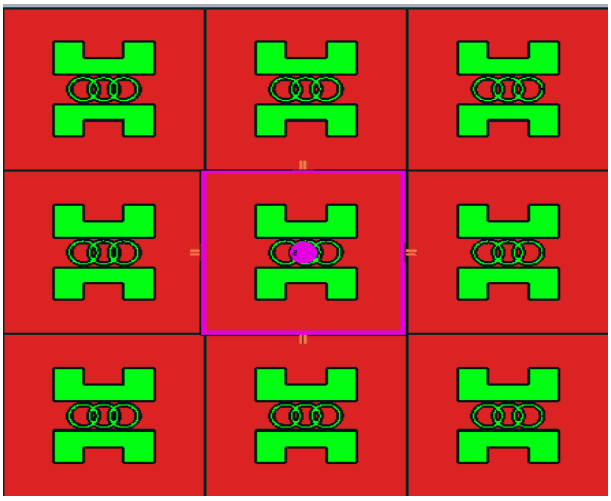
CHAPTER-6

DESIGN AND METHODOLOGY

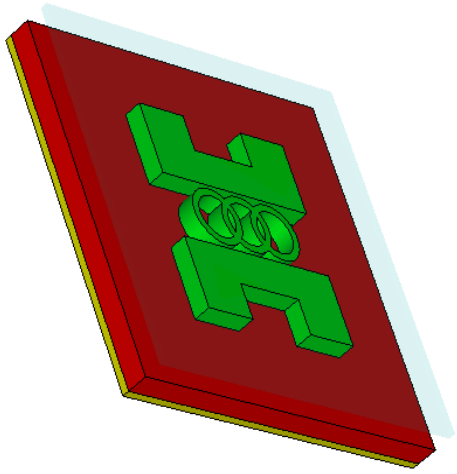
The conventional metamaterial (MM) absorbers generally consist of three different layers: a metallic ground layer at the bottom, a dielectric substrate layer placed in the middle, and a patterned resonator layer on the top. Different resonator structures are added to the top layer to improve impedance matching with free space. This greatly reduces reflection loss [45]. Numerical simulations were performed using CST Simulation Studio to optimize the proposed structure and investigate its optical characteristics. The adopted approach making it a good absorber and a biosensor by maintaining high sensitivity toward variations in the refractive index through detailed parametric analysis.

6.1 Description of unit cell and Periodic boundary conditions

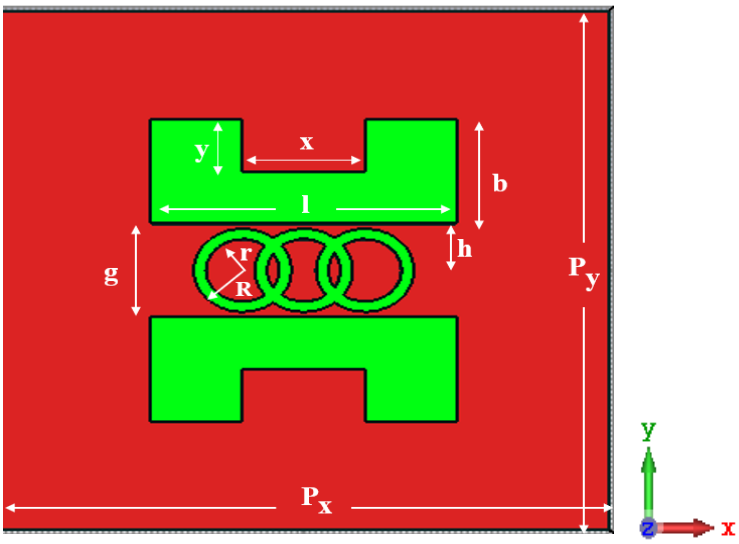
The proposed THz absorber is designed in the form of a 3 × 3 unit-cell array, as illustrated in the figure 10 (a). Each unit cell possesses a periodicity of 100 μm along both the x- and y-directions (Px = Py) and consists of a tri-layer metal-insulator-metal (MIM) structure with a bottom gold reflector, a middle paper dielectric spacer, and a top VO_2 resonator consists of three closed circular ring resonators placed between two rectangular bricks. Figure 10 (b), and (c) present the three-dimensional schematic diagram, front view of the proposed metamaterial unit cell respectively.



(a)



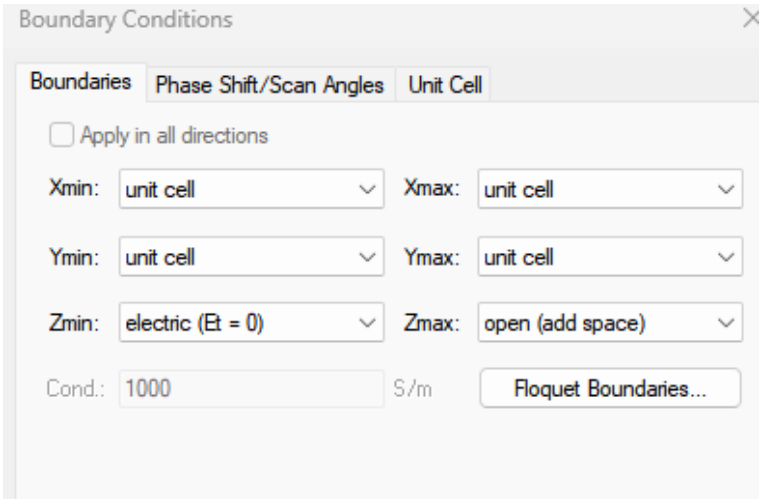
(b)



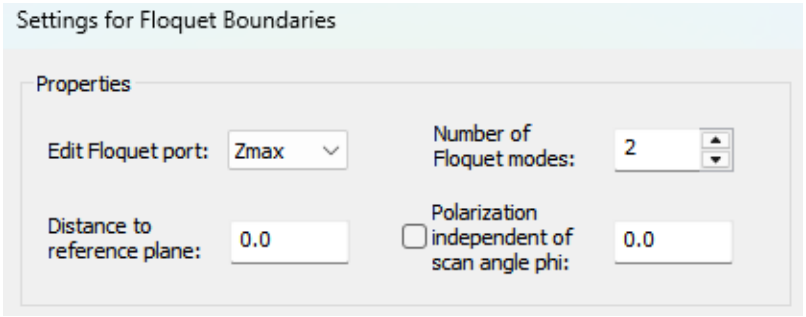
(c)

Fig.10 (a) Layout of 3×3 unit cell array of the proposed THz biosensor **(b)** Three-dimension schematic diagrams of the unit cell **(c)** The structural configuration and the front view of unit cell

The structural design and numerical simulations were performed using CST Microwave Studio. In the simulation setup, unit cell boundary conditions were applied along the x- and y-directions, while open boundary conditions with additional space, equivalent to a perfectly matched layer (PML), were assigned along the z-direction to minimize unwanted reflections. A planar electromagnetic (EM) wave was normally incident from the top surface along the z-axis, ensuring that the electric and magnetic field components remained mutually perpendicular [46]. Furthermore, tetrahedral meshing was employed to improve the accuracy of the simulation, and the frequency-domain solver was utilized to investigate the electromagnetic response of the proposed structure. During the analysis, the magnetic field and electric field polarizations were maintained along the x-axis and y-axis, respectively.



(a)



(b)

Fig.11 Simulation model demonstrating the use of **(a)** periodic boundaries and **(b)** Floquet port settings applied in proposed unit cell

6.2 Choice of materials

In the development of a metamaterial biosensor, the choice of materials for different layers plays a crucial role, as the overall sensing performance strongly depends on the electromagnetic characteristics, absorption efficiency, and tunable behavior of the structure. In the proposed design, gold is used in the bottom metallic layer, paper material is used as the dielectric substrate layer in the middle, and vanadium dioxide (VO_2) used in the top resonator layer.

- Gold is selected for the bottom layer due to its high electrical conductivity of 4.56 x 10^7 S/m and also due to its excellent chemical stability [45]. Gold works well in the THz frequency range as it helps to reflect waves so they do not go through the structure and that makes the absorption performance better. It is also good because it has ohmic losses and it supports strong plasmonic effects, which means the sensor can detect things more clearly and it has better sensing characteristics. Also one more fact that make gold a suitable option is that it does not oxidize or corrode easily which makes the biosensor more stable and reliable over time. That is very important, for the gold biosensor.

- Paper is used as the dielectric substrate because it offers several properties like low dielectric loss, flexibility, lightweight structure, and low fabrication cost etc. It has a dielectric constant of 2.31, loss tangent of 0.003, density (ρ) of 800 kg/m³, thermal conductivity of 0.05 W/K/m, and thermal diffusivity of 4.46 × 10^{-8} m²/s [45]. Also paper material is safe for the environment. It is also biocompatible. This makes paper a good choice, for sensing applications.

- Vanadium dioxide is selected for the top layer because it has good electromagnetic properties and it is good at dealing with THz radiation. It also has high electrical conductivity. This means it can make resonance and keep the electromagnetic fields inside the metamaterial structure really well. So the biosensor we are proposing can absorb things better. Sense things more efficiently. Vanadium dioxide also has the advantage of low optical losses. This makes it a good material for making powerful THz devices. The material helps make resonance responses that're sharp and stable. This is helpful because it means we can get a quality factor be more sensitive and detect things more precisely. Because of all these things Vanadium dioxide is a great material to use for making advanced biosensors that are used to sense things in the body.

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6.3 Methodology of Design

The proposed unit cell was designed using various optimized geometric shapes to enhance the interaction with electromagnetic waves and to improve the absorption performance. To study how the resonator arrangement affects the absorber characteristics, we examined four different structures by changing the number of circular closed ring resonators placed between the rectangular brick shaped elements, as illustrated in Fig. 12. Each structure was analyzed in detail in this section.

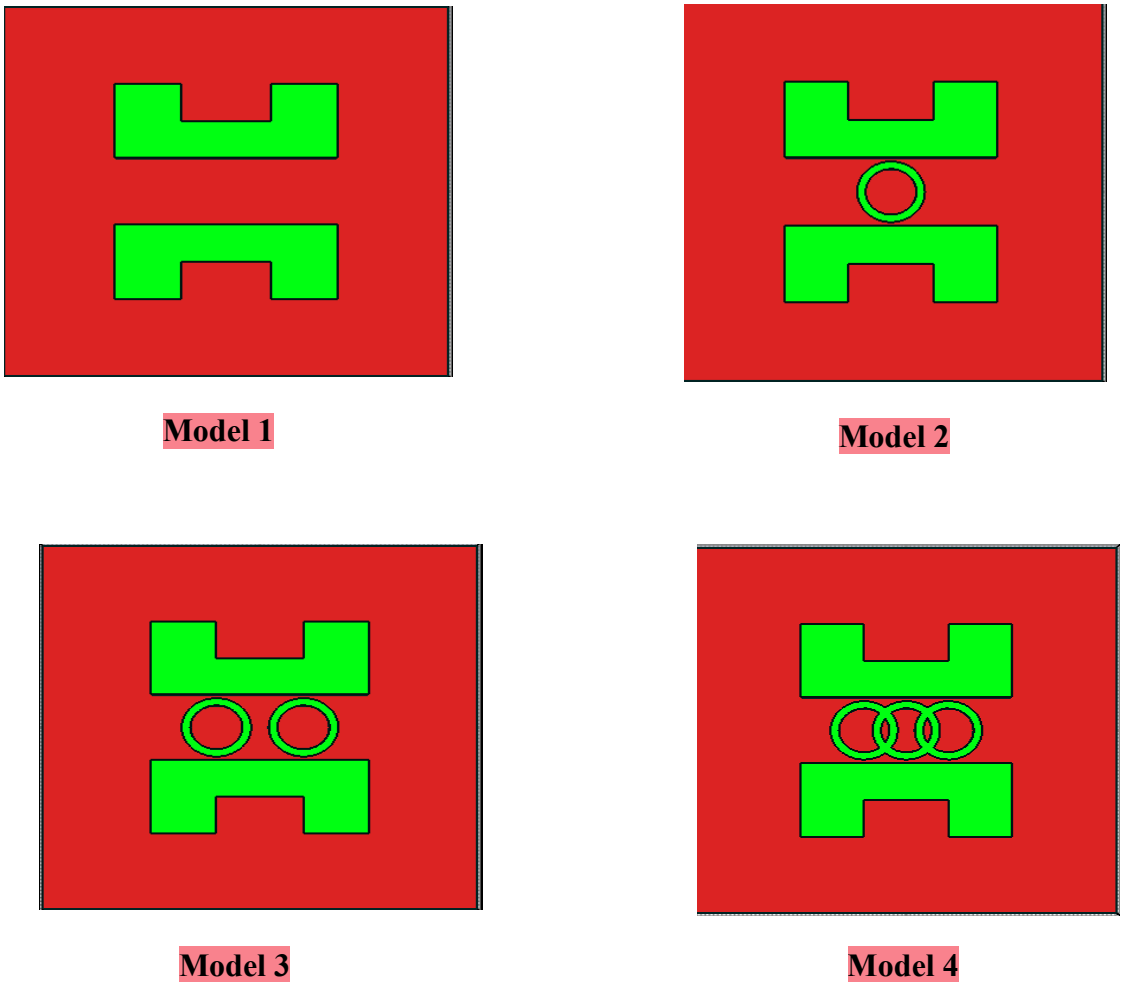


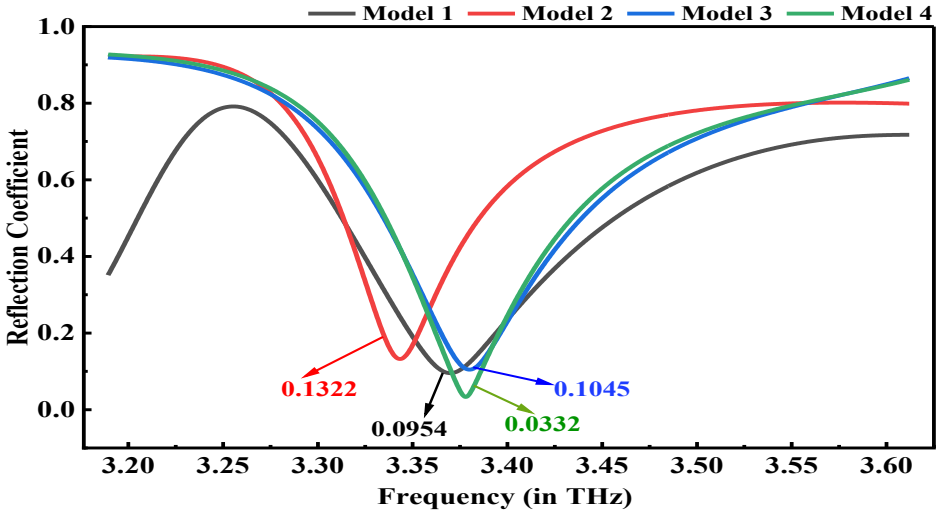
Fig.12 Design generation of proposed unit cell

In Model 1, we used only rectangular bricks without any circular ring resonators. This structure results into low reflection coefficient of 0.0954 and a high absorptivity of 99.08 %. Even though the absorptivity value is high but the absence of ring resonators limited the overall electromagnetic field confinement and resonance enhancement occurs within the structure.

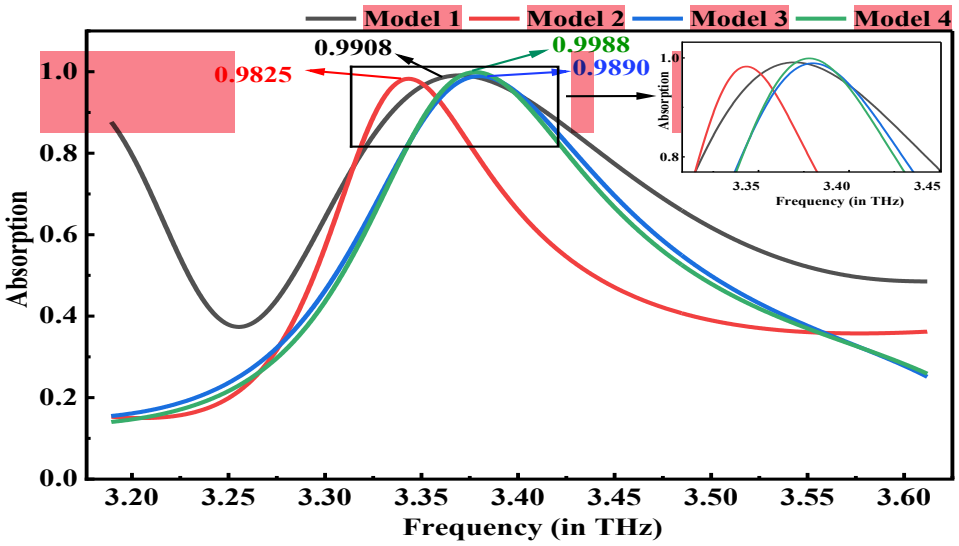
In Model 2, we introduced a single circular ring resonator between the rectangular bricks to improve the interaction. However, the use of only one ring increased the reflection coefficient to 0.1322 but slightly decreasing the absorptivity to 98.25 % as compared to Model 1. This results shows that a single resonating element was not sufficient in order to provide effective impedance matching or strong resonance coupling.

To enhance the performance further, we used two circular ring resonators in between the rectangular bricks as shown in Model 3. Here, the reflection coefficient reduced to 0.1045 and the absorptivity improved to 98.9 %. Although the extra ring improved the confinement of field and also enhanced the electromagnetic interaction but the increase in absorption was still limited. This shows that the resonance characteristics and surface current distribution were not yet completely optimized.

Finally, a significant improvement in absorber performance was achieved in the proposed Model 4, where three intersecting circular ring resonators were incorporated between the rectangular bricks. The presence of multiple intersecting rings greatly enhanced the resonance effect and improved the impedance matching characteristics of the structure. Consequently, the absorptivity increased sharply to 99.88 %, while the reflection coefficient dropped to 0.0332. The enhanced performance can mainly be attributed to stronger localization of electromagnetic fields, improved surface current distribution, and the generation of multiple resonance modes due to the intersecting ring arrangement. In Fig.13 the simulated results for reflection coefficient and absorptivity for all the models are shown.



(a)



(b)

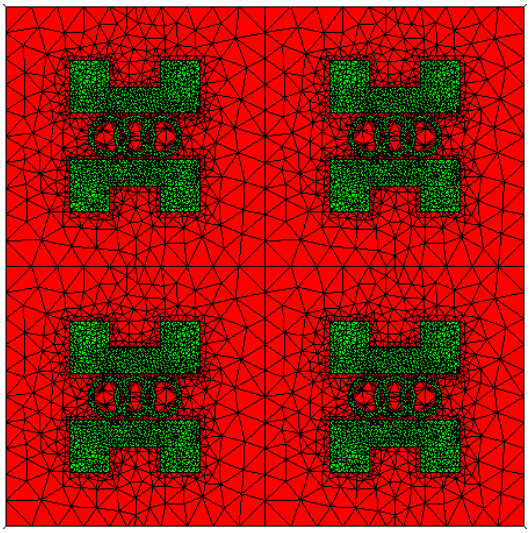
Fig.13 Enhancement of the proposed absorber and response characteristics at various stages of absorber development **(a)** Reflection response and **(b)** Absorption characteristics.

6.4 CST simulation setup parameters (mesh type, ports, monitors)

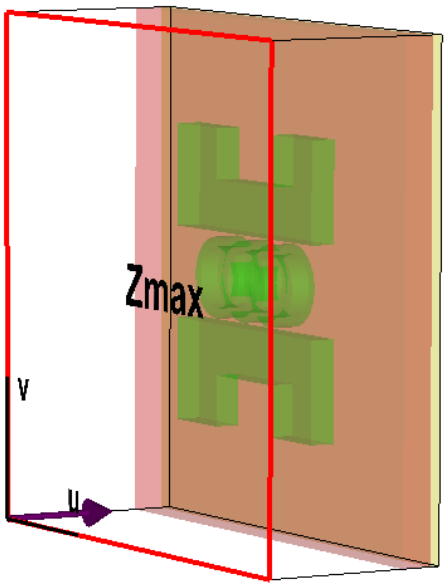
- **Mesh Type:** A tetrahedral mesh with adaptive refinement was employed to accurately capture the intricate geometrical details and variations in the electromagnetic field distribution.

- **Ports:** To excite the metasurface, two Floquet port were applied, allowing plane-wave illumination during the simulation process.

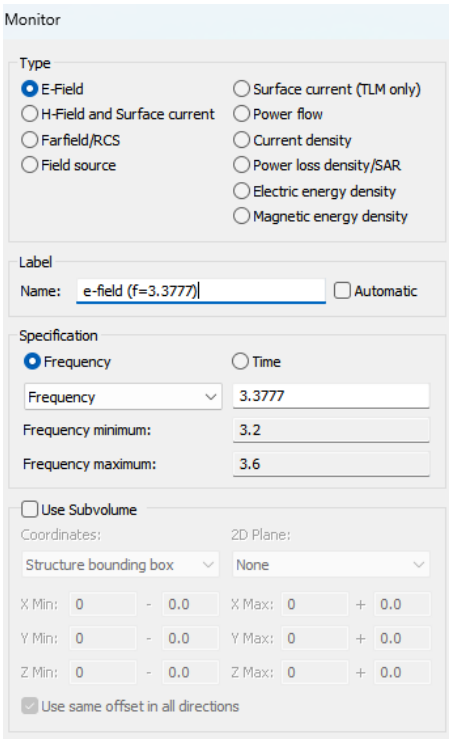
- **Monitors:** Frequency-domain monitors were utilized to observe and analyze important parameters such as absorption characteristics, reflection response, and near-field distributions at selected operating frequencies (3.2 -3.6 THz).



(a)



(b)



(c)

Fig.14 (a) Showing mesh view of the proposed metamaterial biosensor **(b)** Port setup used for electromagnetic wave excitation **(c)** Frequency monitor setup for various analysis

The proposed structure was analyzed using the Finite Element Method (FEM) solver. Periodic boundary conditions were applied along both the x- and y-directions to represent the repeating nature of the design. Along the propagation direction (z-axis), a perfect electric conductor boundary condition (Et=0) was assigned at the Zmin plane for the normally incident plane wave. In contrast, the Zmax plane was treated as an open boundary with extra space provided to ensure accurate wave propagation and proper electromagnetic interaction within the structure.

CHAPTER-7

PARAMETRIC OPTIMIZATION AND ANALYSIS

This section explains the parametric study of the proposed structure (Model 4) to find the optimum design parameters. Optimization was done by varying the different parameters given in Table 1, such as substrate thickness, resonator thickness, and circle radius, individually while the other parameters were kept unchanged. Our aim was to achieve near-perfect absorption . The effect of these parameter changes can be seen in Figures 15–18.

Figure 15 shows how the substrate thickness ($t_{substrate}$) affects the performance of the proposed structure. The thickness was changed from 4 μm to 8 μm with a step of 2 μm. The results show that increasing the substrate thickness causes a red shift in the resonance frequency. This indicates that the interaction between the electromagnetic waves and the structure strongly depends on the dielectric layer thickness. Changes in absorption are also observed. The absorption values are 69.79%, 99.14%, and 94.64%, respectively. The maximum absorption is obtained at 6 μm. This happens because the impedance matching between the absorber and free space becomes better. As a result, reflection loss decreases and the electromagnetic field remains more confined inside the structure. When the substrate thickness is increased further, the absorption starts to decrease due to weaker field confinement.Therefore, the substrate thickness of 6 μm was selected as the optimized value since it provides the maximum absorptivity of 99.14 %.

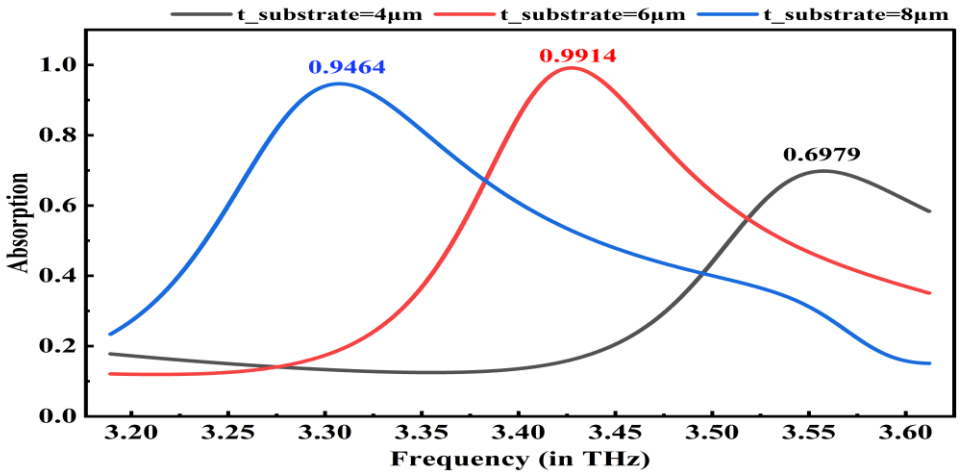


Fig.15. Geometric parameter: Variation in substrate thickness

Figure 16 shows the effect of changing the resonator thickness ($t_{resonator}$) from 2 µm to 6 µm with an interval of 1 µm. The obtained absorption values are 80.83 %, 93.26 %, 99.14 %, 99.81 %, and 97.72 %, respectively. The results indicate that the absorption increases noticeably as the resonator thickness rises up to 5 µm. But when the thickness exceeds 5 µm, the absorption starts decreases. From these results we conclude that among all the tested values, the maximum absorption of 99.81 % is obtained at 5 µm. Therefore, 5 µm was selected as the optimized resonator thickness for the proposed biosensor.

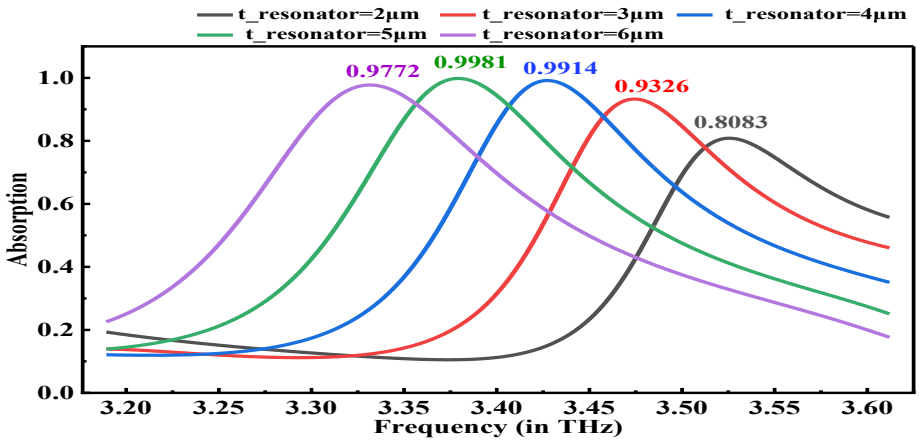


Fig.16. Geometric parameter: Variation in resonator thickness

Similarly, the value of the inner radius of the circular resonator (r) was judged by changing its value from 4 µm to 10 µm in steps of 2 µm, as shown in Figure 17. The obtained absorption values are 99.38 %, 99.81 %, 97.79 %, and 92.26 %, respectively. These results demonstrate that the geometrical dimensions of the circular resonator strongly affect the resonance intensity and electromagnetic field localization. Initially, increasing the radius improves resonance coupling, leading to enhanced absorption performance. However, further enlargement of the radius weakens the interaction between incident wave and the structure and reduces the absorption efficiency. Therefore, the optimum inner radius was determined to be 6 µm, where the maximum absorption of 99.81 % was achieved.

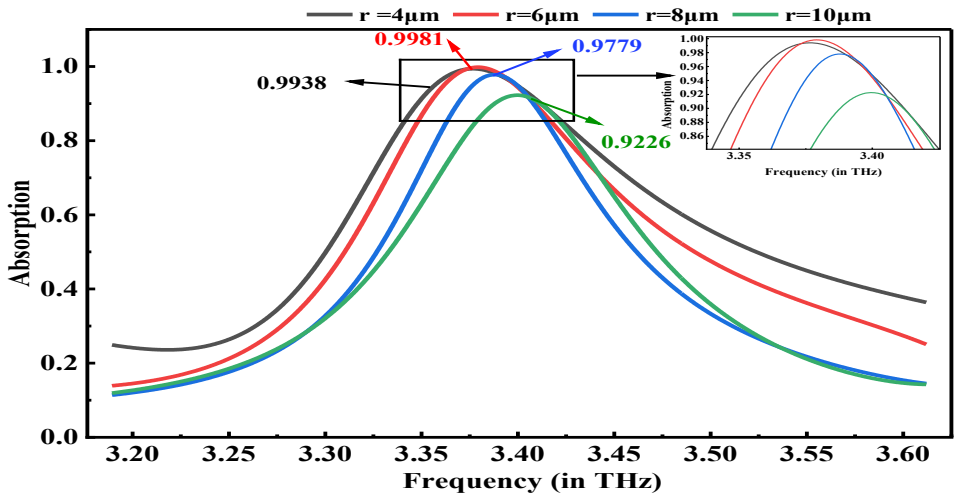


Fig.17. Geometric parameter: Variation in inner radius of circular

In addition, figure 18 illustrates the influence of the half distance between the two brick-shaped resonating structures (h), which was varied from 8 μm to 12 μm with a step size of 1 μm. The results show that the spacing between the resonating elements directly affects the electromagnetic coupling and near-field interactions within the structure. Among all the tested configurations, the highest absorption peak of 99.81 % is obtained at 9 μm, indicating the strongest resonance coupling at this separation distance. When the spacing is increased further, the interaction between the resonating elements becomes weaker, slightly reducing the absorption efficiency. Hence, the optimized half-gap distance was selected as 9 μm, corresponding to a total separation of 18 μm between the two rectangular brick-like structures.

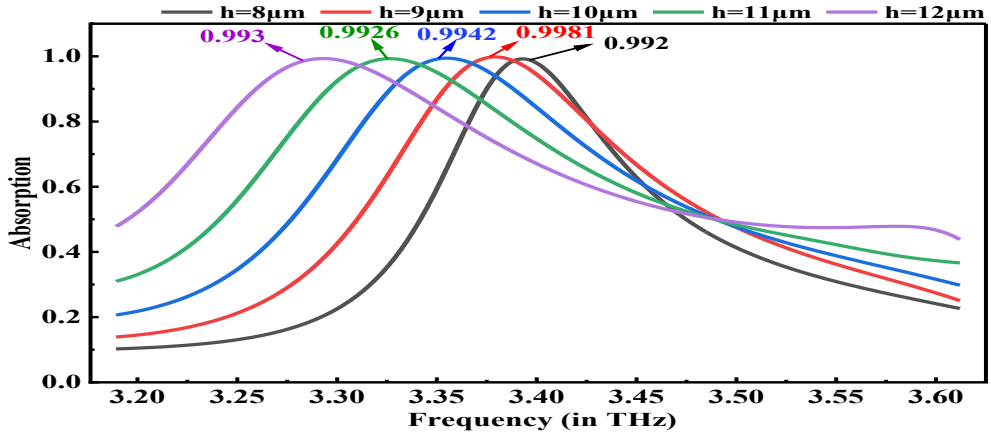


Fig.18. Geometric parameter: Variation in half gap between bricks

Finally, Table1 summarizes the optimized geometrical parameters of the proposed absorber design. These optimized dimensions were subsequently utilized for further simulation studies and performance evaluation of the THz metamaterial biosensor.

Table1. Optimized parameter for the proposed Design

Name	Value(µm)	Description
t_ground	2	Height of ground
t_substrate	6	Height of substrate
l	50	Length of brick
b	20	Breadth of brick
g	18	Distance between bricks
h	9	Half distance between bricks
t_resonator	5	Height of resonator
$P_x = P_y$	100	Length and breadth of unit cell
r	6	Inner radius of circular rings
R	8	Outer radius of circular rings
t_analyte	2	Thickness of analyte
x	20	Length of rectangular brick
y	10	Breadth of rectangular brick

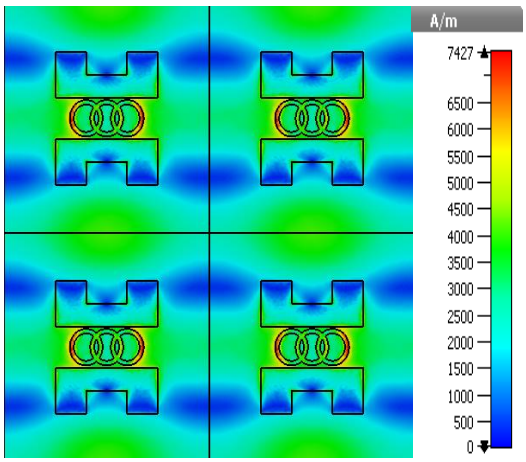
CHAPTER-8

ELECTROMAGNETIC FIELD DISTRIBUTION

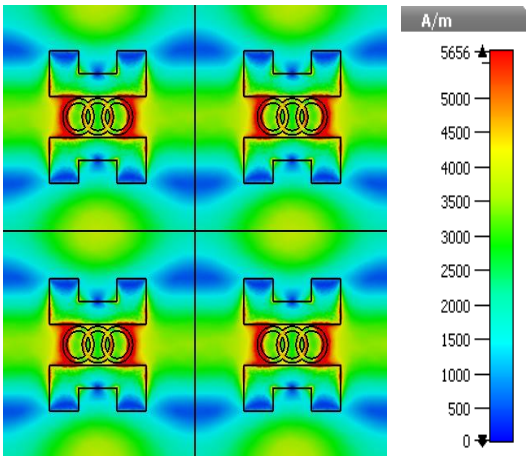
To gain a deeper understanding of the absorption behaviour of the proposed metamaterial structure, the distributions of both electric and magnetic fields were examined at three different frequency conditions, namely below resonance, at resonance, and above resonance frequencies. The simulation results are shown in figures 19 and 20, which shows how the incident electromagnetic waves interact with the resonator geometry at different operating frequencies.

The figures 19(a), 19(b) and 19(c) show us the field distributions of magnetic field at different frequencies. We see the field distributions at 3.3414 THz, then at 3.3777 THz which is the resonance frequency and finally at 3.4658 THz. At the resonance frequency the magnetic field is very strong around the edges of the ring resonators. It is also strong near the sections of the brick-shaped elements. This happens because the metallic layer and the ground plane are connected in a way that they make parallel surface currents between the two metallic layers. This results in a strong magnetic field inside the dielectric region. The magnetic field is trapped inside the structure. This is important for the structure to absorb energy effectively. The magnetic field distributions at the resonance frequency are very important for the structure to work properly. The figures 19(a), 19(b) and 19(c) help us understand the field distributions, at different frequencies especially at the resonance frequency of 3.3777 THz.

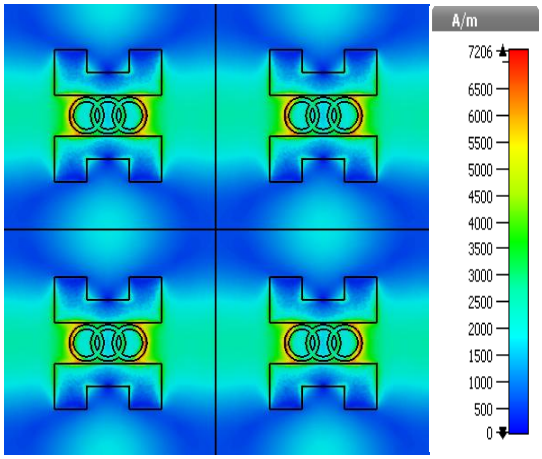
But on the other hand, we observed the magnetic field intensity becomes much weaker at frequencies below and above resonance, as shown in figures 19(a) and 19(c). At these frequencies, the electric field becomes weaker because the surface current excitation is low. This reduces the interaction between the incoming wave and the resonator. As a result, a smaller amount of electromagnetic energy remains trapped inside the structure. Thus, we noticed the decrease in absorption performance when the system moves away from the resonance frequency.



(a)



(b)



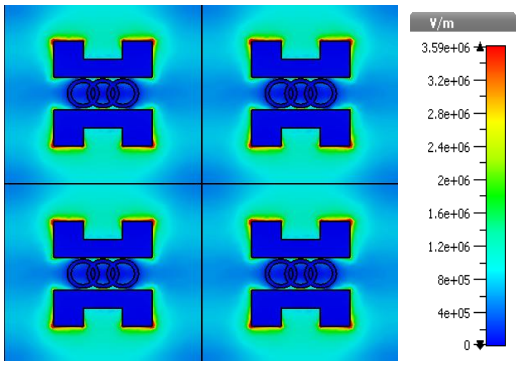
(c)

Fig.19 Real |H| -field distribution at: **(a)** 3.3414 THz **(b)** 3.3777 THz (Resonance Frequency) **(c)** 3.4658 THz

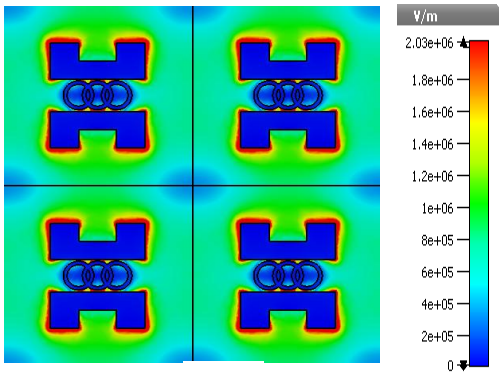
Similarly, Figures 20(a), 20(b), and 20(c) show the electric field distributions corresponding to the same frequencies we talked earlier. At 3.3414 THz (below resonance frequency), only a small amount of electric field concentration is observed which is along the outer boundaries of the brick structures. This is clearly shown in Figure 20(a). At the resonance frequency of 3.3777 THz, a very strong electric field is observed near the edges

of the brick structures and inside the gap between the closed ring resonator and the bricks, as shown in Figure 20(b). The concentration of the electric field in these regions indicates strong resonance and better interaction between the incoming electromagnetic wave and the resonator structure. Due to this effect, maximum absorption is achieved. In comparison, at 3.4658 THz, the electric field strength reduces clearly and is mainly limited to the upper part of the central ring resonator, as presented in Figure 20(c). This shows that the resonance becomes weaker at frequencies above the operating range.

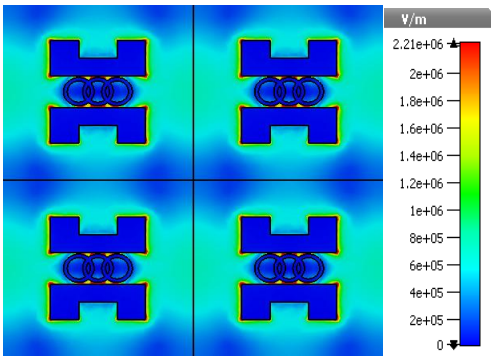
Thus we can say that the combined behaviour of the electric and magnetic field distributions confirms that both resonances work together to improve the absorption efficiency of the proposed design.



(a)



(b)



(c)

Fig.20 Real |E|-field distribution at: **(a)** 3.3414 THz **(b)** 3.3777 THz (Resonance Frequency) **(c)** 3.4658 THz

From the above discussion we conclude that at the resonance frequency i.e. 3.3777 THz, both the electric and magnetic fields become highly concentrated within the resonator structure. This field confinement shows a strong interaction between the incident electromagnetic wave and the metamaterial surface which leads to high efficient energy absorption. The observed behaviour confirms the ability of the proposed design to achieve near-perfect absorption at 3.3777 THz, which is also come from figure 21.

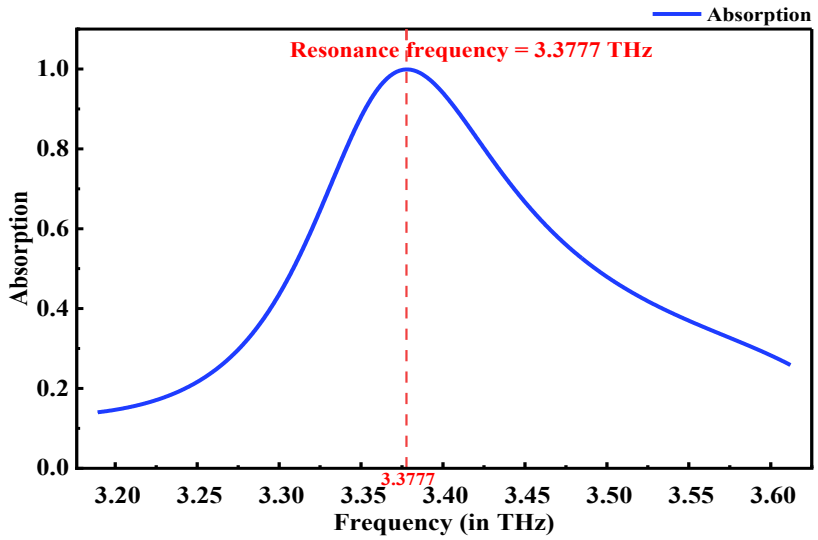


Fig.21 Absorption characteristics of the proposed metamaterial unit cell

CHAPTER-9

RESULTS AND DISCUSSION

9.1 EVALUATION OF REFRACTIVE INDEX SENSOR

A 2 μm thick analyte layer is placed above the resonator so that the proposed absorber can now be used as a sensor. By changing the refractive index (RI) of the surrounding medium this behaviour is studied and observing the changes in the absorption spectrum, as shown in fig. 22(a). The RI is changed from 1.31 to 1.40 with an interval of 0.01 to examine the sensor performance under different conditions. It is found that when the refractive index increases, the absorption resonance shifts towards lower frequencies or higher wavelengths. This shows a clear redshift behaviour. This continuous shift confirms that the proposed structure can detect even small variations in the surrounding refractive index.

The resonant frequencies for different refractive index values are given in Table 2. The results indicate that the resonant frequency continuously decreases when the refractive index increases. This shows a strong interaction between the electromagnetic field and the analyte layer. To study the sensing performance of the proposed structure, a linear fitting was carried out between the refractive index values and the resonant frequencies obtained from the simulation results. Figure 22(b) shows an excellent linear relationship with a coefficient of determination of ($R^2 = 0.993$). The fitted equation is expressed as:

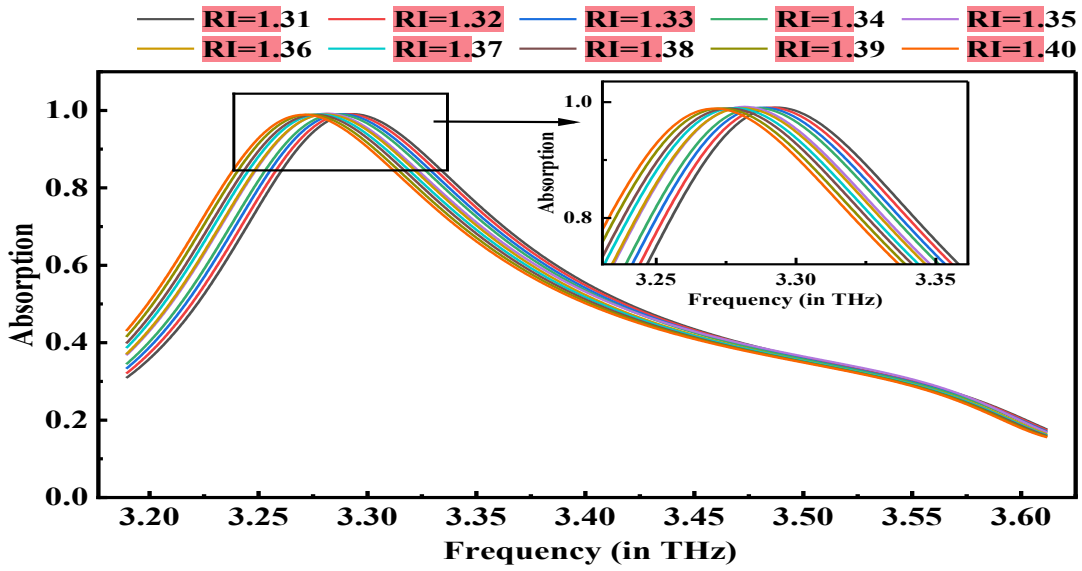
$$f = -0.24703 \times RI + 3.61653 \quad (10)$$

The negative slope of the fitted equation indicates that the resonant frequency decreases from 3.2933 THz to 3.2709 THz as the refractive index changes from 1.31 to 1.40. This inverse relationship proofs the stable and predictable sensing behaviour of the proposed structure. The strong linearity between RI and resonant frequency highlights the suitability of the absorber for refractive index sensing applications. Also, the enhanced confinement of electromagnetic waves around the resonator improves the interaction between the analyte and the sensing structure. This contributes to the improved sensitivity of the device.

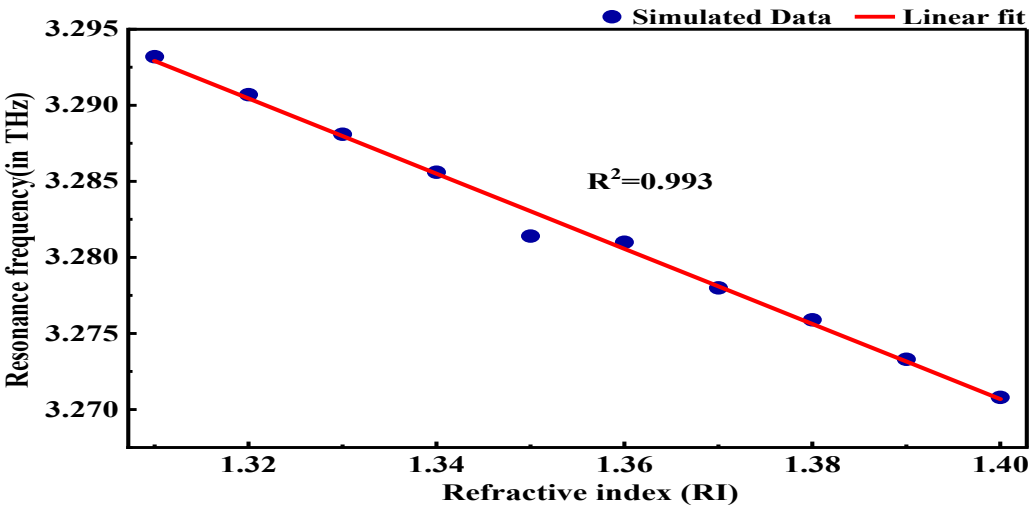
Due to its high sensitivity, the proposed sensor is capable of detecting very small refractive index variations produced by biomolecular interactions. This capability makes the structure highly effective for identifying the changes occurs in biological samples with greater precision. Such performance is used in biomedical sensing, where slight differences in refractive index can help distinguish between normal and infected cells. Hence, the proposed absorber can serve as a promising refractive index-based biosensor for advanced sensing systems.

Table2. Various resonant frequencies (in THz) corresponding to the refractive index

Refractive Index	Resonance frequency (in THz)
1.31	3.2933
1.32	3.2907
1.33	3.2882
1.34	3.2857
1.35	3.2814
1.36	3.2810
1.37	3.278
1.38	3.2759
1.39	3.2734
1.40	3.2709



(a)



(b)

Fig.22 (a) Spectra of absorption for various refractive index **(b)** Linear fitting curve between resonant frequency and refractive index.