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Effect of the thermomechanical properties of hybrid materials on the performance enhancement of nano terahertz antennas

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This study investigates the impact of the thermomechanical properties of hybrid materials, such as polymer substrates and gold or graphene radiating elements, on the performance enhancement of nano terahertz antennas, with a specific focus on the combination of graphene and polyimide. We analyze how the Young's modulus of materials like graphene, Gold, PTFE, polycarbonate and polyimide varies with temperature. Results show that graphene maintains high rigidity with minimal decrease in Young's modulus even at elevated temperatures, whereas gold exhibits a more pronounced reduction. Among polymer substrates, polyimide exhibits increasing rigidity with temperature, making it highly suitable for high-temperature applications. Combining graphene with polyimide to concept terahertz antenna with dimension of 64.97*90.84*1 provides an optimal balance of low reflection coefficients S11 of -20.59dB and high gain of 6.01 dBi, demonstrating excellent performance and stability in the THz frequency range. Hybridizing polymer substrates with graphene or gold antennas merges the mechanical benefits of polymers with the exceptional electrical and optical properties of graphene and gold. This approach facilitates the creation of lighter, more flexible, and durable devices while enhancing performance in terms of sensitivity and resistance across a range of innovative technological applications.

Keywords: Polymer substrates; terahertz antenna; graphene; gold; young's modulus; thermomechanical properties.

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1. Introduction

The terahertz (THz) band, covering frequencies from 0.1 to 10 THz, represents a new frontier in communications and sensor technology [1, 2]. THz antennas leverage this frequency range for various groundbreaking applications. In communications, they enable ultra-fast data rates, which are crucial for next-generation networks [3]. In mechanical engineering, THz antennas facilitate the characterization of advanced materials by enabling the analysis of composite structures and the detection of internal defects without contact [4]. They also support the optimization of polymers and other materials by allowing the testing and development of new formulations with enhanced mechanical properties for specific applications [5]. The THz band, with its unique properties, promises to revolutionize numerous sectors with its unprecedented capabilities in detection, imaging, and communication [6].

The choice of materials for radiating elements and substrates is crucial in the design of patch antennas due to their impact on overall performance, including dielectric permittivity (ϵ_r), dielectric loss (tangent delta, tan δ), substrate thickness, and mechanical and thermal stability [7]. This article emphasizes the importance of mechanical and thermal properties to ensure the antenna's stability and durability under varying environmental conditions, such as temperature fluctuations and vibrations [8]. We will explore the influence of Young's modulus of elasticity of different materials used in printed antennas for the terahertz band, which is known for its diverse applications across multiple research fields [9, 10].

Hybridizing polymer substrates with graphene or gold antennas combines the mechanical benefits of polymers with the exceptional electrical and optical properties of graphene and gold. This approach enables the creation of lighter, more flexible, and more durable devices while enhancing performance in terms of sensitivity and resistance across a range of innovative technological applications. Young's modulus, also known as the modulus of elasticity, measures a material's stiffness. For polymers, this modulus is influenced by factors such as temperature coefficients and molecular structure, which play a crucial role in their mechanical and thermal behavior and impact their compatibility with graphene or gold antennas [11, 12].

In terahertz applications, where antennas must operate with extreme precision, structural rigidity is essential to prevent distortion and performance variations. Additionally, the material's ability to maintain rigidity despite temperature changes ensures stable performance in various thermal environments, which is especially important for systems integrated into devices exposed to fluctuating thermal conditions [13, 14].

Several research papers have explored the use of graphene and gold in terahertz (THz) band applications. For instance, Ref. [15] presents the design of a terahertz circularly polarized antenna. Reference [16] discusses a dual-band patch antenna with a hexagonal shape incorporating graphene, while [17] describes a compact circularly polarized patch antenna [18]. Introduces a wide-band nano patch circular graphene antenna with defected ground structure (DGS), as well as a circular gold antenna. Additionally, [19] highlights recent advances in materials for terahertz metamaterial sensing, and [**?**] provides an analysis and optimization of the band gap of terahertz antennas for wireless body area network (WBAN) applications. Reference [21] focuses on graphene microstrip patch ultrawide-band antennas for THz communications. Finally, [22] features the design of a graphene optical nano patch antenna specifically for terahertz applications.

Other research works have focused on the study of materials, such as [23] study the effect of temperature on elasticity young's modulus of graphene, [12], which discusses the temperature effect on the mechanical properties of graphene sheets under tensile loading, and [24], which focuses on the current advancements in graphene mechanics. The latter encompasses graphene's behavior under tension and compression, fracture, shearing, bending, friction, and dynamic properties, as studied through both experimental and numerical simulations, [9] Employ molecular dynamic (MD) simulations to investigate the tensile and compressive mechanical responses of GCHs under in-plane and out-of-plane directions across a temperature range from 10 to 1800 K, [25] investigates a graphene-based hybrid material microstrip slotted antenna for THz applications, further highlighting the relevance and recent progress in hybrid material antenna designs for terahertz frequencies. Finally, [26] presents an innovative design for a directional cross-dipole antenna with a conformal graphene-based reconfigurable intelligent surface, advancing terahertz connectivity and demonstrating the ongoing evolution of graphene-based THz antenna technologies.

In this paper, we will combine polymer substrates such as PTFE $\epsilon_r = 2.1$, polyimide $\epsilon_r = 3.5$, and polycarbonate $\epsilon_r = 2.9$, each with a thickness of 3 μm, with radiating elements made of graphene and gold to achieve optimal performance for terahertz antennas. These polymers are chosen for their exceptional dielectric properties and structural advantages: PTFE's stable and non-reactive fluoropolymer structure, polyimide's heat-resistant aromatic structure, and polycarbonate's durable and impact-resistant carbonate linkage structure. Graphene, with its single layer of carbon atoms arranged in a hexagonal lattice and its high Young's modulus, provides superior mechanical stability, making it ideal for robust applications. Gold, with its face-centered cubic (FCC) crystalline structure, offers malleability and ease of shaping, though it may not provide the same level of mechanical stability under significant stress. The combination of these materials leverages the strengths of both the polymers and the conductive elements, resulting in terahertz antennas that are highly efficient and mechanically resilient.

2. Choice of antenna structure

A pentagonal slotted patch antenna is presented in Fig. 1, it is fed by microstrip line of 50 Ω. Gold and Graphene of 1μm of thikness are used for radiation element (patch) and three polymers materials are used as susbstrates materials : PTFE $\epsilon_r = 2.1$, polyimide $\epsilon_r = 3.5$ and polycarbonate $\epsilon_r = 2.9$ with 3 μm of thikness. The dimension of antenna are calculted using equations [27]:

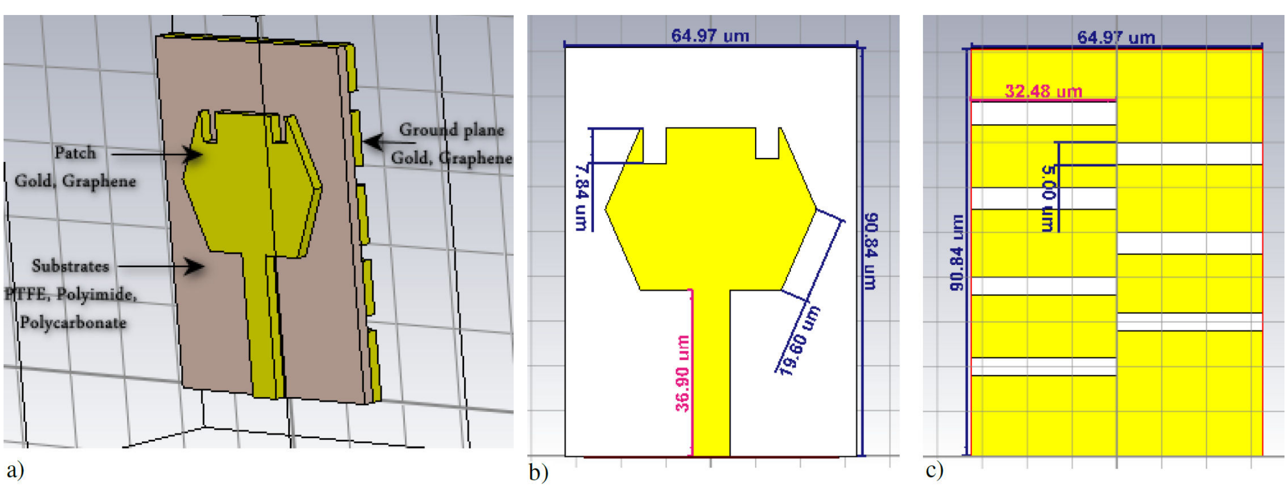

FIGURE 1. Pentagonal slotted patch antenna, a) side view, b) patch, c) ground plane.

TABLE I. Young's modulus parameters.

Materials		$E_{0,\text{Materiaux}}$ (MPa)	T_0(°C)	$\alpha_{\text{materiaux}}$ (1/°C)
Radiation element materials (patch)	Graphene	1000*10^3	20	-0.5e^{-3}
	Gold	79*10^3	20	-2.5e^{-3}
Materials for polymers susbstrates	PTFE	500	20	-0.002
	Polycarbonate	2300	20	-0.0015
	Polyimide	2000	20	0.001

$$w = \frac{1}{2f_r\sqrt{\mu_0\epsilon_0}}\sqrt{\frac{2}{\epsilon_r+1}}, \tag{1}$$

$$\epsilon_{\text{eff}} = \frac{\epsilon_r+1}{2} + \frac{\epsilon_r-1}{2}\left(1+12\frac{h}{w}\right)^{-0.5}, \tag{2}$$

$$\frac{\delta L}{h} = 0.412\frac{(\epsilon_{\text{eff}}+0.3)(\frac{w}{h}+0.264)}{(\epsilon_{\text{eff}}-0.258)(\frac{w}{h}+0.8)}, \tag{3}$$

$$L = 0.412\frac{c}{2F_r\sqrt{\epsilon_{\text{eff}}}} - 2\delta L, \tag{4}$$

$$L_{\text{eff}} = L - 2\delta L, \tag{5}$$

$$Lg = ll + 2L + 6h, \tag{6}$$

$$Wg = 2L + 6h, \tag{7}$$

where h substrate thickness, fr the resonant frequency, ϵ_r dielectric constant, ll the length of the line, Lg length of both substrate and ground plane, and Wg width of both substrate and ground plane.

2.1. Calculation of Young's modulus of elasticity as a function of temperature

The primary thermomechanical property analyzed in this study is the Young's modulus of elasticity of the materials used for the radiating elements (graphene, gold) and polymer substrates (PTFE, polycarbonate, polyimide). The research specifically investigates how the Young's modulus varies as a function of temperature for each material, as this directly impacts the mechanical rigidity and thermal stability of terahertz (THz) antennas [28]. The Young's modulus of elasticity is a fundamental thermomechanical property that quantifies a material's stiffness, defined as the ratio of stress (force per unit area) to strain (deformation) in the linear elastic region of the material's response. In the context of terahertz (THz) antennas, this property is critical for both the radiating elements (such as graphene and gold) and the polymer substrates (PTFE, polycarbonate, polyimide), as it determines the ability of the antenna structure to maintain its shape and performance under mechanical and thermal stress [28].

In this section, we are interested in the calculation of the Young's moduli of materials as a function of temperature. We chose graphene and gold for the radiating element of the antenna and PTFE, polyimide, and polycarbonate for polymer substrates [29], We used a simplified linear relationship,

$$E_{\text{Materiaux}}(T) = E_{0,\text{Materiaux}}\left(1 - \alpha_{\text{materiaux}}(T - T_0)\right), \tag{8}$$

where $E_{0,\text{Materiaux}}$ (MPa) Young's modulus at a specific reference temperature, T_0 reference temperature in (°C), $\alpha_{\text{materiaux}}$ (1/°C) empirical temperature coefficient.

The values of each parameter at the ambient temperature of 20°C are given in Table I.

2.2. Results of the variation of the Young's modulus for radiation element material of the antenna

In this section, we will examine how temperature affects the stiffness of graphene and gold as a function of their temperature coefficients and atomic structures. Understanding these variations is essential for selecting the most suitable material for applications subject to thermal fluctuations:

The figure shows how the Young's moduli for graphene and gold vary with temperature, using simplified linear models for the coefficients of thermal variation.

- The Young's modulus of graphene decreases with increasing temperature, but this decrease is relatively small, although graphene is extremely rigid, the neg-

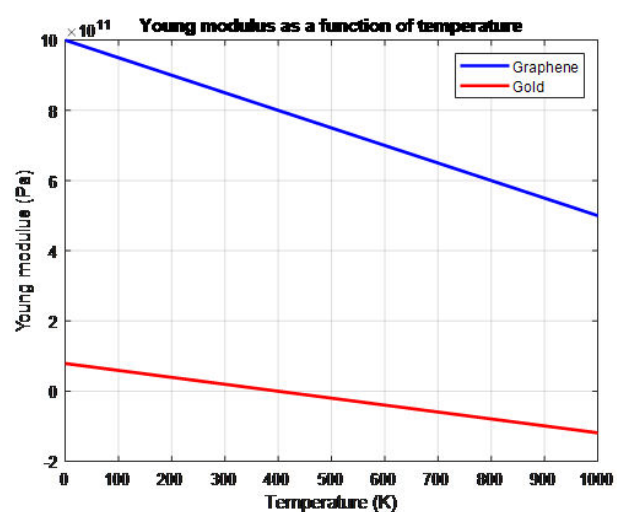

FIGURE 2. Young modulus for graphene and gold.

ative temperature coefficient (very low) means that rigidity decreases slightly with temperature. However, the Young's modulus remains relatively high even at 1000 K.

– The Young's modulus of gold decreases more sharply with increasing temperature, Gold is a metal whose Young's modulus is more sensitive to temperature changes than graphene. The higher temperature coefficient (-2.5e-3) leads to a more significant decrease in Young's modulus as temperature increases.

From the two graphs, we can conclude that graphene with a high young's modulus is more rigid than gold due to its unique atomic structure and binding properties.

2.3. Results of the variation of the Young's modulus for polymer substrate materials

In this section, we will show how temperature affects the stiffness of different polymers as a function of their temperature coefficients and molecular structures. Understanding these variations is crucial to choosing the right material for specific applications subject to temperature variations:

The graphs in the figure show how the mechanical behaviour of materials changes with temperature. The variation of Young's modulus with temperature is influenced by the molecular structure, intermolecular interactions and chemical composition of each material.

– PTFE: The Young's modulus decreases with increasing temperature due to the negative temperature coefficient ($\alpha_{\text{PTFE}} = -0.002$), This means that the material becomes less rigid as the temperature rises.

– Polycarbonate: The Young's modulus decreases with increasing temperature, but at a different rate compared to PTFE ($\alpha_{\text{Polycarbonate}} = -0.0015$). Similar to PTFE, polycarbonate has a negative temperature coefficient, indicating a decrease in rigidity with increasing temperature.

– Polyimide: The Young's modulus increases with increasing temperature due to the positive temperature coefficient ($\alpha_{\text{Polyimide}} = 0.001$), This means that the material becomes more rigid as the temperature rises.

From the three graphs, we can conclude that polyimide and plolycarbonate with a high young's modulus are stiffer than PTFE. Due to its unique thermomechanical behavior. Their ability to maintain high mechanical and thermal performance makes them ideal for applications where high temperature stability is essential [28,30,31].

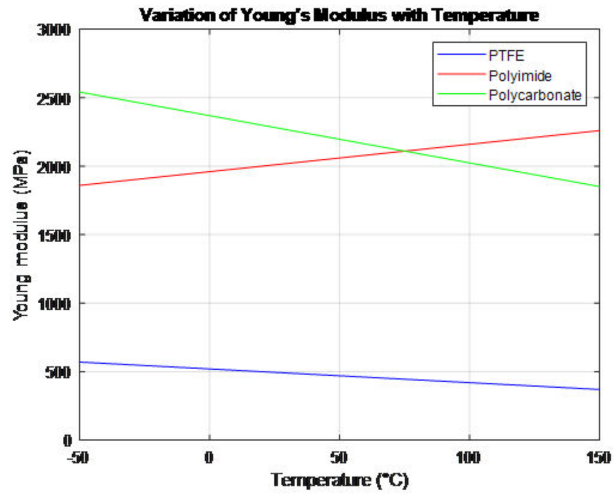

FIGURE 3. Young modulus for PTFE, Polyimide and Polycarbonate.

TABLE II. Thickness and permittivity of PTFE, Polyimide and polycarbonate substrates.

Polymer Substrates material	h	ϵr
PTFE	3 μm	2.1
Polyimide	3 μm	3.5
Polycarbonate	3 μm	2.9

3. Influence of the Young's modulus on the performance of terahertz antennas

We will present the performance results of the terahertz patch antenna at an ambient temperature of 20 degrees Celsius. The Young's modulus of radiating element and substrates material are given in Table I. Table II gives thickness and permittivity of PTFE, Polyimide and polycarbonate substrates.

4. Simulations results with Graphene and polymer substrates (PTFE, Polyimide and Polycarbonates)

After analyzing the simulated graphs in the previous section, we found that graphene and polyimide exhibit high stiffness as a function of temperature. We will now present the simulation results for the combination of graphene and gold, which are the materials chosen for the radiating element, combined with the polymer substrates of the patch antenna. This combination aims to improve the reliability, accuracy and robustness of the devices [25]. For this analysis, we used Table I, which shows the Young's moduli of each material at an ambient temperature of 20 degrees Celsius. Graphene material characteristics for the patch and ground plane are: chemical potential $\mu_c = 2$ eV, relaxation time $\tau = 1$ ps andthickness of 1 μm. The simulation results in terms of S11 and antenna gain are presented in the next section.

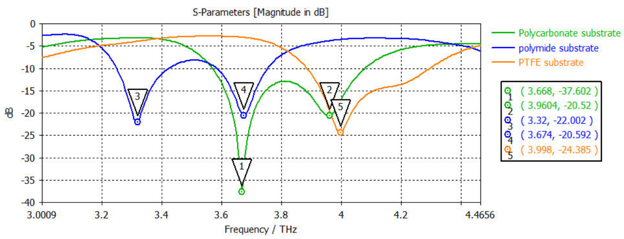

FIGURE 4. Return loss S11 of pentagonal terahertz antenna with Graphene and polymer substrates (PTFE, Polyimide and polycarbonate).

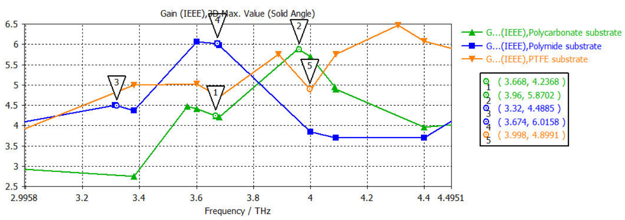

FIGURE 5. Gain of pentagonal terahertz antenna with Graphene and polymer substrates (PTFE, Polyimide and polycarbonate).

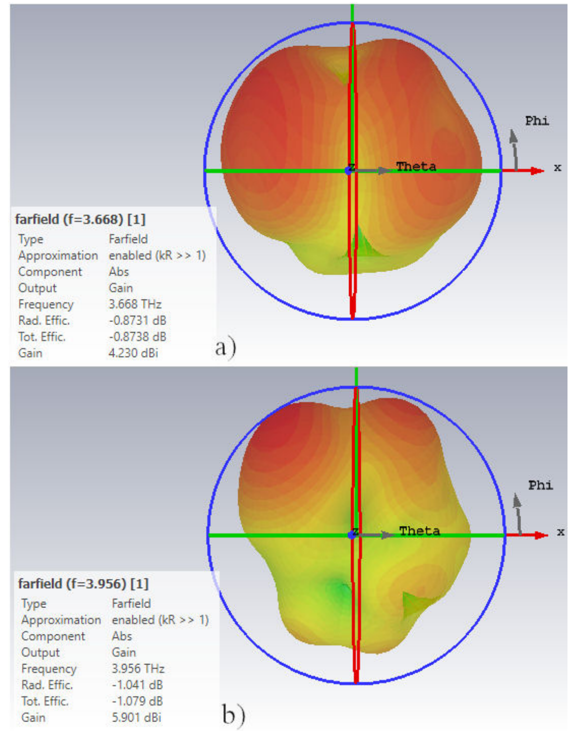

FIGURE 7. 3D radiation pattern of the proposed pentagonal patch antenna with polycarbonate substrate at a) 3.668 THZ; b) 3.956 THz.

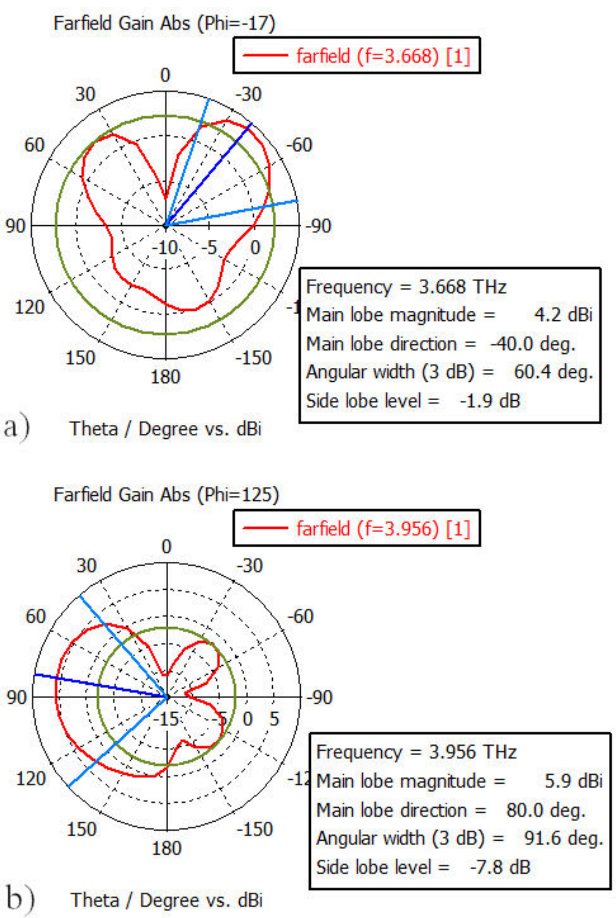

FIGURE 6. Polar radiation pattern of the proposed pentagonal patch antenna with polycarbonate substrate at a) 3.668 THZ; b) 3.956 THz.

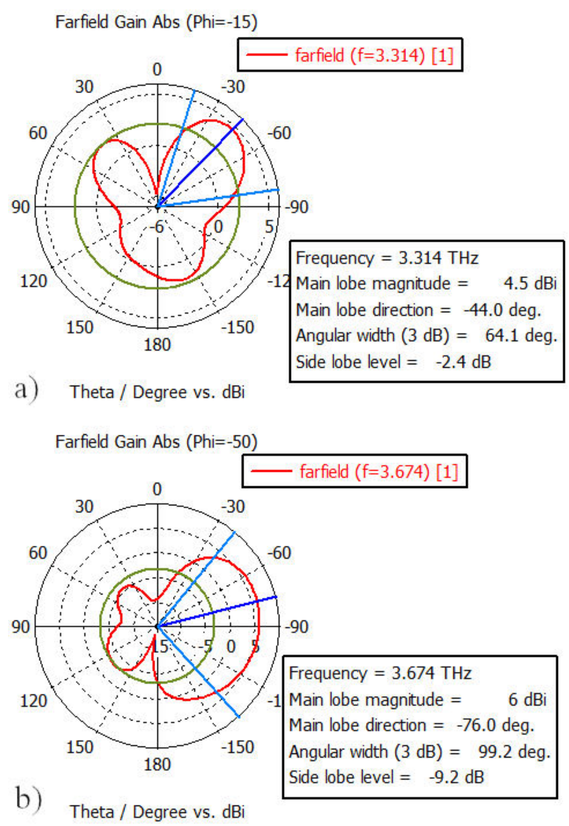

FIGURE 8. Polar radiation pattern of the proposed pentagonal patch antenna with polyimide substrate at a) 3.314 THZ; b) 3.674 THz.

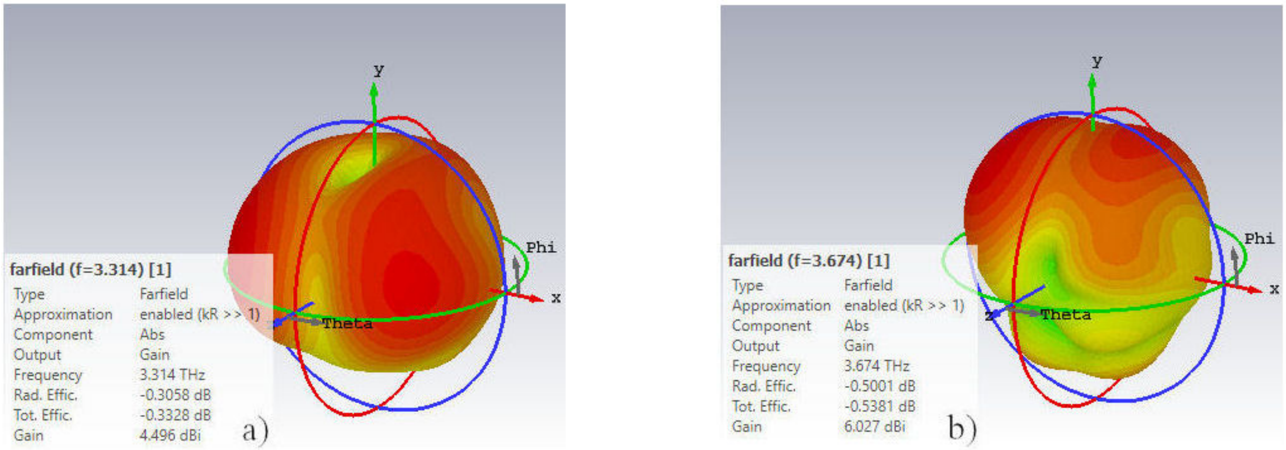

FIGURE 9. Polar radiation pattern of the proposed pentagonal patch antenna with polyimide substrate at a) 3.314 THZ; b) 3.674 THz.

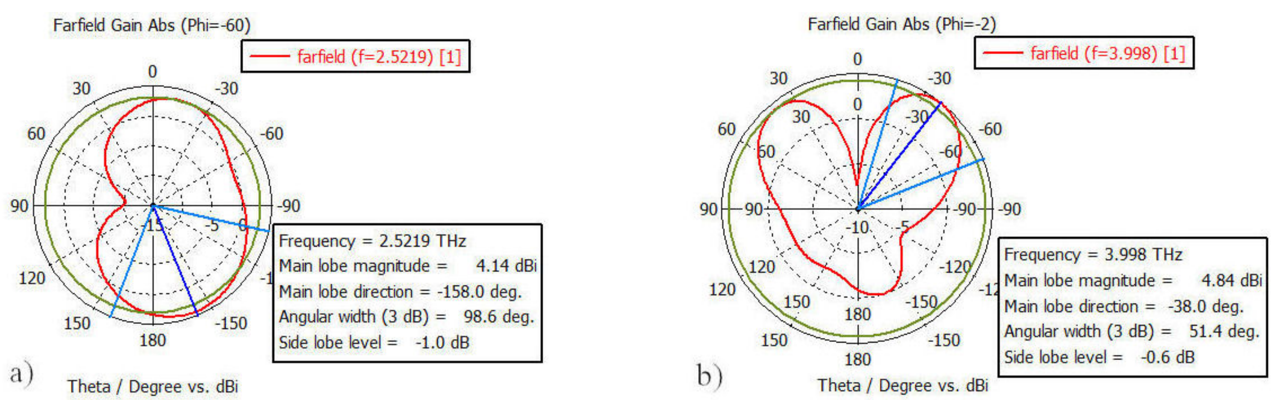

FIGURE 10. Polar radiation pattern of the proposed pentagonal antenna with PTFE substrate at a) 2.521 THZ; b) 3.998 THz.

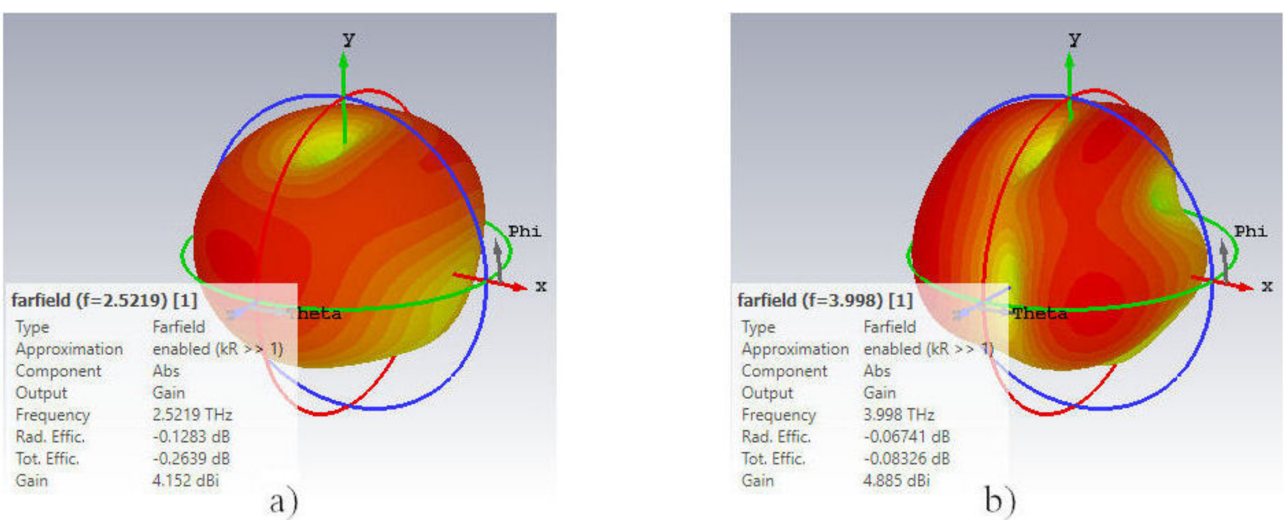

FIGURE 11. 3D radiation pattern of the proposed pentagonal patch antenna with PTFE substrate at a) 2.521 THZ; b) 3.998 THz.

- The S11 parameter is crucial for assessing the efficiency and performance of an antenna, particularly regarding impedance matching and minimizing reflection losses. Generally, for antennas, an S11 below -10 dB across the operational frequency band is desirable, indicating that less than 10% of the energy is reflected and more than 90% is transmitted.

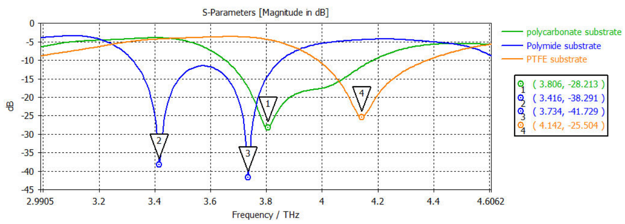

FIGURE 12. Return loss S11 of pentagonal terahertz antenna with Gold and polymer substrates (PTFE, Polyimide and polycarbonate).

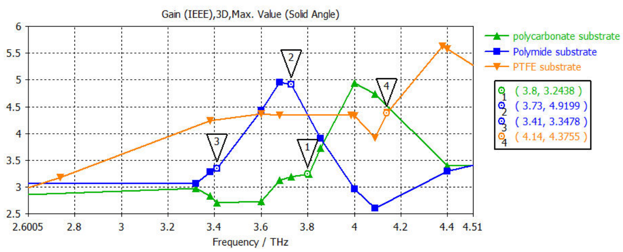

FIGURE 13. Gain of pentagonal terahertz antenna with Gold and polymer substrates (PTFE, Polyimide and polycarbonate).

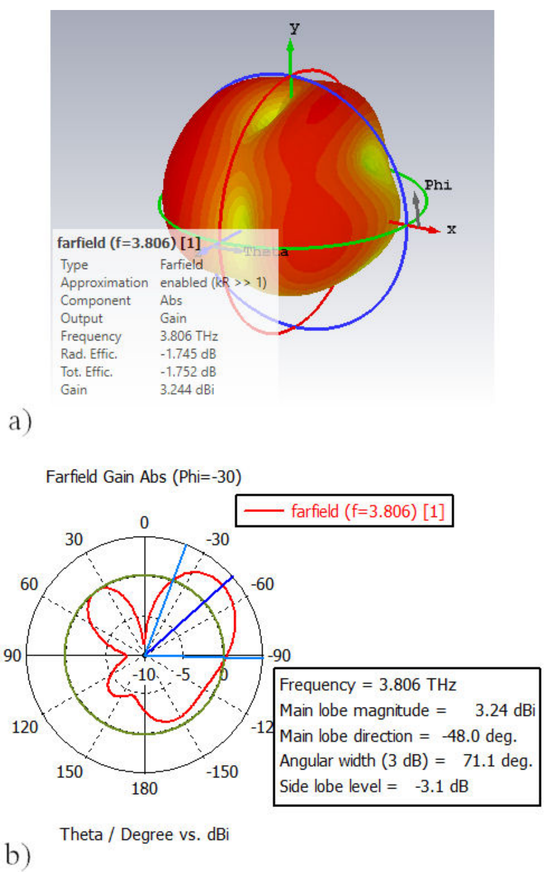

FIGURE 14. a) Polar radiation pattern b) 3D radiation pattern of the proposed pentagonal patch antenna with polycarbonate substrate at 3.806 THz.

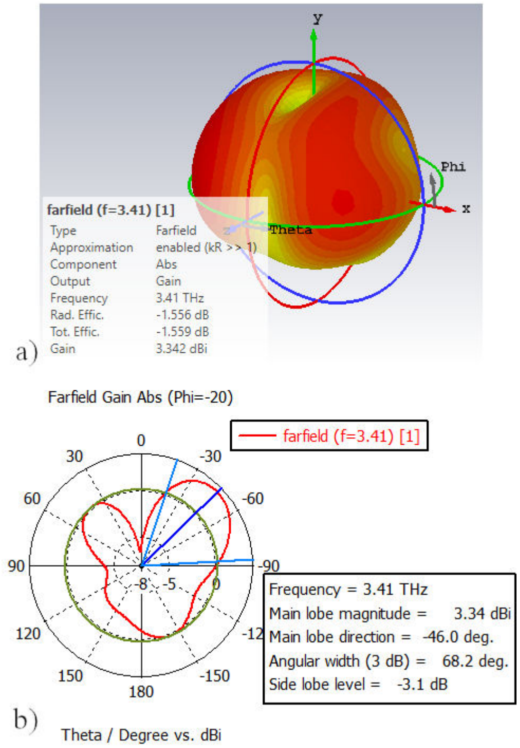

FIGURE 15. a) Polar radiation pattern b) 3D radiation pattern of the proposed pentagonal patch antenna with polyimide substrate at 3.41 THz.

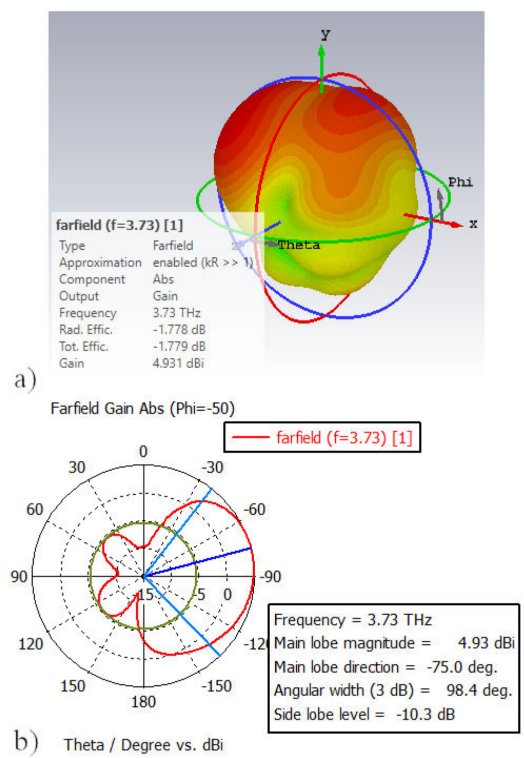

FIGURE 16. a) Polar radiation pattern b) 3D radiation pattern of the proposed pentagonal patch antenna with Polyimide substrate at 3.73 THz.

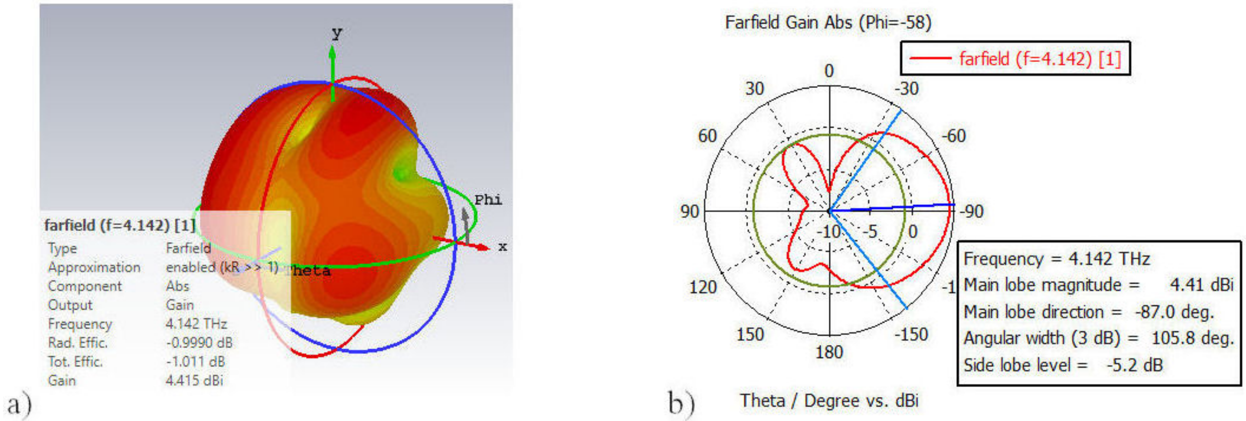

FIGURE 17. a)Ppolar radiation pattern (b) 3D radiation pattern of the proposed pentagonal patch antenna with PTFE substrate at 4.142 THz.

TABLE III. simulations results.

Radiating element	Polymer substrates	frequency (dB)	S11 (dBi)	Gain
Graphene	PTFE	3.998	-24.385	4.8991
	Polycarbonate	3.668	-37.602	4.23
		3.96	-20.52	5.87
	Polyimide	3.32	-22.00	4.488
		3.674	-20.59	6.0158
GOLD	PTFE	4.142	-25.504	4.41
	Polycarbonate	3.8	-28.213	3.24
	polyimide	3.416	-38.291	3.34
		3.734	-41.729	4.93

- Gain is a crucial parameter in antenna design and RF systems, indicating how well an antenna directs energy in a specific direction compared to an isotropic radiator (an ideal antenna that radiates equally in all directions).

5. Simulations results with Gold and polymer substrates (PTFE, Polyimide and Polycarbonates)

We presented in this section the simulation results in term of S11 parameter and Gain of gold pentagonal patch antenna with polymers substrates material:

6. Results discussion

After examining the performance of various radiating elements and polymer substrates in the terahertz (THz) band, it appears that the combination of graphene with polyimide stands out due to its particularly interesting results, it offer both mechanical and thermal stability, ensuring reliable antenna performance in environments with significant temperature fluctuations [28, 30, 32]. Indeed, this combination offers an excellent balance between a very low reflection coefficient (S11) and high gain. For frequencies of 3.32 THz and 3.674 THz, the reflection coefficients (S11) are -22.00 dB and -20.59 dB, respectively, indicating very good antenna matching. Furthermore, the gains are 4.488 dBi and 6.0158 dBi, demonstrating remarkable efficiency in signal transmission and reception.This directly supports the development of THz antennas that are robust, reliable, and high-performing under a wide range of operating conditions. Although gold with various polymers can offer good performance, the combination of graphene with polyimide is generally more advantageous for applications requiring high performance and great stability over varying temperatures. Polyimide, known for its thermal stability and remarkable rigidity, retains its mechanical and dielectric properties even at high temperatures. When combined with graphene, which also exhibits excellent thermal stability and exceptional mechanical rigidity due to its two-dimensional structure and strong covalent bonds, the entire antenna structure can operate reliably over a wide temperature range. This combination is thus particularly suited for terahertz applications where temperature variations can impact performance, offering a promising solution for advanced technologies in the terahertz frequency spectrum.

To highlight the significance of our work, we have compared the simulation results with those from previous and recent literature, as shown in Table IV. The table indicates that the pentagonal patch antenna with graphene achieves a high gain of 6.01 dBi, outperforming all the referenced designs. Additionally, the use of polymer substrates contributes to the development of lighter, more flexible, and more durable devices, while improving performance in terms of sensitivity and resistance for a variety of innovative technological applications.

TABLE IV. Comparison of proposed work with previous literature.

	Substrate material	Frequency (THz)	S11(dB)	Gain (dBi)
[32]	RT Duriod 6010(ϵ_r = 10.2)	2.270	-22.39	4.8
	Silicon(ϵ_r=11.9)	3.254	-42.67	5.3
[33]	Polyimide(ϵ_r = 4.3)	0.445-0.714	-26.4	5.4
[22]	Silicon(ϵ_r=11.9)	3.930	-54.96	5.4
	Duroid 3210(ϵ_r=10.8)	4.010	-63.1	5.06
	Alumina (ϵ_r=9.9)	4.085	-41.32	5.25
	Roger RO4003C(ϵ_r=3.55)	3.24	-48.77	4.346
	Roger 5880 (ϵ_r=2.2)	2.76	-23.317	4.504
[34]	Not mentioned	2.14	-24.65	4.71
		5.41	-25.86	6.61
[35]	Silicon(ϵ_r=11.9)	2.58	-33.7	2.58
		4.41	-10.56	1.22
[18]	Rogers RO4003C(ϵ_r=3.55)	3.26	-30.706	3.437
		4.69	-55.54	5.008
		6.95	-26.812	6.62
Proposed work Gold petagonal patch antenna	PTFE(ϵ_r=2.1	4.142	-25.504	4.41
	Polycarbonate(ϵ_r=2.9)	3.8	-28.213	3.24
	Polyimide(ϵ_r=3.5)	3.416	-38.291	3.34
		3.734	-41.729	4.93
Proposed work **Graphene** pentagonal patch antenna	PTFE(ϵ_r=2.1)	3.998	-24.385	4.8991
	Polycarbonate(ϵ_r=2.9)	3.668	-37.602	4.23
		3.96	-20.52	5.87
	Polyimide(ϵ_r=3.5)	3.32	-22.00	4.488
		3.674	-20.59	**6.0158**
Results discussion				

7. Conclusion

The analysis of Young's modulus variations with temperature reveals significant differences between materials. Graphene maintains a high Young's modulus with minimal decrease even at elevated temperatures, due to its unique atomic structure and strong covalent bonds. In contrast, gold shows a more pronounced reduction in Young's modulus with increasing temperature, highlighting its greater sensitivity to thermal changes. Among polymer substrates, polyimide stands out with its increasing rigidity as temperature rises, unlike PTFE and polycarbonate, which exhibit a decrease in rigidity with higher temperatures. This property of polyimide, combined with the stability of graphene, results in a particularly advantageous combination for terahertz applications. The combination of graphene and polyimide offers a superior balance between low reflection coefficients (S11) and high gain, making it ideal for high-performance and temperature-stable terahertz antennas. This pairing ensures reliable operation across a broad temperature range, providing an optimal solution for advanced terahertz technologies where both performance and thermal stability are critical.

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