Tuneable Graphene Metamaterial Absorbers: Tailoring Absorption with Fermi Energy

Thesis Submitted in Partial Fulfilment of the Requirements for the Degree of

MASTER OF SCIENCE

in

Physics

by

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CERTIFICATE BY THE SUPERVISOR

Certified that **Jitesh Sachdeva** (2K22/MSCPHY/65) has carried out their search work presented in this thesis entitled **“Tunable Graphene Metamaterial Absorbers: Tailoring Absorption with Fermi Energy”** for the award of Master of Science from Department of Physics, Delhi Technological University, Delhi under my supervision. The thesis embodies results of original work, and studies are carried out by the student himself and the contents of the thesis do not form the basis for the award of any other degree to the candidate or to anybody else from this or any other University/Institution.

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Date:

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I, **Jitesh Sachdeva(2K22/MSCPHY/65)** student of M.Sc physics, hereby certify that the work which is being presented in the thesis entitled **"Tuneable Graphene Metamaterial Absorbers: Tailoring Absorption with Fermi Energy"** in partial fulfilment of the requirement for the award of the degree of Master in Science, submitted in the Department of Applied Physics, Delhi Technological University is an authentic record of my own work carried out during the period from May 2023 to May 2024 under the supervision of Dr. Yogita Kalra.

The matter represented in the thesis has not been submitted by me for the award of any other degree of this or any other institute.

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This is to certify that the student has incorporated all the corrections suggested by the examiner in the thesis and the statement made by the candidate is correct to the best of our knowledge.

ACKNOWLEDGEMENTS

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Abstract

This paper explores the design of graphene-based metamaterial absorbers for electromagnetic waves using a surface conductivity approach. We propose a novel design utilizing circular graphene patches on a substrate with a refractive index of 2.0. We investigate the impact of varying Fermi energies within the graphene on both the absorption properties and the effective surface conductivity of the metamaterial. Our findings demonstrate the ability to achieve tunable absorption characteristics, including narrowband and broadband regimes, by manipulating the Fermi energy of the graphene patches. This research paves the way for the development of graphene-based metamaterial absorbers with tailored absorption properties for various applications.

TABLE OF CONTENTS

List of Figures

Chapter 1
Introduction

1.1 Metamaterials

Ever since, metamaterials have become an area of scientific research in material science because of the control they provide the unprecedented control in determining the interaction of light with matter [1]. Unlike natural materials, whose properties are defined by their atomic composition, metamaterials realize their functionality through the design of micro- and nano-structures. These generally consist of sub-wavelength building blocks, in a periodic or non-repeating pattern, to interact with electromagnetic waves in exceptional ways.

The theoretical basis for metamaterials was set by the work of Veselago in 1967 through his prediction of left-handed materials (LHMs) with a simultaneously negative permittivity and permeability [2]. It became a window that ushered in the possibility of negative refraction, where light bends in the opposite direction of its conventional material. The experimental demonstration of the existence of left-handed materials by Shelby et al. in 2001 actually proved it using microwaves [3].

In optics, they promise to give rise to miniaturized waveguides and super lenses with advanced functionalities [4]. Metamaterials have also been demonstrated to build a cloaking device that guides light waves around an object, without scattering, to make them invisible [5]. This can have vital impacts in the medical field, where sensitive tissues can be protected during diagnostic procedures. More than that, the ability to control light-matter interactions opens up the potential for novel sensors with extraordinary sensitivity, as demonstrated by Liu et al. using metamaterial perfect absorbers [6].

Within the broad field of metamaterial research, this work focuses on. (insert your research area within metamaterials). We contribute to this field by investigating the design, properties, and possible applications of these materials.

1.2 Terahertz Technology

Terahertz Technology is a fascinating region within the electromagnetic spectrum. It lies between Microwaves and visible light. This unique range offers number of advantages in its applications and research fields with immense future possibilities. Although Terahertz radiation is not new in the field of research, it still has great potential and possibilities waiting to be discovered.

1.2.1 Advantages of THz Technology

The leading property of terahertz radiation is its penetrating power. Terahertz waves have relatively lower photon energy, if compared to high energy radiation. This allows terahertz waves to penetrate opaque surfaces without causing any harm to the material, making them perfect for any non-destructive measurement and imaging applications[7]. Additionally, THz spectroscopy takes complete advantage of its position in electromagnetic spectrum. Most of the molecules show resonance with their vibrational and rotational frequencies within the terahertz region. This advantage allows terahertz radiation to paves way for the characterisation technology in characterising specific molecules or group of molecules within the sample. Besides that, because of their shorter wavelength, in contrast to microwaves, terahertz radiation provides a much precise resolution. This allows us to identify even smaller details with the help of terahertz radiation [8][9].

1.2.2 Applications of THz Technology

The unique qualities of terahertz technology allow us to employ this tool in several settings. Out of which security screening stands at the top. Terahertz radiation can penetrate clothes and baggage materials without causing any injury to human skin, making it an efficient tool for security screening. Weapons and illegal substances can be easily detected by terahertz waves without posing any risk to human health, unlike traditional X-rays [9]. Terahertz radiation's non-ionising nature and tissue penetration properties makes it favourable for bio-imaging applications as well. THz technology can even detect early-stage cancers, it can monitor tissue health and even record psychological processes [10]. Additionally, terahertz technology can be used for Material characterisation. It can specifically identify certain molecular behaviours which makes it a useful tool for characterisation purposes. Applications like detection of defects and analysis of crystalline structures is a cherry on the top.

1.2.3 Future Research Possibilities

Even though it's been while since scientists started studying terahertz waves, there are still enormous discovery possibilities waiting to be unlocked in this region. Current focus of researchers regarding THz technology aims towards detectors, enhanced sensitivity, and increased bandwidth. These fields will also allow us to further make improvements in THz spectroscopy infrastructures, which will allow us to better understand the structure of complex molecules and their behaviour. Plasmonic metamaterials has a ton of research possibilities which are incomplete without terahertz radiation. Plasmonic metamaterials also paves the way for light manipulation applications.

1.3 Graphene

Graphene is a monolayer of graphite, made of purely carbon atoms. These atoms are arranged in a honeycomb lattice. Discovery of graphene has turned out to be a gift for researchers for its revolutionary properties. In fact, when merged with terahertz technology, it's synergistic effects are off the charts providing researchers uncountable ideas/possibilities/work areas.

1.3.1 Graphene's Strengths for THz Applications

When it comes to tunability in terahertz technology, graphene stands as the top contestant. Electrical conductivity and carrier density of graphene can be adjusted to an extent just by applying voltage, which allows us to dynamically control how terahertz waves interact with graphene. Graphene also has near zero resistivity or a very high electrical conductivity, even higher than best conductive metals which results in minimal resistive losses, which is one of the must have property when working with terahertz devices. Graphene's thickness also plays a vital role when it comes to the applications. The ultrathin structure of graphene allows us to confine the THz waves into nanoscale dimensions, enabling us to precisely control the propagation of THz waves [11].

1.3.2 Synergistic Effects

Graphene and terahertz technology when combined together unlocks new pathways and revolutionary research ideas. If we look at graphene-based modulators, we can efficiently modulate the phase and intensity of terahertz waves. Graphene modulators if used efficiently, can even encode information onto terahertz waves, allowing us to achieve much higher bandwidths in our communication systems [12]. Additionally, graphene's unique ability to sustain surface plasmons makes it a perfect candidate for the development of very sensitive THz detectors. These detectors can play an important role in a range of applications, including biomolecular sensing and security screening with exceptional sensitivity[13].

1.3.3 Research Frontiers

There is a never-ending list of research possibilities in this domain. Current focus of scientific research is integrating graphene with other materials to enhance their properties even further. So composite materials with graphene is one of the major research frontiers here. In the metamaterial domain, graphene and terahertz radiation walk with hand in hand together. Metamaterials based on graphene can very effectively manipulate terahertz radiation in unconventional ways allowing us to apply the science for applications never imagined before. Additionally, research on microfabrication techniques for graphene-based THz devices is crucial for their miniaturization and integration into practical applications.

1.4 Gadolinium gallium garnet (GGG)

Gadolinium gallium garnet (GGG) is a synthetic crystalline material with chemical formula $Gd_3Ga_5O_{12}$. It belongs to the garnet group of minerals, which are known for their unique crystalline structures and wide range of applications in optics and electronics.

1.4.1 Benefits of GGG

GGG shows high transparency in a broad range of optical wavelengths, from visible to near-infrared regions. This allows it to be an excellent substrate material for optical applications where minimum absorption and light scattering are critical.[14]

GGG, on the other hand, has good thermal conductivity, allowing optical components to maintain their thermal stability and enabling efficient heat dissipation, which prevents thermal damage to sensitive metamaterial structures during device operation.[15]

The GGG lattice constant is compatible with many types of epitaxial layers, including those used in the fabrication of metamaterials. The small lattice mismatch avoids strain and defects in the layers deposited, ensuring high crystalline growth and, hence, optimal optical performance.[16]

Because the intrinsic optical losses are low, GGG can support high-quality factor, Q, optical resonances in metamaterials. This is very important for applications, including filters, sensors, and modulators, where high efficiency and low losses are required.[17]

Chapter 2
Literature Review

Graphene possesses unusually high absorption across a wide range of wavelengths, some of which are optical. This makes it ideally suitable for a large number of optoelectronic applications. Bonaccorso et al. indicate that the reason graphene can absorb 2.3% of incident light across the visible spectrum is its unique electronic structure [18].

One of the major advantages regarding graphene is its tuneable absorbance due to the variation of the Fermi energy. This makes the material very promising for next-generation photodetectors and sensors. Ju et al. demonstrated in their work that the application of a gate voltage can change the optical conductivity of graphene, which changes the absorbance [19].

Graphene-based photodetectors have come a long way because of their broad spectral sensitivity and fast response times. According to Mueller et al., the graphene photodetectors present high responsivity, which can be operated at high speeds, making it feasible for telecommunications and imaging applications. The tuneable nature of graphene's absorbance enhances its functionality in photodetector design [20].

High surface area and functionality make graphene suitable for use in gas and chemical sensors. Schedin et al. in 2007 reported that graphene can detect individual gas molecules by change in electrical conductivity, which is related to absorbance properties. Functionalized graphene will be sensitive to a particular gas in a selective way, enhancing the sensitivity and specificity of the sensor [21].

THz waves have the property of penetrating most non-conducting materials and are being researched for use in non-destructive testing and imaging for applications in various disciplines, such as medical diagnostics, security screening, and industrial inspection. Ferguson and Zhang summarized, in the same paper, that THz imaging can be used for the detection of defects in materials and the identification of chemical substances [22].

THz spectroscopy turns out to be a powerful tool when it comes to molecular spectroscopy as it a very detailed information can be extracted about vibrational and rotational modes of the molecule by using it. Thus, the chemical composition can be clearly obtained from terahertz spectroscopy. Jepsen P. U states that one can identify unique molecular fingerprints using THz spectroscopy and hence use it for chemical and biological sensing [12].

Graphene's high carrier mobility allows it to be used for making efficient THz detectors. The development of sensitive graphene THz detectors at room temperature was shown by Vicarelli et al., showing the capacity of the material for practical THz applications [23].

Graphene supports surface plasmons tunable in the THz frequency range. Ju et al. showed that one can create tunable THz plasmonic devices through nanostructuring graphene, thereby enhancing the interaction between THz waves and the material [10].

GGG has high optical transparency and low optical loss in a wide range of wavelengths, starting from the visible to the near-infrared. This property is absolutely crucial for applications requiring minimal absorption and scattering of light. In the study by Flory et al. (1993), GGG presented good transmission properties, supporting the fabrication of optical devices of high quality. [21]

GGG is a material with high thermal conductivity and a significant melting point, which in total results in its thermal stability. This is important for enabling the devices to exhibit consistent performance levels under changing thermal conditions and prevent thermal damage to sensitive components. The mechanical hardness and stability of GGG provide structural support, ensuring the durability and longevity of the devices built upon it. The study by

Babulanam et al. (1987) pointed out these thermal and mechanical properties of GGG, making the material a good candidate for a substrate material.[22]

The lattice constant of GGG closely matches that of various epitaxial films, for example with yttrium iron garnet (YIG). This close matching reduces lattice mismatch, and therefore defects, in the epitaxial layers. Good epitaxial growth is important for the performance and reliability of advanced optical and electronic devices. An excellent example of this is shown in a paper by Chen et al. 1994, where lattice matching allows high-quality epitaxial growth of thin films on GGG substrates.[23]

GGG shows significant magneto-optical properties because of the gadolinium ions, whose presence in the material gives a very large magneto-optical effect. The property is helpful for applications in Faraday rotators and optical isolators, where light is to be controlled through magnetic fields. The high Verdet constant of GGG enhances its effectiveness in these applications, as highlighted in a study by Hogan (1953). [24]

Chapter 3
Materials, Design and Formulation

We employed COMSOL Multiphysics software to simulate the proposed metamaterial design. The substrate material selected for this study is gadolinium gallium garnet (GGG), within which a graphene sheet is embedded.

3.1 Formulation

In terahertz domain, graphene's properties can be described in terms of its surface conductivity. And surface conductivity further depends on interband and intraband transitions. [1] So,

$$\sigma = \sigma_{\text{inter}} + \sigma_{\text{intra}}$$

$$\sigma_{\text{inter}} = \frac{e^2}{4\hbar}[H(\frac{\omega}{2}) + i\frac{4\omega}{\pi}\int_0^{\infty}\frac{H(\Omega) - H(\frac{\omega}{2})}{\omega^2 - 4\Omega^2}] [1]$$

$$\sigma_{\text{intra}} = \frac{2k_b T e^2}{\pi\hbar^2}\ln(2\cosh\frac{E_F}{2k_b T})\frac{i}{\omega + i\tau^{-1}} [1]$$

Where,

$$H(\Omega) = \frac{\sinh(\frac{\hbar\Omega}{k_B t})}{\cosh(\frac{\hbar\Omega}{k_B t}) + \cosh(\frac{E_F}{k_B T})} [1]$$

T is temperature,

E_F is fermi energy

ω is the frequency of the E.M. wave.

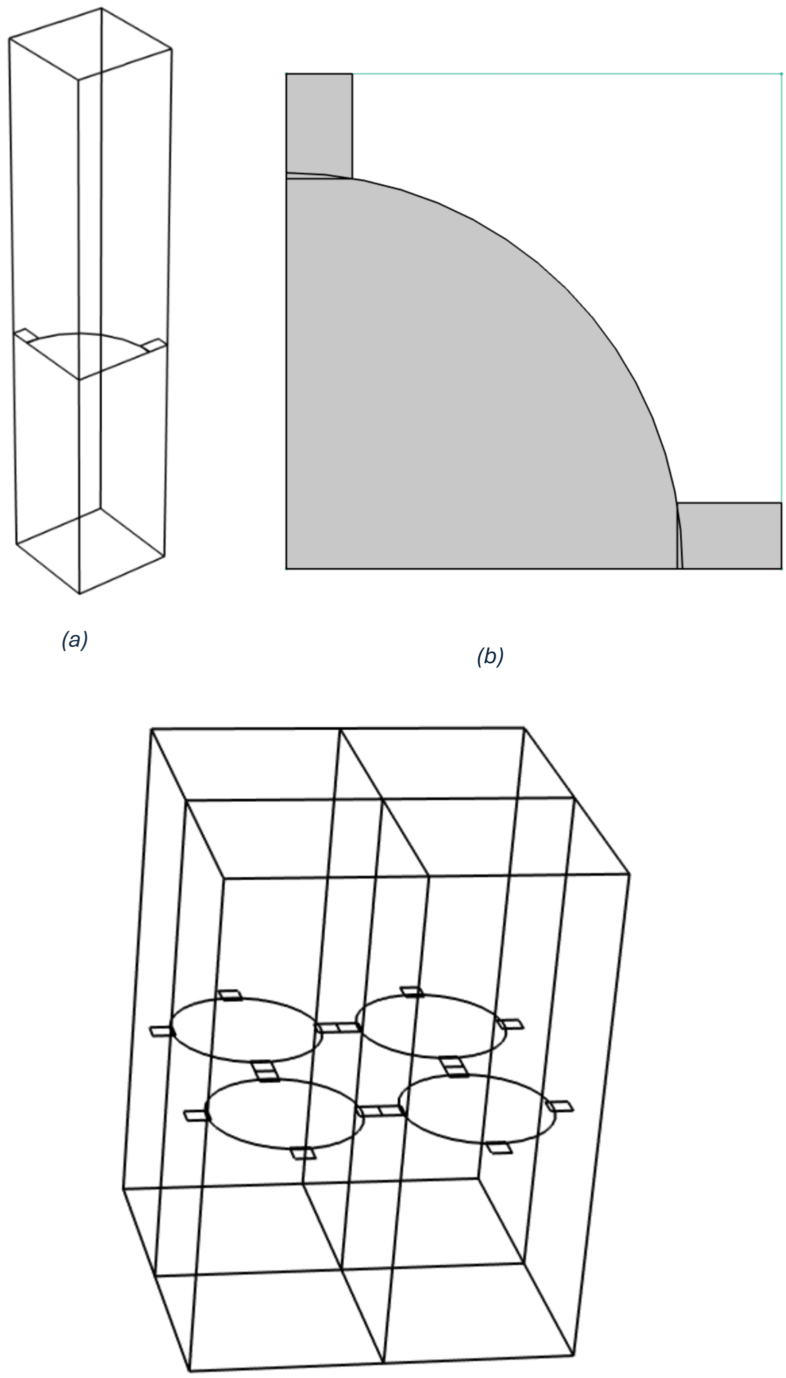
τ is the relaxation time.

3.2 Structure and Dimensions

To ease the simulation process we will make use of mirror symmetry and will only design one-fourth of the unit-cell.

Substrate material used is gadolinium gallium garnet (GGG) with a refractive index of 2. The substrate takes the shape of a cuboid with a square base. Length of the cuboid substrate is 40um with the side of square base being 15um. Relaxation time is $1\times10^{-13}s$.

Graphene sheet embedded is of circular shape with 4 nodes attached to circle after 90° arc distance. Fig 2.1(b) shows the structure of graphene sheet inside unit cell from top view.



(a)

(b)

(c)

Figure 3.1:(a) Structure of one-fourth unit cell used for simulation process. (b) Structure of Graphene sheet embedded inside the substrate. (c) Full visualization of 4 unit cells combined together

The structure of the unit cell is defined by dimensions of 40 µm in height, 15 µm in width, and 15 µm in length. Within this unit cell, a graphene sheet is embedded at a height of 17.6 µm. The graphene sheet features a circular segment with a radius of 6 µm, and rectangular nodes with a length of 2 µm and a breadth of 1.584 µm. The remaining volume of the unit cell, excluding the graphene sheet, consists of the substrate material, gadolinium gallium garnet (GGG).

Given the application of mirror symmetry in our design, only one-fourth of the unit cell needs to be modeled. Consequently, the dimensions used for simulations are adjusted as follows: the radius of the quadrant is 6 µm, the length of the rectangular node is 1.584 µm, and the breadth of the node is 1 µm.

Chapter 4
Results and Discussion

This simulation was conducted to study the absorbance and conductivity of graphene sheet embedded in gadolinium gallium garnet (GGG), with focus on the effect of varying fermi energy in terahertz region of optical frequency.

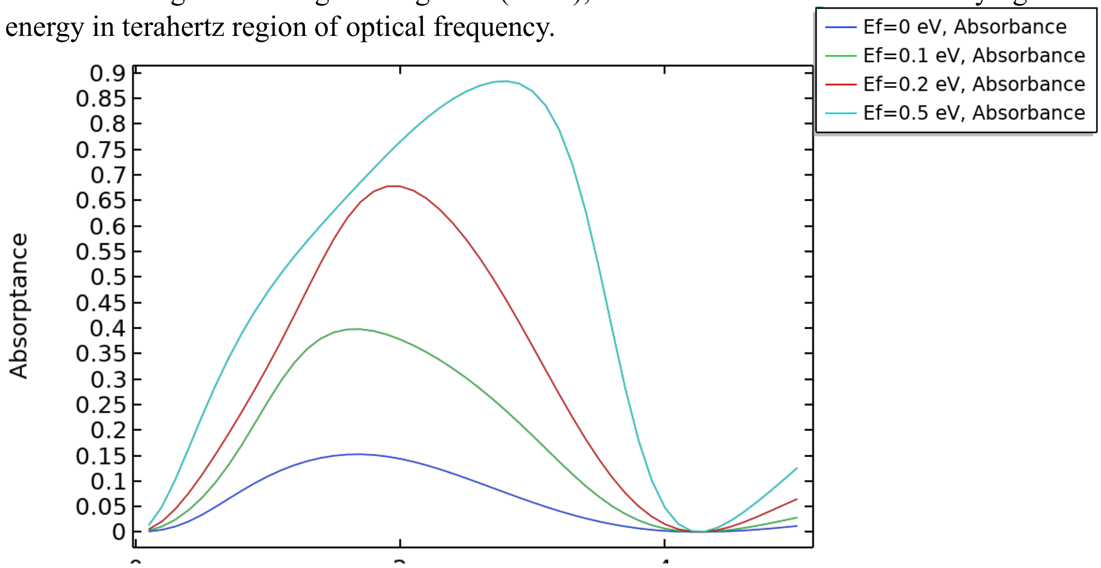


Figure 4.1: Absorbance of Graphene sheet with GGG as substrate and varying frequency at different fermi energies

4.1 Absorbance Traits

4.1.1 Absorbance Dependence on Fermi energy

From the obtained results (Fig: 3.1) we can observe that,

When fermi energy is 0eV(blue line), absorbance of graphene peaks between 0.1 to 0.15. When fermi energy is 0.1eV(green line), absorbance of graphene peaks between 0.35 to 0.4. When fermi energy is 0.2eV(red line), absorbance of graphene peaks between 0.65 to 0.7. When fermi energy is 0.5eV(cyan line), absorbance of graphene peaks between 0.85 to 0.9.

In general the trait that can be clearly observed here is, that with the increase in fermi energy, absrobance increases significantly. Also, with the increase in fermi energy, the peak shifts towards higher frequency spectrum (towards right).

4.1.2 Absorbance Dependence on Frequency.

As it can be observed in figure 3.1, absorbance increases with frequency for all cases till about 1.5 terahertz and and falls back to 0 after peaking a certain value. The peaks shifts slightly towards right with increase in ferrmi energy.

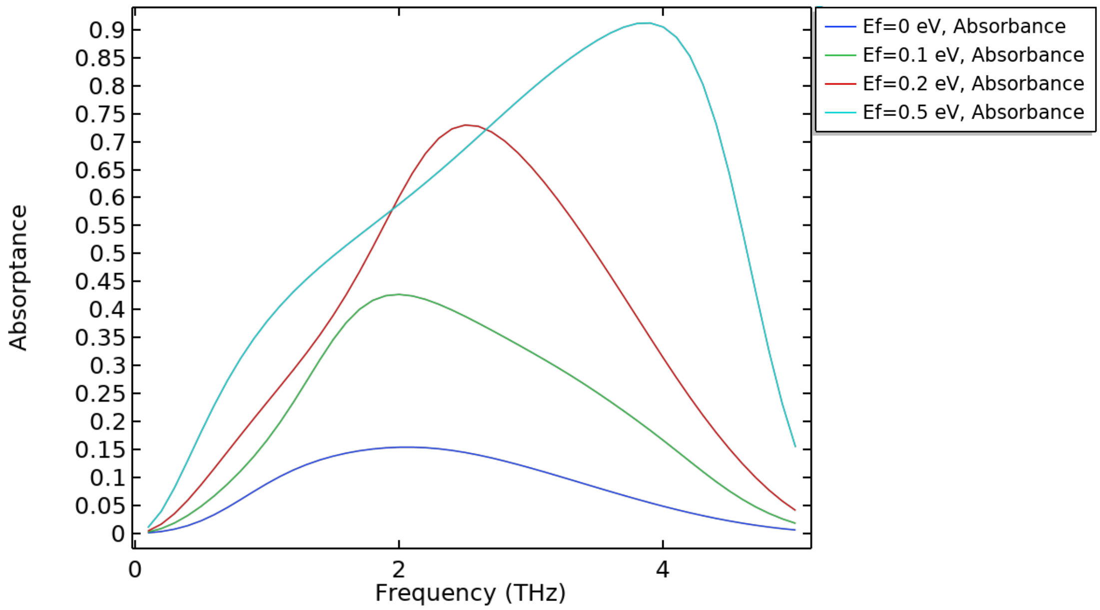


Figure 4.2: Absorbance of Graphene sheet with substrate of refractive index 1.53 and varying frequency at different fermi energies

4.1.3 Absorbance Dependence on Refractive index of the substrate.

It can be observed from figure 4.2 that if we tend choose a substrate with lower refractive index, or in another words if we decrease the refractive index of background material in our simulation, we observe a shift in the peaks towards right i.e., peaks are now attained at a higher frequency value. Similarly if we increase the refractive index of our substrate, the trait that can be observed is, the graph of absorbance slighlty compreses towards left with peaks also shifting towards lower frequencies.

Hence a tunable graphene based absorber metamaterial in terahertz spectrum is attained, which can be tailored further by varying its fermi energy.

4.2 Conductivity Traits

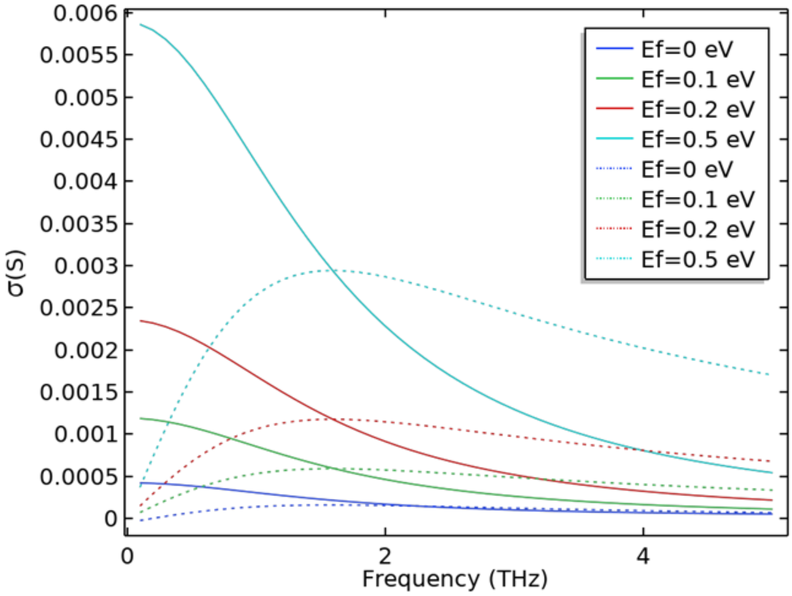


Figure 4.3: Conductivity of Graphene sheet vs Frequency at different fermi energies. Solid line: Real part, Dotted line: Imaginary part

From the results we can clearly observe that both real and imaginary parts of conductivty increases with increase in fermi energy. Thus conductivity of graphene which already surpases even the best conducting metals can be enhanced further by increasing it's fermi energy. Furthermore, the peaks of both real and imaginary part of conductivty rises with increase in fermi energy. Which also indicated that at higher fermi energy levels graphene can support higher frequency conductive modes.

The increase in magnitude of both real and imaginary parts of the conductivity with fermi energy suggests that there is an increase of carrier density within the sheet which had an enhanced interaction with terahertz radiation.

Chapter 5
Future Scope

Further development of graphene-based THz detectors, sensitivity and response time can be the subject of research. Devices with improved performance may result from investigating novel graphene heterostructures, such as graphene combined with other two-dimensional materials.

The bandwidth and data transmission capabilities of current and upcoming 5G networks can be improved by combining graphene-based THz components. Techniques for effortless integration and graphene device tuning for telecom infrastructure can be the subject of future research.

The combination of graphene and THz technology enables new breakthroughs for imaging and sensing. Graphene-based THz detectors have revealed the potential for room-temperature operation and high sensitivity, which is very important for medical imaging, security screening, and non-destructive testing. Efficient THz radiation generation and detection may, in turn, bring about new diagnostics and improved imaging capabilities.

Graphene's electronic properties are tunable, which allows one to develop ultrahigh-sensitive THz-spectroscopy tools and use them for a variety of material characterization and chemical analysis in samples, which can even be employed for monitoring the environment. The high spectral resolution achievable with graphene-based THz devices could significantly improve the detection and identification of chemical and biological substances.

It is foreseen that some of the mentioned unique properties of graphene at THz frequencies will be useful for quantum computing applications. For the purposes of qubit manipulation and the execution of quantum operations with high precision, THz graphene plasmonics could be a very useful element. Research is in progress for the development of graphene-based THz quantum gates and circuits; they could contribute to the advancement of quantum computing technologies.

The combination of graphene's biocompatibility and electrical properties promotes the use of graphene in biomedicine, for both THz biosensing and medical diagnostics. Being non-ionizing, THz radiation can effectively penetrate most common materials, making it the primary region for monitoring biological tissues. Based on graphene, new techniques for diagnostics and new stages in the detection and treatment of disease could be expected from THz devices.

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Co-Authors:	Ankush Dewan, Yogita Kalra

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