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Integer-PSO-Optimized Checkerboard Dual-Band Terahertz Metamaterial Absorber for Biomedical Sensing Applications †

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Abstract

This paper presents a checkerboard-patterned terahertz (THz) metamaterial absorber engineered for wideband dual-band absorption. The absorber consists of a gold metal layer patterned on a polyimide substrate, forming a unit cell structure with dimensions of 85 μm × 85 μm. At the core of the design is a square metal patch of 67 μm × 67 μm, which is divided into a 5 × 5 grid of 25 smaller cells. An integer-coded Particle Swarm Optimization (PSO) algorithm is employed to generate the pattern, where an input value of '1' retains the metal in a cell, and a '0' results in the removal of metal from that cell, resulting in a digitally optimized checkerboard pattern. The substrate height is also optimized and fixed at 7 μm to enhance resonance characteristics. The PSO algorithm is run for 50 iterations, with the fitness function defined as the number of frequency points at which the absorption exceeds 90%. The finalized design achieves two distinct absorption peaks with high efficiency: 99.53% at 3.434 THz with a 90% absorption bandwidth of 212 GHz and 99.35% at 3.823 THz with a bandwidth of 177 GHz. While the absorption performance is already significant, it can be further improved by increasing the number of PSO iterations, albeit at the cost of higher computational complexity. The proposed absorber demonstrates strong potential for biomedical sensing, as validated through its ability to differentiate between cancerous and non-cancerous breast and blood cells. This work paves the way for fully automated, algorithm-driven metamaterial design strategies in the THz regime, particularly for applications in non-invasive biomedical diagnostics.

Keywords: terahertz metamaterial absorber; dual-band; cancer detection; sensitivity; biomedical sensor

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1. Introduction

Terahertz (THz) radiation, positioned between microwave and infrared wavelengths, exhibits unique characteristics that make it valuable for biomedical sensing, spectroscopy, and security screening. A metamaterial absorber is defined as an engineered material that effectively absorbs incident electromagnetic radiation [1]. A special category of these structures are the THz metamaterial absorbers (TMAs) that can absorb THz radiation. The absorption peaks of TMAs can be tailored by modifying material properties or altering the unit cell design, enabling precise control over the absorption spectrum. This versatility and tunability position TMAs as a critical element in the advancement of THz technologies and applications. Researchers have achieved multi-band, broad-band, and tunable TMAs, often employing traditional design approaches involving modifications to the unit cell [2–4]. The conventional design methodology necessitates alterations to the unit cell to achieve the desired absorption characteristics, a process that can be time-consuming and labor-intensive. An alternative approach involves automating the design process using optimization algorithms. Many researchers have used this approach to design unique TMAs. A swastika shapted design has been optimized using firefly algorithm to achieve dual-band characteristics [5]. Deep learning was employed in [6] to optimize the TMA to achieve wide band absorption characteristics. A Taguchi deep neural network was employed to optimize a graphene based TMA to achieve wide band characteristics [7]. A machine learining framework was developed to design a multi-band absorber in THz range [8]. Another deep learning approach has been presented in [9] to design a multi-band TMA. While reducing manual effort, these approaches still require considerable effort and time to design the initial unit cell, which is followed by parameter optimization to achieve the desired characteristics. Furthermore, this approach can be restrictive, limiting the degree of structural freedom. An alternative is to design the structure entirely using optimization algorithms. Although computationally intensive, this approach offers greater structural freedom and can facilitate achieving the desired absorption characteristics. For detection applications, absorbers with a high Figure of Merit (FoM) are desirable [8–10]. Several investigations have explored multiband absorbers utilizing multiple metallic resonators; for example, ref. [11] details a quad-band absorber design employing four resonators of distinct sizes. Similarly, refs. [12,13] utilized triple and dipolar resonances to construct quad-band absorbers. THz metamaterial absorbers can also be utilized to sense changes in refractive index [14].

This work introduces a novel terahertz (THz) metamaterial absorber meticulously designed for efficient, dual-band absorption. The absorber incorporates a digitally optimized checkerboard pattern, created using a Particle Swarm Optimization (PSO) algorithm, to achieve high absorption peaks at 3.434 THz and 3.823 THz. This design, consisting of a gold layer on a polyimide substrate, demonstrates significant potential for biomedical sensing, specifically for distinguishing between cancerous and non-cancerous blood and breast cancer cells. The manuscript is organized into four sections. The subsequent section details the design methodology and unit cell structure. The third section presents the simulation results and discusses the sensing capability of the design. The conclusion section outlines the future scope of this work.

2. Design Methodology and Unit Cell Structure

The design and optimization of the terahertz metamaterial absorber unit cell were carried out through a co-simulation framework integrating Ansys HFSS with Python, where the PyAEDT library enabled automated communication between the two platforms. To achieve optimal performance, a PSO algorithm, implemented using the PySwarm library in Python, was employed. In each iteration, the PSO algorithm updated the design parameters of candidate solutions, which were then applied to the HFSS model through PyAEDT. HFSS subsequently simulated the modified unit cell and generated the corresponding absorption spectrum, which was returned to Python for fitness evaluation. The fitness function was defined as the number of frequencies exhibiting absorption greater than 95%, serving as the optimization target. The design space consisted of 27 variables, where 25 binary variables defined a checkerboard distribution of metal patches on the central square (parameter a): with '1' indicating the presence of a metal patch and '0' its absence; while the remaining two continuous variables controlled the overall square dimension (a) and substrate height (h). This automated co-simulation process enabled systematic exploration of the design space, allowing the PSO algorithm to iteratively refine the geometry until the desired broadband, near-perfect absorption characteristics were obtained. The steps involved in the design methodology are shown in Figure 1.

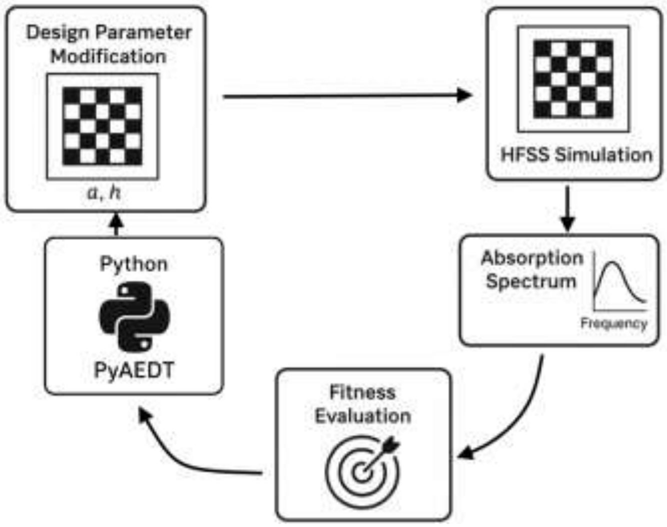


Figure 1. Proposed structure of metamaterial absorber: (**a**) top view; (**b**) side view.

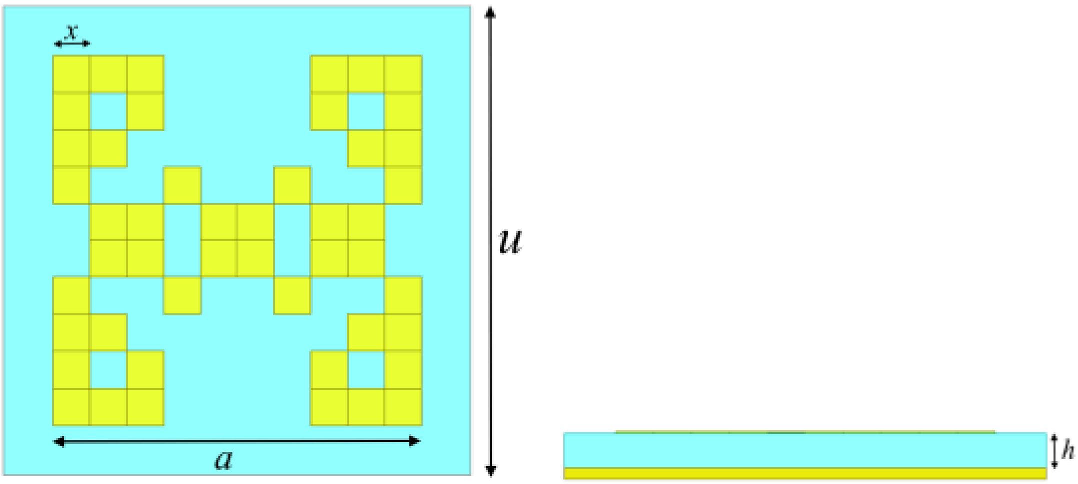
The fitness function of the PSO simulates a periodic structure within HFSS based on input numerical data. Initially, it prepares the input array, extracts key dimensions and parameters, and creates a "dielectric" box in HFSS. A checkered pattern of gold patches is then generated, defined by a binary sequence within the input array, establishing a repeating motif of gold elements atop a dielectric base. Subsequently, the design is mirrored along the x axis and the y axis to complete the structure. This ensures that the structure is symmetric. The structure is then simulated in HFSS, and the resulting reflection coefficient data is extracted, processed in Python to calculate absorption values, and optionally saved to a CSV file. The algorithm returns the number of frequencies exceeding a specified absorption threshold. PSO then uses the fitness values to improve the design over subsequent iterations. The pseudo-code for the algorithm is shown below:

Algorithm 1. To calculate the fitness

```
INPUT: An (Array of Numbers), pl (Boolean)
OUTPUT: Result (Number or String)

BEGIN

// 1. Data Preparation
An_flat = Flatten(An)   // Convert An to a 1D array

// 2. Extract Parameters
N = Length(An_flat) − 2
Un = Slice(An_flat, 0, N)
h = An_flat[N]     // Integer − Height
a = An_flat[N + 1]   // Integer − Dimension (Width, etc.)

// 3. Create 'dielectric' box in HFSS
CALL CreateHFSSBox(origin=[0, 0, b], sizes=[u, u, h], name="dielectric", material=polyimide)

// 4. Calculate Simulation Parameters
Nx = IntegerSqrt(Length(Un))
```

```
Ny = Nx
ax = a/(2 ∗ Nx)
ay = a/(2 ∗ Ny)

// 5. Create Checkered Pattern in HFSS
count = 0
FOR i = 0 TO Ny − 1 DO
FOR j = 0 TO Nx − 1 DO
IF Un[count] == 1 THEN
start = [(u − a)/2 + j ∗ ax, (u − a)/2 + i ∗ ay, h + b]
CALL CreateHFSSBox(origin=start, sizes=[ax, ay, t], name="top", material="gold")
count = count + 1
ENDIF
ENDFOR
ENDFOR

// 6. Mirror 'top' boxes in HFSS
CALL MirrorObjects("top", origin=[u/2, 0, b + h], vector=[u/2, 0, 0])
CALL MirrorObjects("top", origin=[0, u/2, b + h], vector=[0, u/2, 0])

// 7. Run HFSS Analysis
CALL RunHFSSAnalysis()

// 8. Extract Data for Plotting
plot_data = CALL GetHFSSPlotData()

// 9. Create HFSS Report
report = CALL CreateHFSSReport(plot_data[1])

// 10. Extract Solution Data
solution = CALL GetSolutionData(report)

// 11. Export Solution to CSV (with Error Handling)
TRY
CALL ExportSolutionToCSV(solution, "data.csv", separator=";")
EXCEPT
CALL DeleteHFSSObjects(["dielectric"] + CALL GetHFSSObjectNames("top"))
RETURN 0    // Indicate Failure
ENDTRY

// 12. Process Data
df = CALL ReadCSV("data.csv", separator=";")
x = CALL GetColumnValues(df, 0)
y = CALL GetColumnValues(df, 1)
y = 10**(y/20)
y = 1 − (y**2)
indices = CALL FindIndices(y, > 0.95)
   CALL DeleteHFSSObjects(["dielectric"] + CALL GetHFSSObjectNames("top"))
RETURN Length(indices)
END ALGORITHM
```

Figure 2 illustrates the unit cell design of the terahertz metamaterial absorber that was obtained using the PSO. The absorber utilizes gold for both the top and bottom layers, chosen for its high conductivity (4.10×10^7 S/m). Polyimide is used as the substrate, having a dielectric constant of 3 and a loss tangent of 0.06. Through the PSO optimization, the dielectric spacer height, denoted as *h*, was determined to be 6 µm, and the central square dimension, *a*, was found to be 67 µm. The unit cell's overall dimension is *u* = 85 µm. The bottom gold layer, *b*, was taken to be 2 µm thick to effectively block electromagnetic wave transmission and the thickness of the top gold layer was taken as *t* = 0.4 µm. The simulation were performed using the Ansys HFSS and master slave boundary conditions were used to obtain the absorption spectrum. The PSO algorithm was run for 50 iterations. The parameters of the PSO algorithm are: number of particles: 4; dimensions: 27; inertia weight: 0.9; cognitive parameter: 0.5; social parameter: 0.3.



(**a**) (**b**)

Figure 2. Unit cell of the PSO optimized structure (**a**) top view (**b**) side view.

3. Results and Sensing Performance

The unit cell was simulated using the Ansys HFSS software. The absorption (*A*) is measured using the reflection coefficient (s_{11}) and the transmission coefficient (s_{12}) using Equation (1):

$$A = 1 - |s_{11}|^2 - |s_{12}|^2 \tag{1}$$

The thickness of the bottom ground plane is more than the skin depth of gold and it prevents the transmission of electromagnetic waves. Thus, the transmission coefficient is almost negligible. The absorption spectrum of the checkered patterned absorber is shown in Figure 3. Also, shown in the figure are its absorption spectra at different polarization and incidence angles. The designs offers two distinct absorption peaks with high efficiency: 99.53% at 3.434 THz with a 90% absorption bandwidth of 212 GHz and 99.35% at 3.823 THz with a bandwidth of 177 GHz.

The absorption spectra of the design varies slightly with the polarization angle. However, with the incidence angle, the shift is more pronounced. The absorption spectrum also varies with the changes in the refractive index of the surrounding medium. This shift in the absorption spectrum is due to changes in the impedance matching, which can be exploited to detect different biological samples [10]. It is known that cancerous and non-cancerous tissues have different refractive index. Cancerous breast cell has a refractive index of 1.399, while non-cancerous breast cell has a refractive index of 1.385 [10]. Similarly cancerous blood cell has a refractive index of 1.39, while non-cancerous blood cell has a refractive index of 1.376 [10]. The absorption spectra of the proposed design, when surrounded by these different biological tissues is shown in Figure 4.

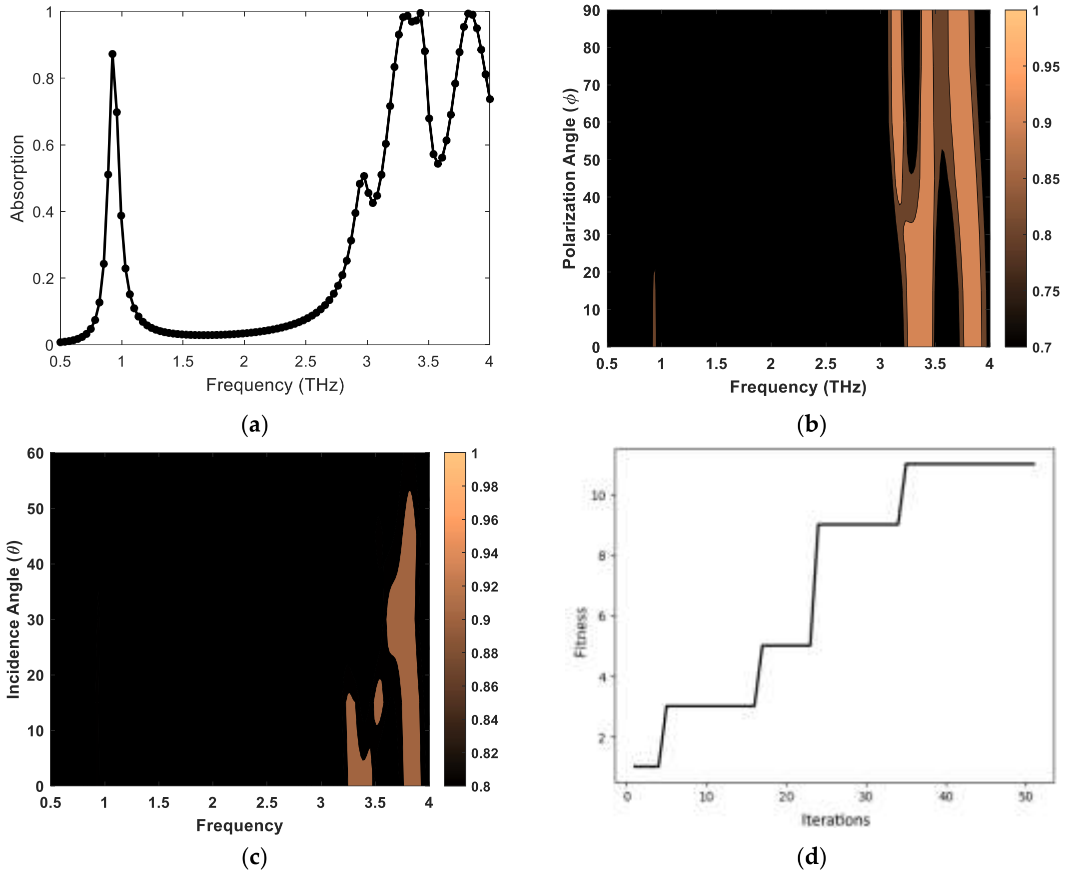


Figure 3. The absorption spectrum of the checkered pattern design at (**a**) normal incidence and polarization angle = 0°; (**b**) at other polarization angles (**c**) at other incidence angles (**d**) convergence curve of the PSO

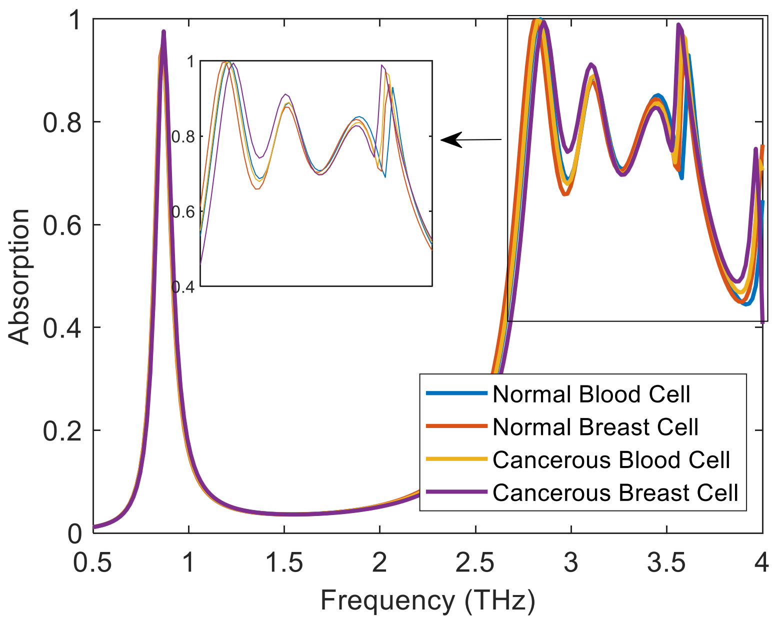


Figure 4. Absorption spectra for different biomedical samples.

From the Figure 4, it can be clearly observed that different biomedical tissues have noticeably different absorption spectra. These shifts in the absorption spectra can be used to detect the biomedical samples accurately.

4. Conclusions

This work presents the successful design of a dual-band terahertz metamaterial absorber with wideband characteristics in both absorption bands. The methodology utilizes an algorithm-driven approach, specifically through the use of a PSO algorithm to generate a checkerboard pattern. The resulting absorber achieves remarkable absorption rates at two distinct frequencies, demonstrating the power of automated design strategies for achieving targeted performance characteristics. Furthermore, the demonstrated ability to differentiate between cancerous and non-cancerous cells validates the potential of this design for advanced biomedical sensing applications. This research not only advances the field of terahertz metamaterial design but also establishes a pathway toward fully automated, algorithm-driven strategies, promising greater efficiency and customization in the development of innovative THz devices for non-invasive diagnostics.

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