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Study of Electric Field Enhancement in Arrow-Pentagonal HfO_2/GaN/Au Multilayer Nanoantenna for Thermal Energy Harvesting

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Abstract **-** This study presents the design and simulation of a novel arrow-shaped pentagon nanoantenna optimized for thermal energy harvesting at 28.3 THz. The proposed design is an enhancement of a conventional pentagon nanoantenna, demonstrating higher electric field enhancement compared to the original structure. Additionally, the performance of hybrid multilayer configurations, including two-layer and three-layer designs, is investigated. Among these, the three-layer structure exhibits the highest electric field enhancement. The hybrid design incorporates moderate-permittivity Gallium Nitride (GaN) and high-permittivity Hafnium Oxide (HfO_2) as dielectric materials, further improving the nanoantenna's performance. The proposed energy harvester offers an efficient solution for the wireless capture and conversion of thermal energy. This will allow for sustainable energy harvesting and reduce our dependence on conventional energy sources.

Keywords**:** Arrow Pentagonal Nanoantenna, Metal-Insulator-Metal (MIM), Gallium nitride (GaN), Hafnium oxide (HfO_2), Electromagnetic (EM).

1. Introduction

Global energy demand has significantly increased in recent decades due to population growth, industrial progress, and the escalating intensity of human activities globally. The increasing need for energy requires the advancement of novel methods to produce clean and economical energy sources [1]. Solar electromagnetic (EM) radiation provides a reliable and sufficient energy source for the Earth. Approximately 30% of solar radiation is reflected by the atmosphere, 19% is absorbed by atmospheric gases and subsequently re-emitted to the Earth's surface at wavelengths within the 7-14 μm range, while the remaining fraction is absorbed and re-emitted predominantly in the infrared (IR) spectrum, peaking at a wavelength of 10.6 μm (28.3 THz) [2]. The extraction of infrared energy from waste heat also offers a significant opportunity for sustainable energy generation. Waste heat sources generally exhibit temperatures between 400-2000 K, which correspond to wavelengths from 2-11 μm.

Nanoantennas have emerged as a promising solution for harvesting this IR radiation. Nanoantennas engineered at nanoscale wavelengths can efficiently capture EM waves, producing alternating current (AC) oscillations at frequencies corresponding to the incident waves. A rectifying nanodiode is integrated with the nanoantenna to convert the harvested energy into direct current (DC) power. Additionally, low-pass filters and step-up DC-DC converters are frequently utilized to supply power wirelessly to loads [3]. Recent research has investigated diverse nanoantenna designs, assessing their performance through the measurement of the electric field distribution on the antenna's surface or within its gap region [2].

Plasmonic nanoantennas exhibit exceptional EM wave confinement abilities; nonetheless, they are limited by substantial ohmic losses at terahertz frequencies. In contrast, dielectric nanoantennas, characterized for their low-loss characteristics, provide better harvesting efficiency relative to metallic counterparts. However, this comes with lower EM wave confinement. To overcome these limitations, hybrid nanoantennas have been proposed, utilizing the significant electric field enhancement of metals in conjunction with the low-loss characteristics of dielectrics. This combination implies a promising method for enhancing electric field intensities. Metal-insulator-metal (MIM) structures have attracted significant attention for their capacity to confine incident light within insulating spacer layers efficiently [4]. This study investigates the electric field enhancement in a nanoantenna structure, achieved by incorporating a dielectric layer with varying permittivity above the metallic framework. Gallium nitride (GaN) and hafnium oxide (HfO_2) are employed as insulating materials to optimize field enhancement and improve energy harvesting efficiency.

GaN performs as an essential substrate material in numerous nanotechnology applications, such as optoelectronics, optical sources, high-intensity light emitters, and satellite solar-cell arrays. Gallium Nitride (GaN) exhibits numerous advantageous characteristics, including a wide direct bandgap of 3.4 eV, a substantial critical electric field of 3 MV/cm, carrier mobility comparable to that of silicon, and high thermal conductivity. Furthermore, it is a crack-resistant semiconductor, making it highly suitable for advanced applications [5]. The moderate refractive index provides excellent confinement of EM fields within nanoantenna structures [6].

Furthermore, HfO_2 is a prominent ceramic material, esteemed for its remarkable dielectric properties (κ = 20-30), establishing it as an exceptional high-κ candidate for present and future nanotechnologies [7]. HfO_2 is characterized by its exceptional chemical stability, optical transparency, wide bandgap of 5.1 eV, and high melting point of 2758°C, thereby increasing its utility in advanced material designs [8][9].

This study presents the design of a novel arrow-shaped pentagonal nanoantenna optimized for operation at a frequency of 28.3 THz. A standard pentagonal antenna was initially designed and afterward modified into an arrow-pentagonal configuration to improve electric field intensities in the gap of the structure. Furthermore, hybrid structures utilizing GaN and HfO_2 as insulating materials have been added above the metallic nanoantenna, keeping the original height of the antenna.

2. Design and Simulation of Nanoantenna

The pentagonal nanoantenna was designed using CST Microwave Studio software. The substrate consists of a 1.15 μm thick silicon layer, with a 115 nm thick copper film working as a backplane at the bottom of the antenna. The antenna is made of gold (Au), having a height of 100 nm.

Perfectly matched layers (PML) are used as absorbing boundary conditions for removing artificial reflections. The EM fields in the nanoantenna gap are characterized using a Cartesian coordinate system, with the x- and y-axes located in the antenna plane and the z-axis oriented perpendicular to this plane. The EM field in the nanoantenna gap is calculated based on the assumption of plane wave illumination having a magnitude of 1 V/m, with polarization directed along the antenna axis.

2.1. Design of Arrow Pentagon Nanoantenna

The side length of the pentagonal antenna (L) can be determined by inscribing it within a circle of radius (r). The relation between L and r is defined accordingly.

$$L = 2r sin\left(\frac{\pi}{5}\right) \tag{1}$$

The resonant frequencies, including those of the dominant mode and higher-order modes, can be determined using the formula provided [10].

$$f_{np} = \frac{X'_{np} c}{2\pi r\sqrt{\epsilon_r}} \tag{2}$$

Where, X'_{np} are the zeros of the derivative of the Bessel function $J_n(x)$of the order n, as is true for TE mode, however for the lowest order modes, X'_{np}= 1.84118. c is the velocity of light and ϵ_r is permittivity of the substrate material.

Nanoantenna structures exhibit significant sensitivity to their geometric arrangement. Parameters including shape, size, aspect ratio, and spatial arrangement are crucial in determining their resonance characteristics, field enhancement abilities, and spectral performance. A novel geometry, referred to as the arrow bowtie nanoantenna, was presented in [11] as an improvement over the classical bowtie design. This geometry provides enhanced EM field confinement, higher directivity, increased output power, and wider bandwidth. In this paper, the arrow pentagon structure is designed with a rear-side cut angle of 62.5° while maintaining the original dimensions of the other sides. Fig 1 (a) and (b) show a three-dimensional view of the pentagon and arrow pentagon nanoantenna structures. Where h_a, h_b, and h_c denote the thickness of the antenna, backplane, and substrate, respectively. L is the side length of the antenna and θ is the rear angle.

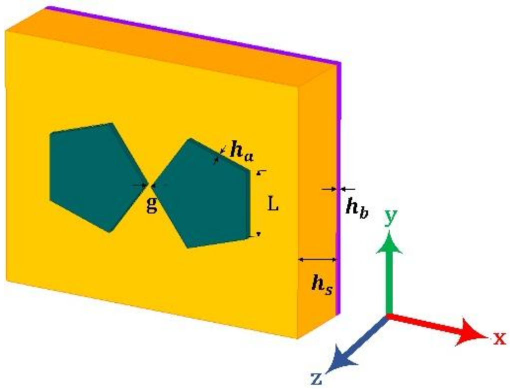

Fig 1 (a): pentagon nanoantenna.

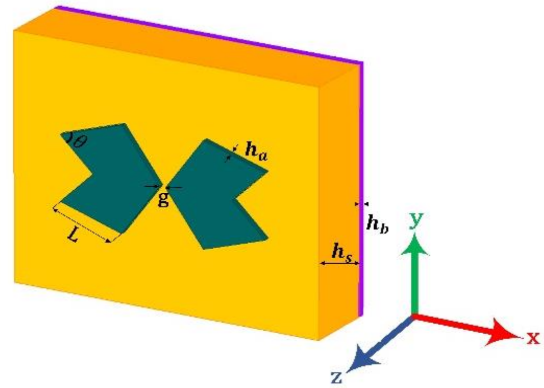

Fig 1 (b): arrow pentagon nanoantenna.

2.2. Design of multilayer structures

The GaN and HfO_2-based bilayer arrow pentagon antennas are shown in Fig 2 (a) and (b). Fig 2 (c) shows a multilayer nanoantenna structure comprised of three layers where GaN is sandwiched between gold and HfO_2 layers.

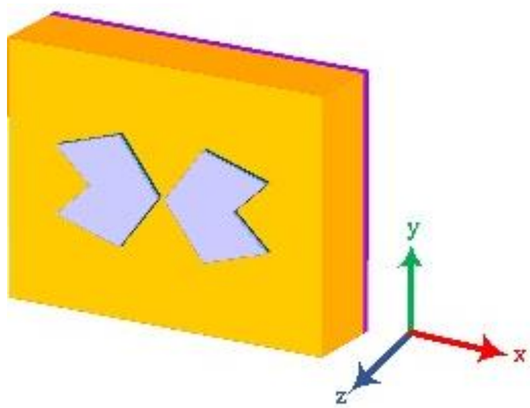

Fig 2 (a): GaN/Au nanoantenna.

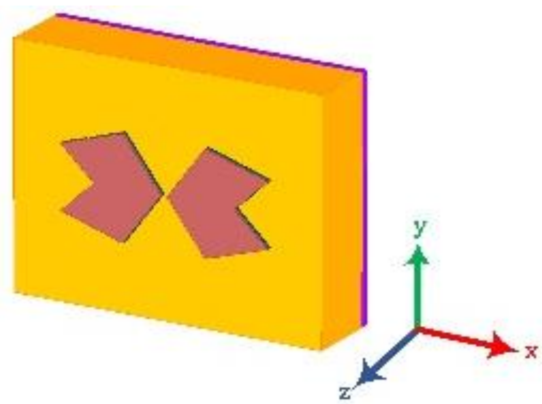

Fig 2 (b): HfO_2/Au nanoantenna.

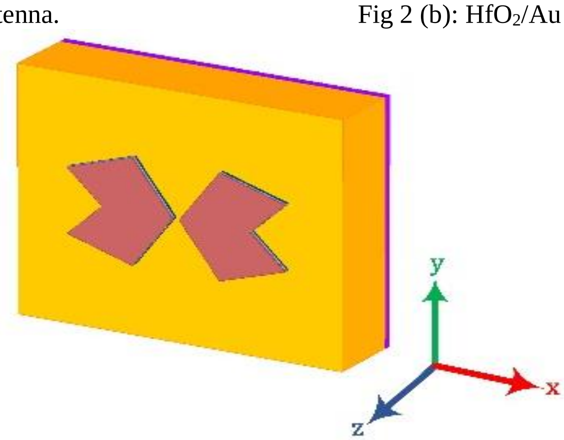

Fig 2 (c): HfO_2 /GaN/Au nanoantenna.

The bilayer structure is designed by placing GaN or HfO_2 layers above the gold layer. The thickness of the antenna kept constant at 100 nm. A filling factor (FF) of 0.5 is used which is defined as [12];

$$FF = \frac{H_{Au}}{H_d + H_{Au}} \quad (3)$$

Where H_{Au} and H_d are the total thickness of the gold and dielectric layer, respectively. For the three-layer structure, the value of FF is 0.3333.

3. Results and Discussion

The electric field enhancement factor in the gap region is formulated as:

$$F = \frac{|E_{gap,peak}|}{|E_{inc,peak}|} \quad (4)$$

Where, $|E_{gap,peak}|$ is the magnitude of the electric field calculated in the subwavelength gap of the nanoantenna, and $|E_{inc,peak}|$ is the magnitude of the electric field of incoming light. The electric field enhancement factor of arrow pentagon antenna is compared with pentagon antenna shown in the Fig 3 (a) and 3 (b). From the results, it is clear that the proposed antenna has 2.59 V/m more enhancement than the pentagonal antenna. This explains that antenna parameters change by varying their geometry. The electric field enhancement factors of bilayer nanoantenna structures consist of GaN/Au and HfO2/Au, which are shown in Fig 3 (c) and 3 (d). This shows that the hybrid structures have more field enhancement compared to a single layer.

The three-layer structure has the highest field concentration compared to the other four structures. This is shown in the Fig 3 (e). An explanation for the increased electric field enhancement observed in the multilayered antenna is its higher refractive index. By inserting a moderate dielectric layer between a metal and a high dielectric material, the effective refractive of the whole structure is increased. This characteristic allows for more abrupt transitions at the antenna/air and antenna/substrate interfaces, hence enhancing energy confinement inside the antenna's center area [12].

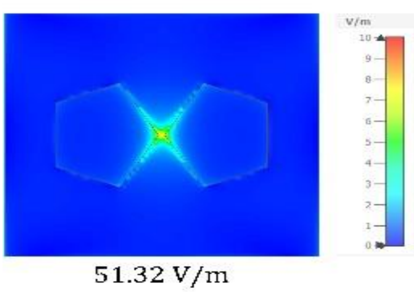

Fig 3 (a): E-field inside pentagon nanoantenna.

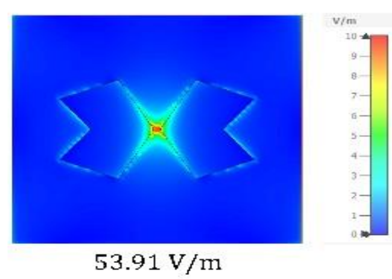

Fig 3 (b): E-field inside arrow pentagon nanoantenna.

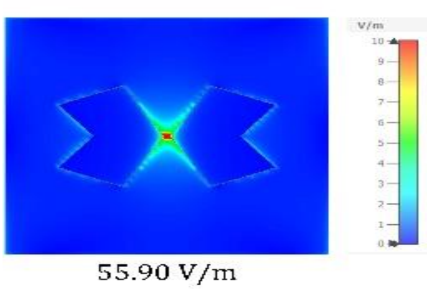

Fig 3 (c): E-field inside GaN/Au nanoantenna.

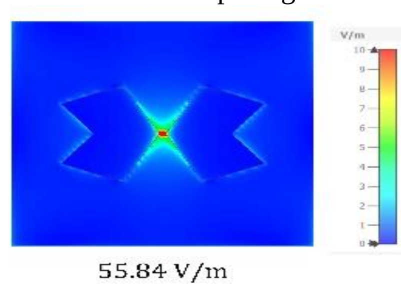

Fig 3 (d): E-field inside HfO_2/Au nanoantenna.

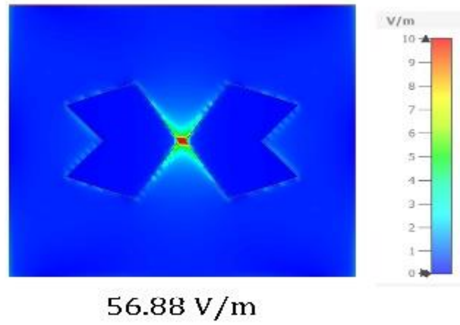

Fig 3 (e): E-field inside HfO_2 /GaN/Au nanoantenna.

The reflection parameters and impedance values of all five nanoantennas are compared in Fig 4.1, Fig 4.2 and Fig 4.3. Also, the results are tabulated in Table 1. From the table, it can be concluded that S_{11} is the maximum for a pentagonal antenna and minimum for HfO_2 /GaN/Au nanoantenna. A magnitude of -37.38 dB is observed at a frequency of 28.3 THz, indicating that the designed multi-layered structure achieves optimal resonance at this frequency. Based on the comparison of impedance values, it can be inferred that the structures exhibit impedance values close to that of free space (approximately 377 Ω). Although the HfO_2/GaN/Au nanoantenna demonstrates a lower real component of Z_{11}, it also shows a minimal imaginary component of Z_{11}, indicating reduced losses. These results suggest that the multilayer structure is a promising candidate for enhanced electric field concentration and, consequently, for energy harvesting applications.

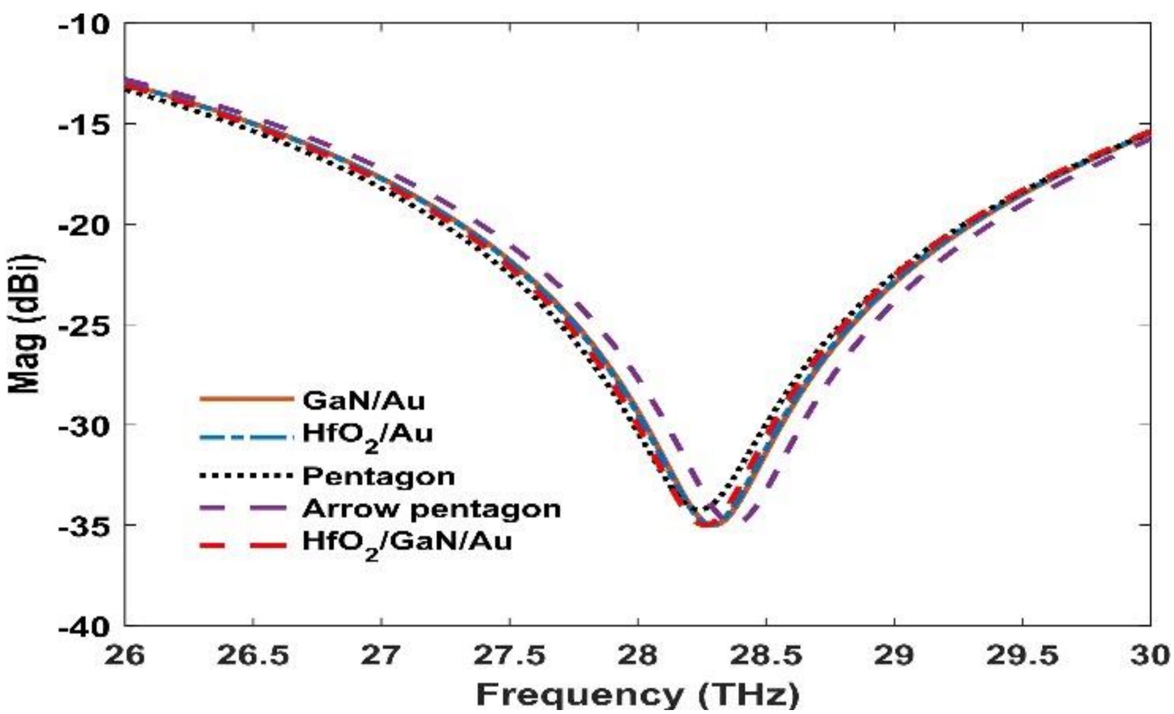

Fig 4.1: S_{11} parameters of the arrow pentagon nanoantenna at 28.3 THz

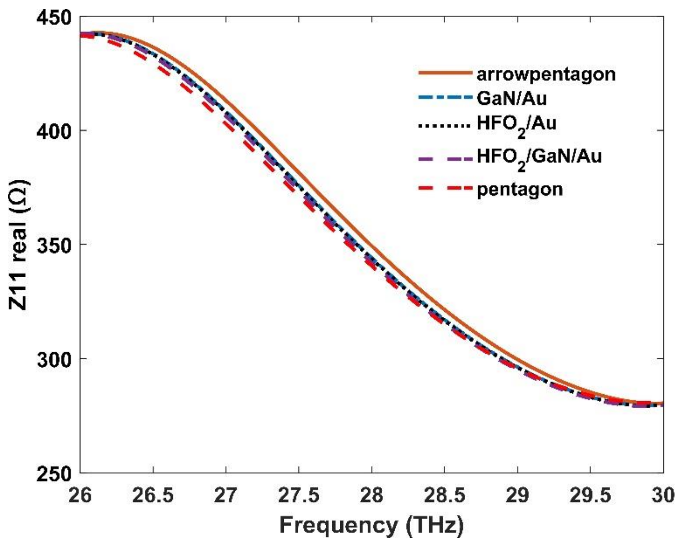

Fig 4.2: Z_{11} (real) of the arrow pentagon nanoantenna at 28.3 THz

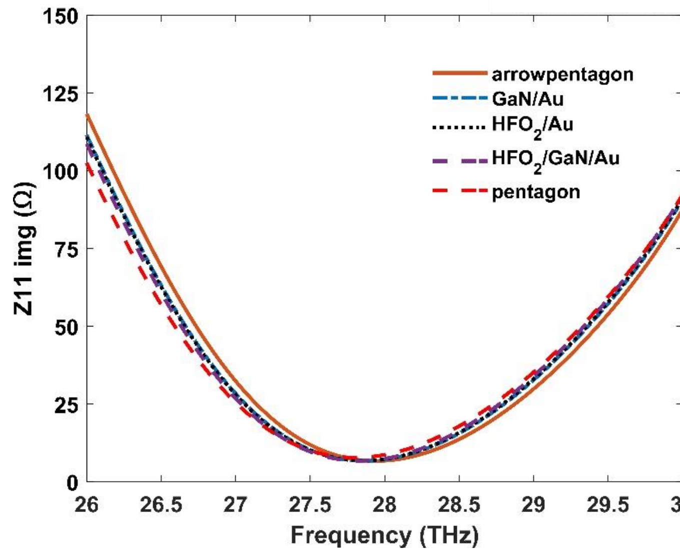

Fig 4.1: Z_{11} (Imaginary) parameters of the arrow pentagon nanoantenna at 28.3 THz

Table 1: Comparison of simulation results of five nanoatennas

Nanoantenna	S_{11}	Z_{11} (real)	Z_{11} (Imaginary)
Pentagon	-34.22	324.55	13.12
Arrow pentagon	-34.94	331.95	9.69
GaN/Au nanoantenna	-35	327.15	11.05
HfO_2/Au nanoantenna	-34.96	326.78	11.23
HfO_2 /GaN/Au nanoantenna	-37.38	325.54	8.66

4. Conclusion

In this study, we conducted a numerical analysis of the electric field enhancement factors for a pentagon-shaped nanoantenna, focusing on the optimization of antenna parameters to achieve maximal field enhancement. A novel arrow-pentagon antenna, derived from the pentagon design, was developed, and the influence of symmetry breaking on field enhancement within the antenna gap was investigated. The electric field enhancement was further improved by incorporating bi-composite structures of GaN/Au and HfO_2/Au, as well as tri-composite structures of HfO_2/GaN/Au. These high-permittivity materials were employed to analyze the behavior of the electric field at a frequency of 28.3 THz. The proposed multilayer antenna demonstrates significant potential for applications in harvesting thermal energy from the environment wirelessly.

Acknowledgments

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