Major Project
Report

STUDY OF SCATTERING BY LINEAR CHAIN OF CYLINDRICAL NANOPARTICLES

Submitted in partial fulfillment of

the requirements for the award of the degree of

Master of Technology

Nano Science and Technology

Submitted by
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(2K15/NST/09)

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Contents

LIST OF FIGURES

CERTIFICATE

This is to certify that the work which is being presented in the report entitled **‘Study of Scattering by linear chain of cylindrical nanoparticles’** submitted by SONAM DOGRA (2K15/NST/09) student of second year M. Tech in the DEPARTMENT OF APPLIED PHYSICS AND with specialization in NANO SCIENCE AND TECHNOLOGY is a record of students work carried out by him under my guidance and supervision during the year 2016-17.

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DECLARATION

I hereby declare that all the information in this document has been obtained and presented in accordance with the academic rules and ethnic conduct. This report is my own, unaided work. I have fully cited and referenced all material and results that are not original to this work. It is being submitted for the degree of Master of Technology in Engineering at Delhi Technological University. It has not been submitted before for any degree or examination in any other university.

(SONAM DOGRA)

ABSTRACT

Optical nanoantennas for visible and infrared radiation can strongly enhance the interaction of light nanoscale matter by their ability to efficiently link propagating and spatially localized optical fields. This ability unlocks an enormous potential for applications ranging from nanoscale optical microscopy and spectroscopy over solar energy conversion, integrated optical nanocircuitry, opto-electronics and density of states engineering to ultra-sensing as well as enhancement of optical nonlinearities. Thus the useful results prompt us to implement a more systematic and further exploration on nanoantennas of some specific configuration of interest. This dissertation is the study of various works in the field of optical nanoantennas, thereafter design and analyze optical nanoantennas.

The focus of this thesis is to put on the investigations of single and multiple dielectric nanoparticles for their near-field and far-field radiation properties. In particular, we elaborately design and carefully analyze such structures to perform their functions as the nanoantennas operating in the optical regime. The Generalized Kerker's conditions are studied in detail to understand scattering of light by nanoparticles of various shapes and sizes.

A study on the accurate behavior of single dielectric nanoparticles is done as to how the scattering of incident field by the nanoparticle enables it to exhibit unidirectional scattering at wavelengths where first and second Generalized Kerker's conditions are fulfilled.

An appropriate numerical approach with the use of FEM is developed for a more effective calculation of nanoantennas covering the broad frequency range including visible and infrared region. Comprehensive investigations are carried out and presented in detail on various factors which have significant impacts on the nanoantenna's performance in the optical region. The software used is COMSOL MULTIPHYSICS whose operation is dependent on the finite element analysis method. The software calculates scattering cross section, far-field pattern and directivity for the optical nanoantenna MATLAB is also used for mathematical computation as and when required.

ACKNOWLEDGEMENT

I take this opportunity to express my gratitude and thanks to the respected Assistant Professor of DTU formerly DCE, Dr. Ajeet Kumar for his valuable technical suggestions and constant encouragement. This project would not have been completed successfully without the patient, insightful and able guidance of my mentor. I greatly appreciate the words of encouragement. I am highly indebted to him for allowing me to carry out my project in computational lab.

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(SONAM DOGRA)

CHAPTER-1

INTRODUCTION

1.1 THESIS MOTIVATION AND APPROACH

Electrical engineers during twentieth century developed radio and electronic antenna to direct electrical signals. Electrical connection can be established between the radio receiver/transmitter with the help of RF antenna. On the other hand, to direct free propagating optical radiations, optical nanoantenna is used. Optical nanoantennas are classified into two types-dielectric nanoantenna and plasmonic nanoantenna. High losses and absorption effects of plasmonic nanoantennas posed limitations on their use. High permittivity dielectric nanoantennas support both magnetic and electric modes of resonance, have low losses at optical frequencies and show sharp resonances. These features make the dielectric nanoantennas beneficial over plasmonic nanoantennas. In this discourse, a chain of dielectric cylindrical nanoparticle is being designed. The nanoparticle chain supports forward scattering which makes it a promising candidate for futuristic nanophotonic applications. Forward scattering is observed where generalized kerker's conditions are satisfied. Scattering cross-sections are calculated by Finite Element Method in COMSOL MULTIPHYSICS software. Influence of the orientation of nanoparticle chain and increasing number of chain elements is being studied.

1.2 OBJECTIVE

Below given are the main objectives of this discourse:

- To study the basics of optical nanoantennas, their features, applications, history and recent developments.
- To learn a new method called the Finite Element Method for scattering cross-section calculations.
- To learn the implementation of designs in COMSOL multiphysics software.
- To study the designing and modeling of a new nano-structure i.e. all-dielectric cylindrical nanoparticle chain.

- To study the impact of orientation of the nanoparticle chain along different axis, on the scattering behavior of electromagnetic field.
- To study the influence of increasing number of chain elements on the scattering properties.

1.3 THESIS ORGANIZATION

The remaining thesis is organized as below:

Chapter 2 includes the literature survey of the research papers studied during the course of the project. It discusses in detail about the nanoantennas, their applications like spectroscopy, spasers, superemitters, microscopy etc., the two types of nanoantennas i.e. plasmonic nanoantennas and dielectric nanoantennas in detail.

Chapter 3 includes the calculational method and the software used. Finite element method being used is explained in detail and discusses about COMSOL multiphysics and MATLAB.

Chapter 4 discusses about the designing of cylindrical nanoparticle. Calculation of scattering cross-section with the help of the equations involved in the software. The evaluation of wavelength where kerker's first condition is satisfied and also the wavelengths where electric and magnetic dipoles are being created.

Chapter 5 includes the designing of the linear chain of cylindrical nanoparticles and also the analysis of the far field plots for a chain of 3 nanoparticles. Analysis of the directivity and far field plots when the orientation of the chain is varied along different directions.

Chapter 6 includes the final conclusions and results obtained from the previous analysis and the future scope involved with the design being created in the field of nanophototnics and nanoantennas.

CHAPTER-2

OPTICAL NANOANTENNA

The wavefront of the incident radiation of light can be controlled and directed by the use of mirrors, diffraction elements and lenses. This type of operation makes use of the wave nature of electromagnetic fields and hence for manipulation at subwavelength scale, this is not responsive.

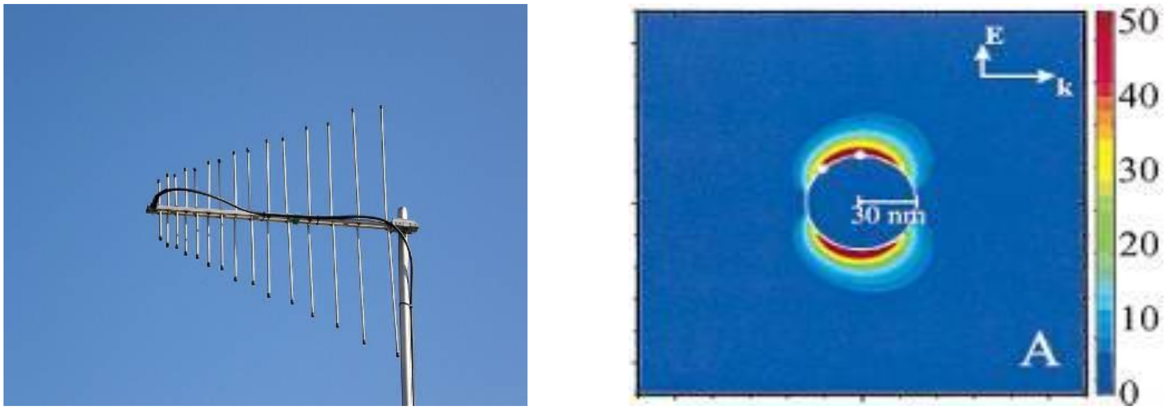


Figure 1: Example of RF antenna (left, of dimensions of several centimeters) and optical antenna (right, 60 nm Ag nano-sphere resonant at 369 nm)

Antennas are an important elements in devices like radios, television etc which make use of electromagnetic waves at microwave and radiowave spectrum. Optical nanoantennas have been a topic of great interest in many applications from near-field microscopy to molecular and biomedical sensors, optical communication, solar cells and optical tweezers [1-7]. In light emitting devices, electron and hole combine to release a photon. On the other hand, just the reverse process takes place in photovoltaics. Optical antennas can help in increasing the absorption efficiency in photovoltaics and efficient release of energy in light emitting devices.

The characteristic dimensions of an optical antenna are of the order of wavelength of light and hence their fabrication requires accuracy upto 10 nm. Fabrication in such a small scale can be done in nanoscience and nanotechnology using top-down or bottom-up method. Top-down methods include ball milling [11, 12], electron beam lithography [13, 14] etc. whereas bottom-up methods include sol-gel technique, atomic layer deposition etc. At nano-scale, size related properties come into picture. These give rise to various challenges against nano-scale fabrication. Although, optical antennas can be widely applicable but the fabrication issues make them non-existent till date.

The development of the antenna concept initially started with the works of Edward Synge [8] in the year 1928. He localized optical radiations on a sample surface by colloidal gold particles. Later, in 1985 John Wessel [9] suggested for the first time that gold particle can work as an antenna. However, it was only in 1995 that the proposed idea was demonstrated experimentally by Dieter Pohl and Ulrich Fischer [10]. Many studies then were carried out by various other researchers and developed optical antennas of various shapes and sizes.

2.1 OPTICAL ANTENNA

Antennas are crucial elements of modern day communication systems. They act as transducers between localized fields and freely propagating radiations [15]. Antennas are the elements which convert propagating fields to electric currents and vice versa. Nano optics is a branch of physics that deals with control and manipulation of optical signals by some specifically designed nanostructures. In nano optics, radiations should be efficiently directed and transmitted between the nano elements. These nano elements can be transmitters or receivers. They can be of various shapes i.e. cylindrical, conical, cuboidal etc. They can be single nano object or their clusters.Optical antenna, analogous to its radiowave and microwave counterparts, is a device that can effectively convert freely propagating optical radiations to localized energy at subwavelength scales. Optical antennas work at higher frequencies as compared to their radiowave counterpart and hence their characteristic size is very small (down to few nanometers). Small size poses many challenges towards their fabrication.

Efficiency and directivity are the two characteristic features of an antenna. Efficiency is defined as the transfer of currents to freely propagating waves or vice versa. On the other hand, directivity is defined as concentrating the electromagnetic energy in desirable regions of space and blocking the coupling of these radiations in undesirable regions of space. Both, a high efficiency and a high directivity are achieved by optimizing spatial distribution of currents.

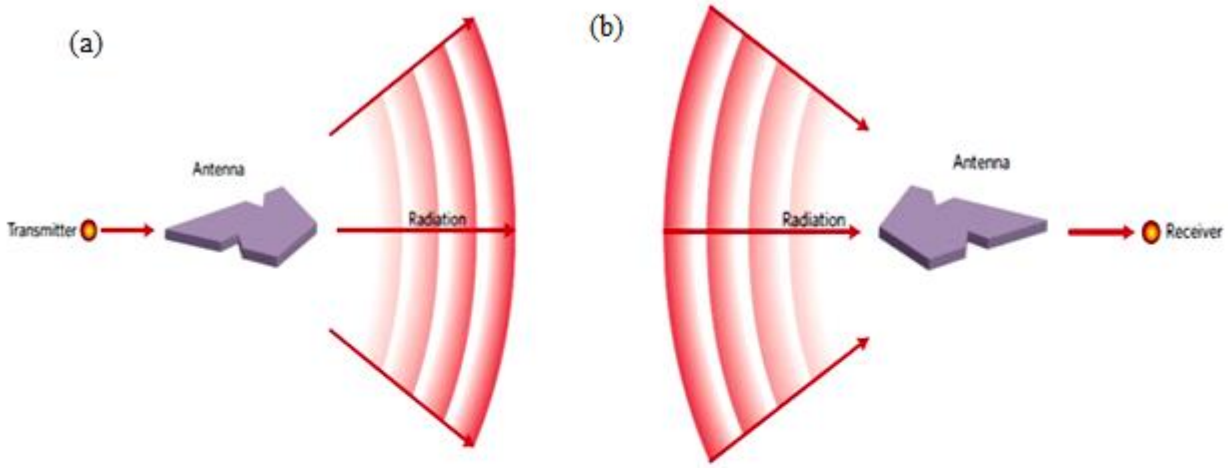


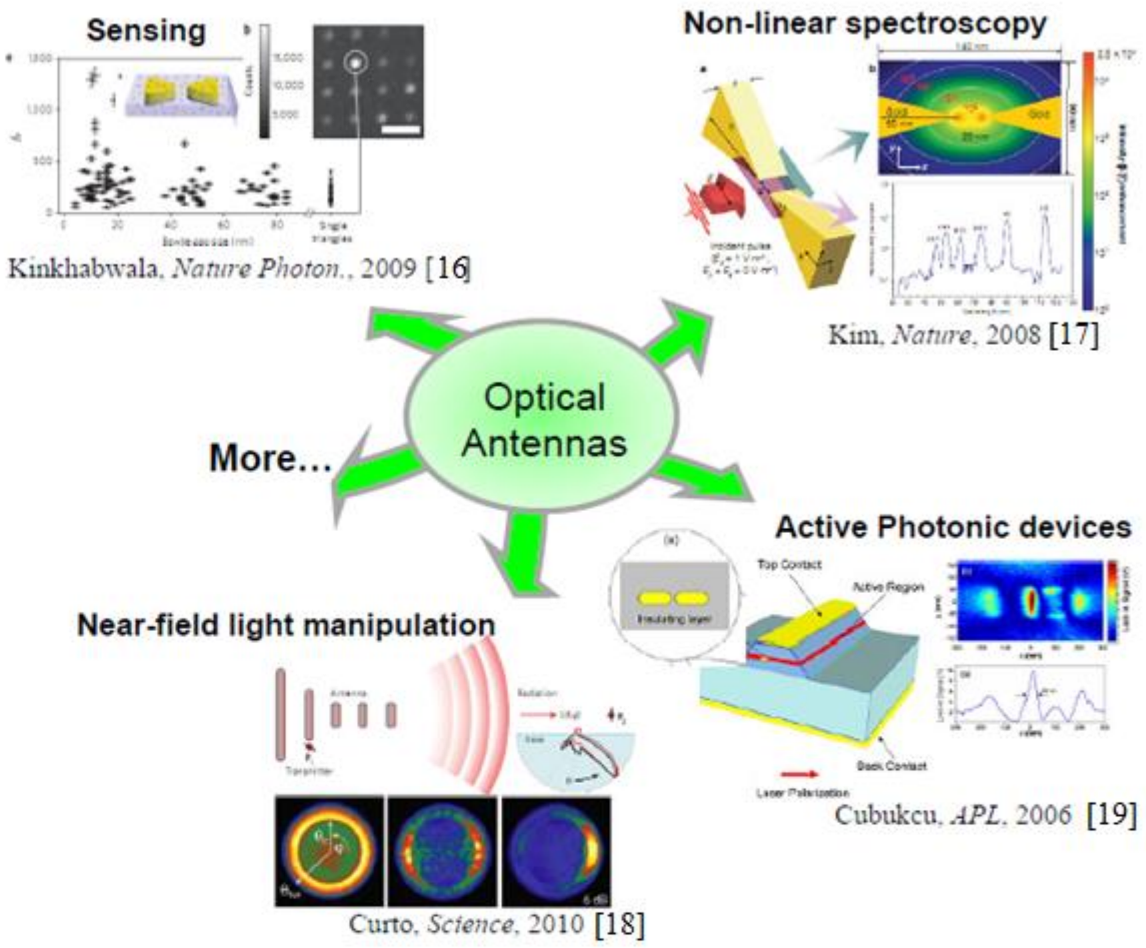
Figure 2: Optical antenna (a) transmitter antenna (b) receiver antenna. Each antenna can be used as a transmitter or receiver antenna simultaneously. [3]

Optical nanoantennas can be of receiving type or radiating type. Receiving nanoantennas are those which convert freely propagating fields into near fields. On the other hand, those nanoantennas which convert near fields to freely propagating fields are called transmitting type. In microwave antenna, waveguide is used to deliver energy. Whereas in case of optical nanoantennas, due to their sufficiently small size, plasmonic-waveguides are used. Plasmonic waveguides are used because of their ability to achieve subwavelength scale confinement and relatively long propagation. They can transform waveguide modes to freely propagating radiations in transmitting nanoantennas. Receiving nanoantennas transform freely propagating radiations to waveguide modes or they can transform optical radiations to strongly confined fields.

Optical nano antennas are broadly of two types – plasmonic nano antennas and dielectric nano antennas. Plasmonic nanoantennas are made of metal nanoparticles, usually Gold and Silver. Some of the examples of plasmonic nanoantennas are dipole nanoantenna, bowtie nanoantenna, yagi uda type nanoantenna etc. The study of nanoantenna started with their fabrication using metals which support plasmonic resonances.

2.2 APPLICATIONS OF OPTICAL NANOANTENNAS

Nanoantennas are promising area of research in the newly emerged field of science called nano-optics due to their ability to bridge the size and impedence mismatch between nano-emitters and freely propagating radiations. They also can also manipulate light on a scale smaller than the wavelength of the incident radiations or sub-wavelength scale. Presently, nanoantennas are used in near field microscopy and high resolution biomedical sensors. In the near future, with the development in nano-optics, nanoantennas will find applications in solar cells, biomedical and molecular sensors, optical tweezers etc.



Sensing

Kinkhabwala, *Nature Photon.*, 2009 [16]

Non-linear spectroscopy

Kim, *Nature*, 2008 [17]

Active Photonic devices

Cubukcu, *APL*, 2006 [19]

Near-field light manipulation

Curto, *Science*, 2010 [18]

Figure 3: The research in optical nanoantenna is driven by wide range of applications. Some of these are shown in this figure.

Research in the field of optical antennas has variety of possible applications that have great advantages to enhanced light-matter interaction. Till now most of the applications have been discussed in reviews of plasmonics and optical antennas [20-24]. Optical nanoantennas have a vast number of nanophotonic applications. In this section we will highlight the some important nanoantenna applications.

i. SCANNING NEAR-FIELD OPTICAL MICROSCOPY:

Topography and optical properties like fluorescence can be measured by near field optical microscopy methods. Various nanoscale imaging tools include microscopic methods such as scanning probe microscope, electron microscope etc. For image of materials having size below 100 nm, optical microscopes are not well suited due to limitations posed by large probe apertures (nearly three times the size of the material to be imaged). To overcome this problem, optical nanoantenna can be used. Nanoantenna needs to be fabricated on the tip of the scanning probe to achieve very high resolution imaging. Here the resonance of the antenna is driven by the localized field of small aperture. By the use of bowtie antenna [25] and $\lambda/4$ [26] antenna, single molecule images of resolution nearly 25 nm (in the latter case) has been achieved. Many experiments have been carried out under this area. Highly controlled probes were manufactured by attaching single or multiple gold nanosphere to the dielectric tip of the optical fiber near-field probe. Such probes can produce images of single molecules of resolution less than the sphere diameter. Using these probes, high resolution images of proteins in their native cells have also been achieved [3, 27, 28].

ii. SPECTROSCOPY

Spectroscopy is the field of science which deals with the measurement of spectra when matter interacts with the electromagnetic radiations or emits it. With the application of nanoantenna, highly enhanced and efficient spectroscopy can be achieved. During spectroscopy process where some nano-object is investigated, nanoantenna is used to enhance both the emission and excitation. Surface enhanced spectroscopy [29] and tip enhanced spectroscopy [30, 31] are the traditionally developed techniques for measurement of light- matter interaction. The Raman scattering involves the absorption and emission of photons which are nearly identical in energy. The total scattering enhancement is usually proportional to the fourth power of the field enhancement. Many developments have been done in these techniques so far since 1970's. Metallic nanostructures are capable of enhancing the local electric field and hence increase the interactions between incident light and specimen placed in its immediacy. Various studies have shown the localization of electric field by single nanoantenna structures but arrays of nanoantennas can even work more efficiently in detecting signals very easily in the far-field. This is caused by various short and long range interactions occurring between the neighboring nanoantennas which lead to changing of resonance characteristics of the array. By moving from isolated nanoantenna to arrays of nanoantenna which are coupled end-to-end through nanogap, it is possible to increase the localization of the electric field even further in these gaps. [32]

iii. SUPEREMITTER :

Light emission, detection and amplification at few photon levels is an interesting area of research in the field of quantum and classical information technology. Optically resonant antenna structures also find a key application in the experimental studies of single emitters coupled to optical antennas. Single photon nanoantenna represents a combination of a quantum system and a nano structure. The nanoantenna is placed in the near field of the fluorescent quantum system. Emission and absorption of precisely single photon at a time can ensured by the quantum system whereas the nano structure ensures the manipulation of the coupling of the emitter to the far-field radiation channels [3, 33]. Nanoantenna based single photon superemitters are envisioned as a structure to control emission, detection and amplification of light at the level of one or more photons at a time. This manipulation of light to be achieved at submicron length scales and subpicosecond time scales. In order to strongly enhance the light-matter interactions, the nanoantenna in the vicinity of the emitter, modify the electromagnetic mode structure around the emitter itself. Emitter placed in the 'hot spot' of the resonant antenna is the source of creation of single plasmons in the resonant mode of the antenna instead of the creation of freely propagating photons. These plasmons are radiatively decayed to produce photons that have the properties of the antenna resonance e.g. its emission spectrum, resonance spectrum, polarization etc.

iv. OPTICAL TWEEZING :

Optical tweezers are the instruments that use light to manipulate microscopic objects as small as a single atom [34]. More recently, it has been demonstrated experimentally that the optical trapping in well-controlled hot spots in the gap of nanoantennas. The large antenna field enhancement allows trapping with lower excitation power and higher efficiency and stability [35, 36]. The momentum associated with light or electromagnetic radiations is linear in nature. The transfer of this momentum to an object leads to the production of forces which are radiative in occurrence. This theory acted as the basic for the design of optical tweezers by the scientist named Arthur Ashkin. He invented optical manipulation technique on microscopic level. Conventional optical tweezers consisted of microscopic objectives or optical lens. These were based on far-field technique and the confinement of light is limited due to diffraction. With the application of nanoantennas in the field of optical tweezing, the limitations imposed by diffraction can be eliminated [48, 49]. Nanoplasmonics and optical tweezing combined to formulate the idea of plasmonic optical tweezers. Unlike optical tweezers which work in the range of microns, plasmonic optical tweezers extends the particle trapping range down to nanometers. For capturing and detection of biomaterials like viruses and vesicles, plasmonic optical tweezers integrated with lab-on-a-chip is a promising technique [50].

v. PHOTOVOLTAICS :

Growing demand for energy and limited resources have resulted in the search of alternative methods for the production of energy in order to meet the growing need. With the purpose of reducing environment degradation and cut on costs of energy, researches have been involved in using sun as the source of energy. ‘Photo’ means light and ‘voltaic’ means voltage, so photovoltaics are the devices which are used to convert light energy to electrical energy. Among the alternatives for generation of energy, solar cells are the ones that have the capability to use sun’s heat energy to generate electrical currents. Less efficiency, complex structures and high costs are the limiting factors for their use. Practically, an isolated solar cell is nearly 20% efficient and a multijunction solar cell is nearly 30% efficient. With the application of nanoantenna in this field, the absorption efficiency can be increased to nearly 85%, which is many times higher. Another advantage of using nanoantennas is that these devices can then be engineered to absorb any frequency of light. The resonant frequency of the nanoantenna can be engineered to absorb a specific wavelength of light by changing the size of the nanoantenna in the array. Plasmonic photovoltaics is one of the most recent fields in nanophotonics which can confined incident radiation in subwavelength range [51]. Standard solar cells are combined with metallic nanostructures, which concentrate and guide light at the nanoscale, leading to a reduction of the semiconductor thickness required, as well as enhancing the broadband absorption of the incident light, which is one of the crucial challenges to modern solar cell technologies [52].

vi. OPTICAL SENSORS :

At visible frequency range, some metals specifically gold and silver, show plasmonic properties. When these materials interact with visible light, group of electrons start vibrating perpendicular to the surface of the material. This creates a wave of oscillating electrons called plasmons. Size of nanoantenna, dielectric material in the vicinity of nanoantenna and nanoantenna material are the factors affecting the wavelength of plasmon oscillatons. In sensing applications, the molecules of material to be sensed get adsorbed near the nanoantenna and cause a shift in the resonant frequency peak. This is how nanoantenna sensors work by showing the resonant frequency peak change. Nanoantenna finds application in biological sensing, chemical gas sensing etc with efficiencies increasing multiple times. Many plasmonic sensors were demonstrated in past for example, sensing based on particle arrays on a fiber facet [39] or on a substrate [40] with sensitivities down to the single-particle level [41, 42]. Mona zaghloul et.al showed a shift of 12 nm in the resonant peak of grapheme covered plasmonic nanoantenna when exposed to sense water vapors [43]

vii. LASING :

Laser is a device that radiates coherent light or other electromagnetic radiation by the emission of photons. A plasmonic nanoantenna implemented to these lasers is known as ‘SPASER’. Spaser is a device that produce stimulated emission of plasmons. Pumping efficiency and intrinsic losses in cavity are the two factors influencing lasing threshold in conventional lasers. Nanoantenna size and geometry can be engineered to resonate at pumping wavelength, emission wavelength or both [44, 45]. Nanoantenna arrays of such particles can efficiently increase absorption, field enhancement [46] and can also tailor the electromagnetic radiations in well defined patterns [47]. Nanoantenna structure combined with a nanocavity can efficiently refuel pumping energy in nanocavity.

viii. PLASMONIC CIRCUITS :

Semiconductor and microelectronic are the two technologies for circuit designing. Both these technologies face serious problems of speed and data transmission rates. With the advancement in the field of nano-optics, these problems can be eliminated. If the electrons in circuits can be replaced by light then speed of operation of the circuits can be significantly increased. Surface plasmons are of two types- localized type and propagating type. Propagating surface plasmon polaritons can be considered for nanophotonic circuits and data transmission. Photonic devices of size smaller than the wavelength of light suffer through limitations of diffraction in fabrication processes. Plasmonic nanoantennas have an advantage due to presence of surface plasmon polaritons which surpass this diffraction limitation. Different metallic nanoparticle structures such as grooves [53], chains [56-59], sharp metal wedges [54], metal slits [55] etc have been designed for guiding these propagating type plasmons to nanophotonic circuits.

ix. THERMAL FIELDS :

Thermally active fields can be easily created by the use of metallic nanoantennas, also called plasmonic nanoantennas. Metallic nanoantennas support localized surface plasmon resonance. Due to this phenomenon local heating of nanoantennas occur. Metals undergo considerable amount of ohmic losses when subjected to radiations of high or optical frequencies. Although, this is considered as a drawback and is the reason behind widespread use of dielectric nanoantennas but in some areas of science, this turns into dramatic advantage. This localized heating plays a vital role in many areas like vapor generation [60, 61], cancer treatment [62], catalysis [63-65], nano-fabrication [66, 67] and nano-manipulation [68,69] etc. metallic nanoantennas can act as nanolocalised sources of thermal energy which can be switched on or off easily by employing low power optical means. Studies show that vapors can be generated by employing the thermal field of the metallic nanoantenna. For instance, Au nanoparticle was studied by Fang Z [60] to demonstrate the formation of nanobubble around the nanoparticle when it is illuminated by resonant light of sufficient intensity. By varying the size of the nanoantenna, microsized bubbles can be achieved and hence light induced vapor generation is possible by implementing the theory of heating caused by surface plasmon resonance in metallic nanoantennas.

2.3 TYPES OF OPTICAL NANOANTENNA :

Optical nanoantennas are broadly of two types and that are (1) metallic nanoantennas and (2) dielectric nanoantennas. Metallic nanoantennas are fabricated by metallic nanoparticles and support surface plasmon resonances. They are also known as plasmonic nanoantennas. On the other hand, dielectric nanoantennas are fabricated by semiconductor material of very high permittivity. Although, plasmonic nanoantennas suffer from various drawbacks such as considerable losses at optical frequencies but they find applications in various fields of science as well. In this section, both types of the nanoantennas are discussed in detail.

2.3.1 METALLIC NANOANTENNA :

The research started in 1928 when a scientist named Richard Hutchinson synge for the first time suggested the use of metallic nanoparticles for confinement of optical field. Later, in 1985 John wessel explained the use of monopoles as nanoantenna. He suggested that a monopole can overcome the diffraction limits and tune the resolving power up to 1 nm. In these nanoantennas, the excitation of surface plasmon resonances of different order occur which cause the confinement of optical fields in their vicinity.

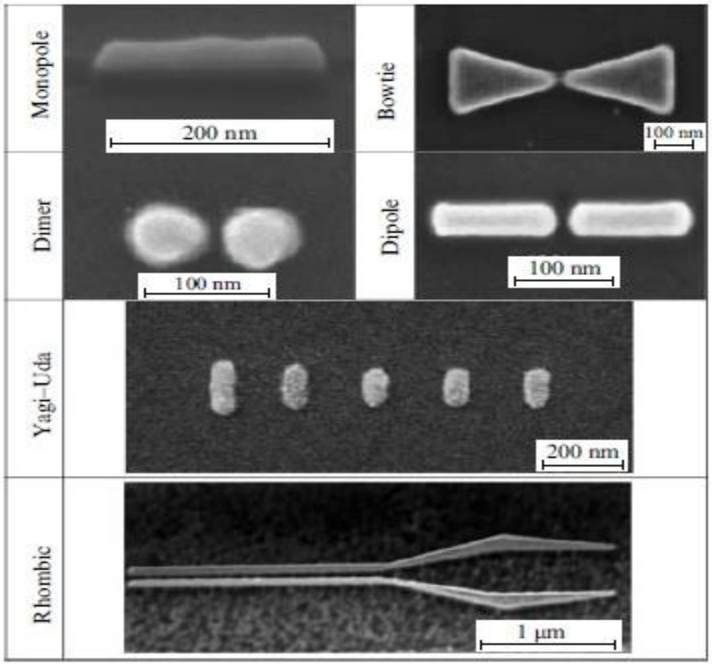


Figure 4: various types of plasmonic nanoantennas. [70]

Metallic nanoparticles confine electromagnetic radiations (incident on them) in their vicinity. Later, it was observed that the magnitude of strength of the confined electromagnetic field is higher in the gap between two or more plasmonic nanoparticles as compared to single elongated nanoparticle. This happened because the confinement in case of two or more plasmonic nanoparticles occurs at a smaller spatial scale. There are many types of plasmonic nanoantennas e.g. monopole , dipole, bowtie, yagi-uda etc. Each of the type of plasmonic nanoantenna has specific property and design.

Plasmonic monopole nanoantenna is the simplest of all the nanoantennas. The factors affecting the characteristics of these nanoantennas are the shape, size, material and the dielectric environment. These nanoantennas find special application where high precision fabrication of nanoparticle arrays is required.

Plasmonic dipole nanoantenna, also called dimer, have the ability of confining electromagnetic field of very high magnitude in the gap between nanoparticles. Research by various authors showed that the dipole nanoantennas can be tuned to work in desired operating regime by introducing materials of different permittivity in the gap. Bowtie nanoantenna finds application in solar cells and ideal absorption coating because they enhance the absorption efficiency. They also have a high value of fluorescence. Plasmonic yagi-uda nanoantenna consists of a reflectror nad one or more directors. These types of nanoantenna show very high directivity.

Plasmonic nanoantennas are fabricated by metal nanoparticles and can be of various shapes and sizes. They are of small size, confine the electromagnetic radiations with very strong magnitude and show high directivity. There exist some of the disadvantages of using plasmonic nanoantennas. In classical antenna theory, it is considered that the electromagnetic field is restricted to the boundary of the metallic nanoantenna. The electromagnetic radiations penetrate into the plasmonic nanoantenna at optical frequency regime. The penetration is described by the skin depth and depends on the permittivity of the material used. So, at optical frequencies the concept of perfect conductor fails. Hence metals suffer considerable amount of losses at optical frequencies. Also, gold and silver (which are major plasmonic materials) are not compatible with CMOS nanofabrication technology. To overcome these disadvantages, nanoantennas made of high dielectric constants came into existence.

2.3.2: DIELECTRIC NANOANTENNAS

These nanoantennas are fabricated by semiconducting materials like silicon, germanium etc which are transparent at optical frequencies and this is the reason they are also called dielectric nanoantennas. Unlike plasmonic nanoantennas where electric resonance of high magnitude is obtained and weak magnetic resonance occurs, in dielectric nanoantennas, both electric and magnetic resonances of high magnitude are obtained. These nanoantennas have gained importance in the past years because both magnetic and electric responses are available at visible frequency range and very low losses in optical regime. Hygen's element is created in these nanoantennas. Many nanoantenna structures can be created by the use of this hygen's element e.g. yagi-uda nanoantenna.

1. HYGEN'S ELEMENT

Hygen's element is a dielectric nanoparticles which is fabricated with material of very high permittivity, in the order of 10-20. These elements show electric resonance and magnetic resonance in the visible spectrum [71]. Both the dipole moments i.e. electric dipole moment and magnetic dipole moment are induced when hygen's element is excited by an emitter. At a particular frequency, the polarizabilities of both the dipole moments has an equal magnitude. Thus with the help of hygen's element, fully dielectric nanoantennas can be fabricated with improved directional properties.

2. OPTICAL MAGNETISM

Electric charges of opposite sign are referred to as a dipole. So, oscillating electric charges of opposite signs can be referred to as an oscillating electric dipole. This oscillatin electric dipole is the source of electromagnetic radiations. Similarly, source of magnetic field in nature is the magnetic dipole. Magnetic monopoles or isolated magnetic poles (i.e. either north pole or south pole) do not exist in nature. A loop of current shrinking to a point can be used for the calculation of magnetic field of a dipole. The split ring resonator or SRR is also an artificial source of magnetic dipole as shown in the figure 5(a) below.

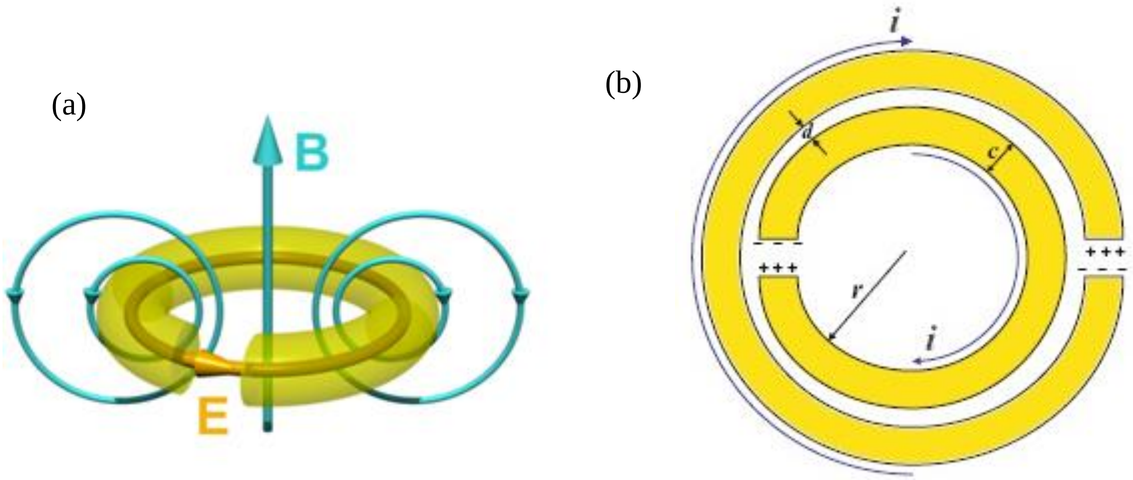


Figure 5: (a) Production of magnetic dipole by split ring resonator (SRR) [72], (b) schematic of split ring resonator showing the direction of currents carried by the two concentric ring.

Split ring resonator is a device used to produce exceptional effects which otherwise are hardly possible. It is built by two concentric rings with slits etched in them and placed such that the two slits are opposite to each other or as shown in the figure 5(b). When electromagnetic radiations interact with this current carrying structure, magnetic dipole is produced which oscillates up and down in a transverse manner at the center of the ring. Split ring resonator finds application in metamaterials.

These type of artificial systems have grown popularity and interest because of the following reasons:

- When incoming electromagnetic radiations interact with these artificial systems, they respond to the magnetic component of the radiations.
- At optical frequencies, they show negative or non unity magnetic permeability.
- The above characteristics are hard to find in naturally existing systems.

Negative refraction [76], clocking [73, 74] and superlensing [75] are some of the material properties which can be designed by these artificial systems. At visible or optical frequencies, intrinsic losses in metals are considerable and cannot be neglected which is the biggest disadvantage behind their use in antenna designing. The alternative approach lies in the use of dielectric materials for this purpose. Dielectric nanoparticles of high refractive index show nearly very low or negligible losses at visible range frequency spectrum. Also, they show strong magnetic response at optical frequencies. High refractive index spherical nanoparticles was used to explain the above two phenomenon. Magnetic dipole resonance of very high magnitude can be attained for a specific range of parameters. Oscillating magnetic field can be achieved at the center of the spherical dielectric nanoparticle as shown in the figure 6

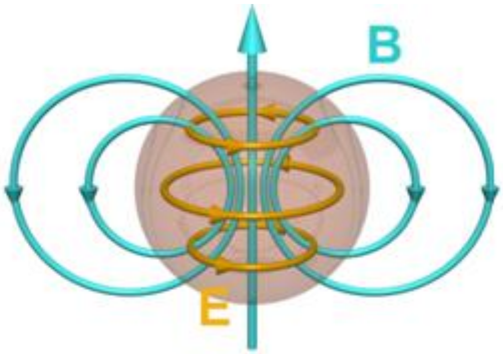


Figure 6: Electromagnetic wave distribution in spherical dielectric nanoparticles [72]

CHAPTER -3

SOFTWARE AND CALCULATION METHODS

3.1 COMSOL

In today's world, computer simulations have become an important part for solving problems in the field of science and engineering. COMSOL Multiphysics is a software package that is used to implement various engineering related problems. Various problems can be simulated, solved and related finite element analysis can be done. 1D, 2D and 3D models can be easily simulated and modeled to look for possible solutions. This software helps in building models which can accurately depict what happens in the real world.

1. Comsol multiphysics is an engineering, design and finite element analysis software. It finds applications in modeling and simulation of systems which are based on physics. These physics based systems are realized by various algebraic equations or ordinary differential equations or partial differential equations. The set of equations used to describe the model in COMSOL Multiphysics software are solved using Finite Element Method in the software itself. Very spontaneous graphical user interface for geometry, material, solver, physics, mesh etc. is also available in the software for quality analysis. These physics interfaces can be employed to perform various studies i.e.
    - (a) Linear as well as non linear studies.
    - (b) Steady (or time independent) and transient (or time independent) studies.
    - (c) Eigen frequency and frequency dependent studies.

There are different modules available for analysis in this software, as given below:

- AC/DC module
- MEMS module
- RF module
- Plasma module
- Heat transfer module
- Acoustic module…. etc.

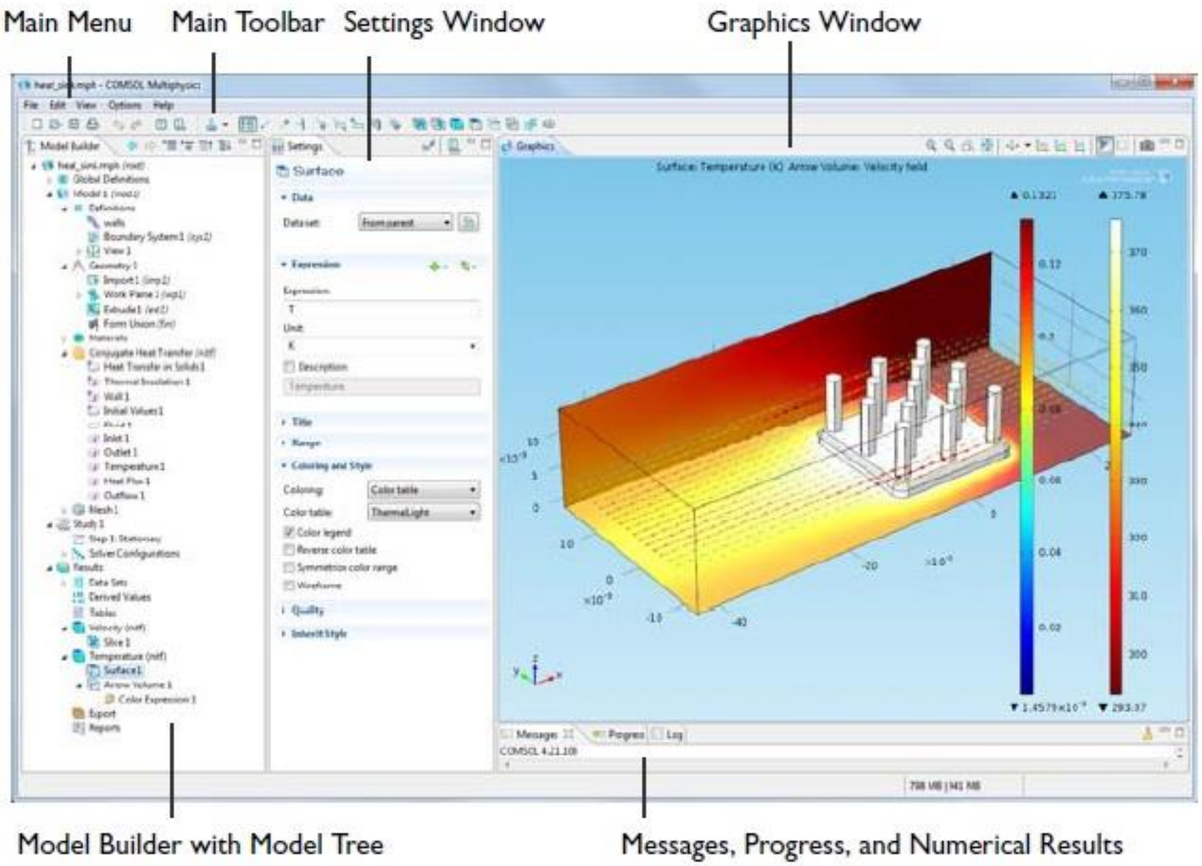


Figure 7 : comsol desktop window showing various tool bars.

2. Comsol desktop is highly organized to help even the beginners to build the model very easily. For achieving simplicity in designing complex realities, comsol multiphysics uses aesthetics, functional form and structure. There are several windows available on the comsol desktop namely model builder, progress, messages, graphics etc. The uncertainty in model building is exempted in this software because there are task-specific tools present. As soon as they are needed, they appear on the desktop.

3. Since the dissertation is on antenna designing, of all the various modules present, RF module is used. RF stands for radiofrequency. For designing of filters, cavities, antennas, waveguides, circuits and metamaterials, RF module is being used by the designers.

Various problems associated with electromagnetic waves like photonics, optics, RF and microwave applications are solved in RF module of COMSOL software. This module is used for component design in various fields which involve electromagnetic waves such as antennas, photonic crystal, waveguides, active photonic devices etc.

4. Pre-processing steps involve following steps:
    - Geometry building
    - Adding surrounding materials and PMLs.
    - Material addition to the design and surroundings.
    - Addition of parameters, variables and constants.
    - Selection and naming of domains

    Any type of shape and size of the nanoantenna can be build in this software. Model building wizard includes these geometry building steps. You can then add the material to the antenna design and the surrounding materials based on one’s choice. PML layers are then added to the model to absorb the scattered fields. Various parameters (like the frequency of radiations incident, wavelength, speed of light, length of the design, radius etc.) related to the design can be added in the parameter window. Domains are to be explicitly specified and named so as to be used later during frequency analysis.

5. Ports of specified power of one’s choice can be added to the designed model. The mode of wave excitation, power level and direction of wave propagation can be changed by changing the location of the ports on the designed model. Perfectly matched layers also known as PML can be added to the model. These layers simulate propagation and excitation of electromagnetic waves in unbounded domain. One can choose between scattered electromagnetic fields and full field.

6. The next step involves meshing of the design. One can use either physically controlled mesh or can mesh the model of one’s choice. Meshing divides the whole geometry in small regions and helps in using weak form of PDEs on larger function space (which

otherwise would create a large amount of error). Various meshing techniques are present e.g. triangular mesh, swept, tetrahedral type etc. COMSOL will automatically mesh the geometry if physics controlled mesh is used. One can also vary the number of elements of mesh being used.

7. Comsol uses finite element method to solve the equations involved in the design. There are variety of numerical solvers available in COMSOL and error control technique which are used along with finite element analysis to solve for the equations related to the model. In frequency domain analysis, one can add study steps to choose among various electromagnetic waves. Parametric sweep can also be assigned to the parameter which is to be solved for.

8. Post-processing data is stored in the form of solution nodes in the result window. Using the solutions one can evaluate various graphs and figures. Volume, surface and layers can be analyzed for the intensity of incident fields on them. Results from comsol can be stored in the form of 3D, 2D, 1D figures and also tables can be plotted from these solutions. The data from these tables can be further used in the software called MATLAB to plot various graphs.

3.2 MATLAB

Matlab stands for MATrix LABoratory. It was developed during 1970s by Cleve Melor and firstly used by researchers of control engineering. Matlab is a tool for visualization, technical computing and computation. It is fourth generation programming language. Using this programming language, following are the works which can be done:

- Plotting graphs, functions and data
- Matrix manipulation
- Algorithm implementation
- User interface creation

- Interfacing with programs that are written in other high level languages namely c, c++, python and fortran etc.

3.3 CALCULATIONAL METHOD USED- FEM

FEM stands for finite element method. For space and time dependent problems, the laws of physics are usually described by partial differential equations (PDE). These PDEs can be easily solved for small geometries but for large geometries, they become more complex and cannot be solved analytically. To solve such complex equations, discretization of the geometry is necessary. The basic idea behind using FEM technique is that it is easier to solve for weak form of PDEs on larger function space than solving for strong form on smaller function space.

Finite element analysis is a numerical method of solving mathematical problems. Traditionally, it was used by the branch of solid mechanics. There are various steps for finite element analysis process and that are as explained below:

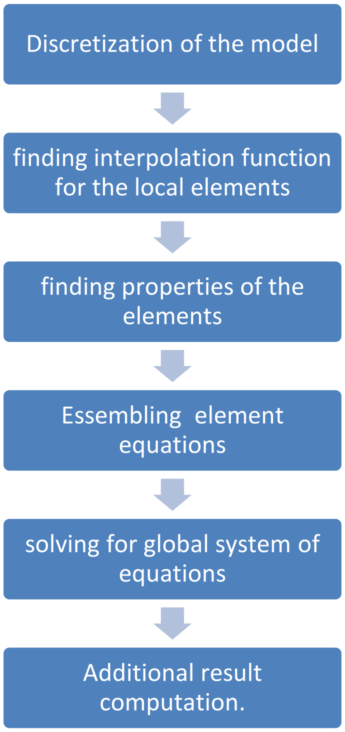


Figure 8: Finite element method step by step process

1. Discretization

Mathematical equations involved in describing the real world models are usually partial differential equations of higher order. Solving such big equations by analytical methods is a tough task. So in order to solve them, approximation is done. The nearness of the approximated result to the exact solution depends on the value of discretization. By discretization, it means that the whole model is divided into small regions. These small regions are called sub-domains. These sub-domains are connected by two or more common points called nodes. More number of sub-domains means that the solution to the problem is more near to the exact value and hence less amount of error.

2. Interpolation function

   The interpolation function plays an important role in solving the problem by finite element analysis method. It is used for the field variables to be interposed over the element. Interpolation function is a polynomial which satisfies the nodal conditions. The number of nodes assigned to the element decides the degree of the polynomial required for this function.
3. Finding properties of elements

   This is the next step involved in the process of solving by FEM. Here, matrix equations describing the relation between the parameters and nodal values of the unknown function are created for the finite elements. Among various techniques and methods available, Galerkin method and Variational method are the two most convenient and generally used methods for this task.
4. Assembling element equations

   The next step after matrix equation establishment for finite element is to combine all the local element equations that were used to describe discretization. We need a global system of equations to assemble the local element equations. This process is called assembly of equations. For connecting these local element equations, we use element connectivities. Before obtaining the solution we need to impose boundary conditions to the system. This is because the element equations do not account for these boundary conditions.
5. Solve for global system of equations

   The global system of equations formed in the previous step is solved to obtain nodal values for the required function. There are various methods available to solve these equations. Usually direct and iterative methods are used to solve them. The global system of equations is symmetric and sparse. The final result of the solution of these equations is the nodal values which are further used to obtain various related information of the model.

6. Additional result computation

   This is the final step in the process involving solution by finite element method. In many models, some additional results are to be calculated based on these obtained nodal values. For example, in problems related to mechanics where the displacement is the result obtained by solving the global equation system, strain and stress are the two additional results that are to be calculated.

CHAPTER – 4

DESIGNING OF DIELECTRIC CYLINDRICAL NANOPARTICLE

In this dissertation, a dielectric cylindrical nanoparticles chain has been designed and simulated using COMSOL Multiphysics software. In this section, the designing of the nanoantenna has been discussed. Also, the scattering properties of the designed nanoantenna are discussed in detail. In the next section, the effect of varying orientation of the nanoantenna chain is explained.

4.1 Nanoantenna design approach and motivation

High intrinsic losses in metallic nanoantennas motivated the study of dielectric nanoantennas. The intrinsic loss in metals, when they are subjected to incident radiations, is an unavoidable problem. Also, split ring resonator used to realize the metallic nanoantennas can work effectively in gigahertz range of frequencies [85-88]. In the optical and near infrared range of frequencies, metals start showing absorption effects i.e. they behave like dielectrics and hence the problems of losses arise. The penetration of the electromagnetic radiations is described by the skin effect in metallic nanoantennas or also called plasmonic nanoantennas as discussed above. So the concept of a perfect conductor doesn’t exist in optical frequency regime. To overcome the problems associated with the metallic nanoantennas, high refractive index dielectric nanoantennas [89-99] were introduced. In dielectric nanoantennas, two types of resonances, i.e. electric resonance and magnetic resonance, occur in the visible region. The magnitude shown by both the resonances is very high in the visible regime and also they can be controlled independently and separately. Previous research and works show that in order to achieve efficient response from the nanoantennas, they should possess both electric and magnetic resonances. All these advantages motivated the use of dielectric nanoantennas over the plasmonic nanoantennas.

Various works were done by many scientists to understand the scattering behavior of nanoantennas. The electromagnetic radiations incident on dielectric nanoantennas give rise to electric and magnetic responses. The studies show that these responses have the ability to effectively engineer the scattering radiations. Magnetodielectric particles show unusual scattering effects and Kerker et al [77] was the first to introduce these effects theoretically. Magnetodielectric particles exhibit both resonances i.e. electric and magnetic. Kerker et al proposed that by varying the values of some specific parameters i.e. magnetic permeability and electric permeability, these resonances can be controlled. He also proposed that when the electric and magnetic dipolar resonances interfere, completely forward or completely backward scattering can be obtained. When sub-wavelength magnetodielectric particle is exposed to electromagnetic waves, asymmetric field radiation with complete forward scattering or zero backward scattering can be obtained under certain combination of electric and magnetic dipolar resonance patterns. This is called first Kerker's condition. Whereas second Kerker's condition produces complete backward scattering or zero forward scattering. At first kerker's condition, the scattering is in the same direction as is the incident radiations and hence it plays a significant role in nanoantenna applications.

Scattering efficiency of high magnitude can be obtained for particles having high electric permittivity because the quality factor of Mie resonances for these particles increases with an increase in permittivity. According to Mie theory, a high magnitude of electric and magnetic dipolar resonances have been demonstrated in visible and near infrared regime both practically and theoretically for nanoparticles fabricated by dielectric material with a very high value of electric permittivity e.g. silicon and germanium [78-81]. By varying the shape and size of silicon nanoparticles, the magnetic and electric resonances can be tuned at a specific frequency [82, 83]. Periodically arranges nanocylinders of silicon have the ability to increase the absorption of light [84].

Here, we propose the designing of array cylindrical nanoantenna for unidirectional scattering in forward direction by applying kerker's first condition for interference of electric and magnetic dipolar resonance. Firstly cylindrical nanoantenna is designed to study the scattering properties. Next, chain of these nano-perticles is designed and analysed for the directional scattering along various directions. The designing is done using COMSOL multiphysics software and the analysis is done by finite element method.

4.2 DESIGNING AND ANALYSIS OF SILICON NANOCYLINDER

Design: A dielectric silicon cylindrical nanoparticle of radius r = 50 nm and height, h = 180 nm is designed. The designing parameters are chosen in a manner that the operating wavelength falls in the visible region. The operating frequency can be varied by changing the designing parameters i.e. radius and height. The nanocylinder is positioned at the origin and surrounded by air. A perfectly matched layer of 50 nm thickness surrounds the entire block containing air and nanoparticle.

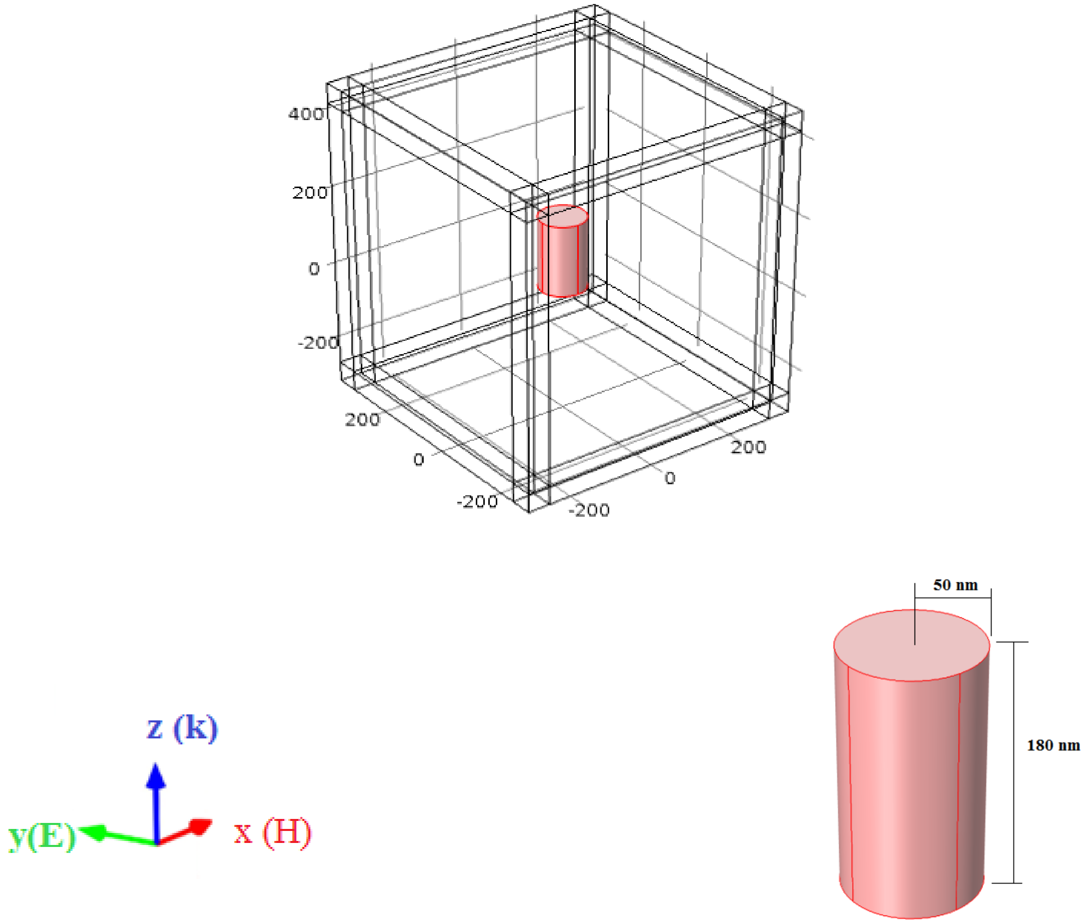


Figure 9: (a) illustrates the orientation of silicon nanocylinder in comsol window (b) shows the axis of orientation (c) shows the dimensions of the silicon nanocylinder

ANALYSIS: The Si nanocylinder is oriented such that the propagation direction of electromagnetic radiation is along the length of the nanocylinder and linearly polarized along y direction. In the visible range of frequencies, electric and magnetic dipoles are created at a particular frequency. As mentioned in the previous chapters, whenever incident light interacts with matter (silicon cylindrical nanoantenna in this case), electric dipoles and magnetic dipoles are created at some specific wavelengths.

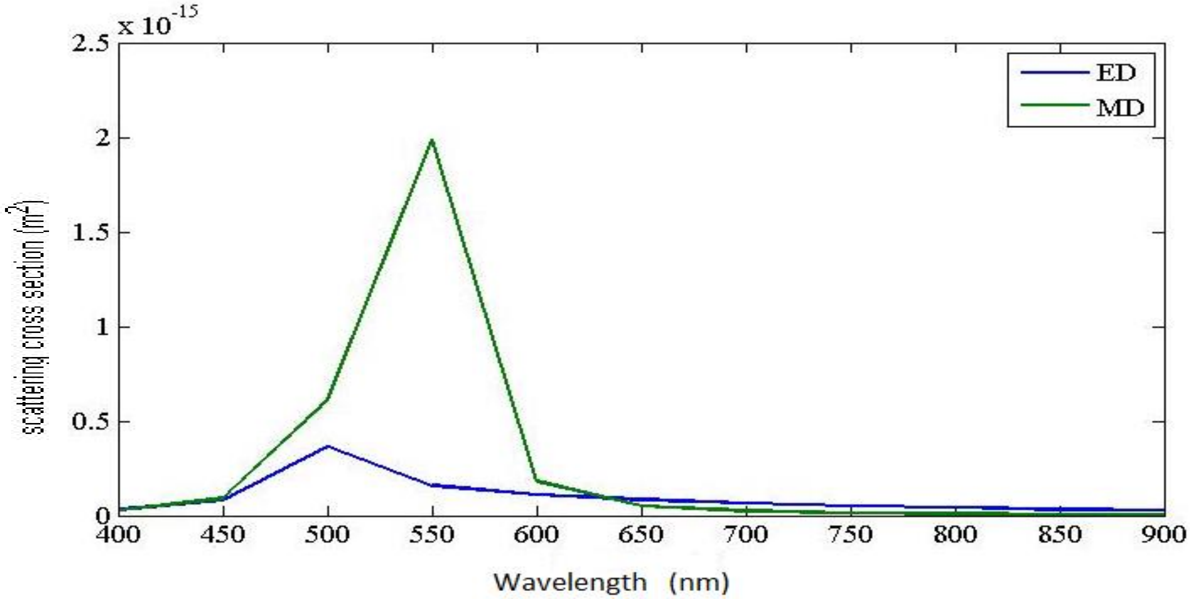


Figure 10: plot showing variation of scattering cross-section with wavelength.

Here electric dipole is denoted by ‘p’ and magnetic dipole is denoted by ‘m’. The equations involved are given below

$$p=\varepsilon_0(1-\varepsilon_r)\oint_V E(r')dV' \ , \quad m=\frac{iw\varepsilon_0(1-\varepsilon_r)}{2C}\oint_V [r\times E(r')]dV' \qquad (1)$$

where, ε_0 is the electric permittivity of free space or vacuum, ε_r is the relative permittivity of the material i.e. nanoparticles, c is the speed of light, $E(r')$ denotes the electric field vector at position vector r' , i is the imaginary part of the complex variable and w denotes the angular frequency. The scattering cross section of the nanoparticles for electric dipole and magnetic dipole is expressed by the equations illustrated below

$$\sigma_{\mathrm{sca}}^{\mathrm{p}}=\frac{<\mathrm{P_{sca,ED}}>}{\mathrm{I_0}} \ , \qquad \sigma_{\mathrm{sca}}^{\mathrm{m}}=\frac{<\mathrm{P_{sca,MD}}>}{\mathrm{I_0}} \qquad (2)$$

where,$\mathrm{I_0}$ is the incident power density, $<\mathrm{P_{sca,ED}}>$ and $<\mathrm{P_{sca,MD}}>$ are the power scattered by electric and magnetic dipoles, respectively, which can be expressed as

$$<\mathrm{P_{sca,ED}}>=\frac{\mathrm{C^2K_0{}^4Z^2}}{12\pi}|\mathrm{p}|^2 \ , \quad <\mathrm{P_{sca,MD}}>=\frac{\mathrm{C^2K_0{}^4Z^2}}{12\pi}|\mathrm{m}|^2 \qquad (3)$$

where, c is the speed of light in vacuum, K_0 and z are the free space wavenumber and free space impedance, respectively. The variation of the scattering cross section for electric and magnetic dipole is plotted against wavelength (nm) as shown in the figure10. The blue curve denotes the plot for electric dipole with the peak at 500 nm. So this shows that at 500 nm the electric dipoles are created. Similarly, green curve is the plot for magnetic dipole and has a peak at 550 nm and hence the magnetic dipoles are created at this particular wavelength. Fig11 shows the 2D radiation patterns showing the distribution of electric field in the nanoparticle.

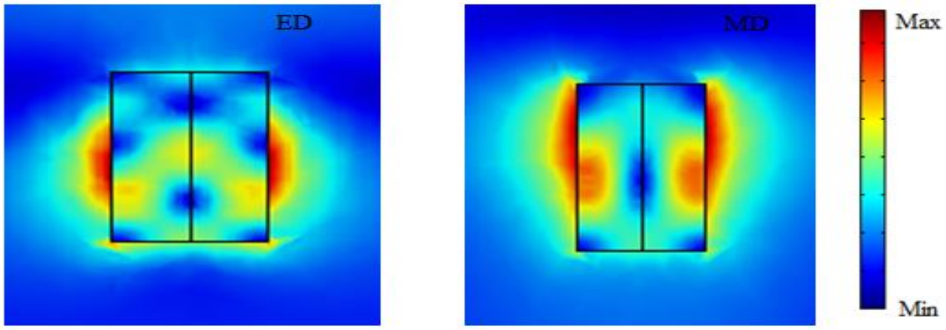


Figure 11: 2D polarization distribution patterns for magnetic dipole (MD) at 550 nm and electric dipole (ED) at 500 nm along with the colour legend.

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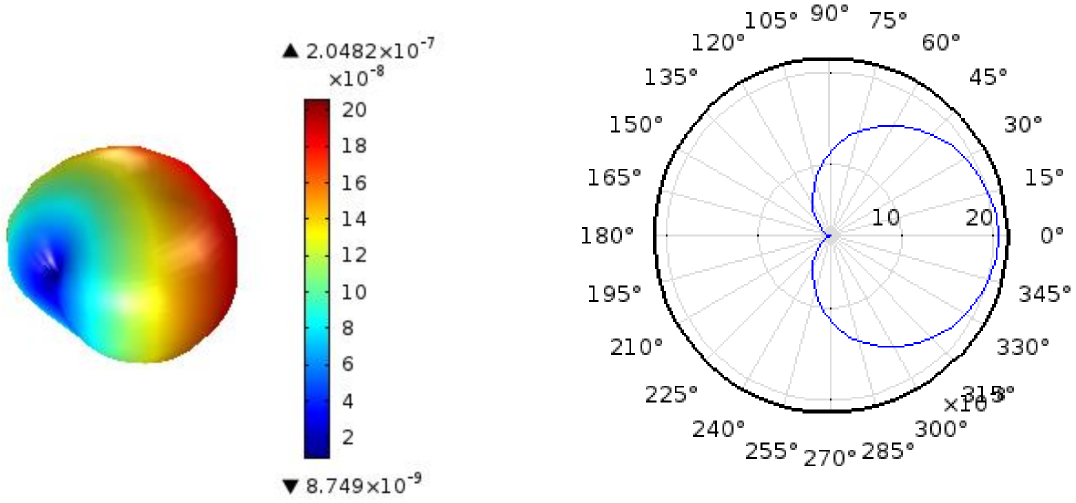

Figure 12: 3D and 2D far field plots at 633 nm for the cylindrical silicon nanoantenna.

The two scattering cross section plots intersect at 633 nm. Far field plot is plotted at this particular wavelength and is shown in figure12. It can be inferred from the plot that there is complete forward scattering or zero backward scattering and hence first generalized Kerker's condition is being satisfied at 633 nm. According to the colour legend, the 3D far field plot shown has maximum electric field intensity at the tip of the plot and it is minimum at zero degrees. Scattering pattern shows highly azimuthal symmetry. Since there is highly forward scattering i.e. the scattering is in the direction of the incident electromagnetic radiation, therefore dielectric cylindrical nanoparticle is highly suitable for nanoantenna application.

CHAPTER-5

DESIGN AND ANALYSIS OF CHAIN OF CYLINDRICAL NANOPARTICLE

In the previous chapter, we designed and analysed cylindrical nanoparticles. In this chapter we will be designing nanoparticles chain of the same cylindrical nanoparticles being already analysed for scattering cross section and far field plots. The chain will be oriented along the three direction and analysed for change in directivity and forward scattering patterns.

DESIGN: The chain of 3 nanocylinders of radius 50 nm and height 180 nm is designed with nanocylinders placed 300 nm apart. Firstly the chain is oriented along the direction of propagation of the incident radiation. Secondly, it is oriented along the direction of the electric field and lastly, it is oriented along the direction of magnetic field.

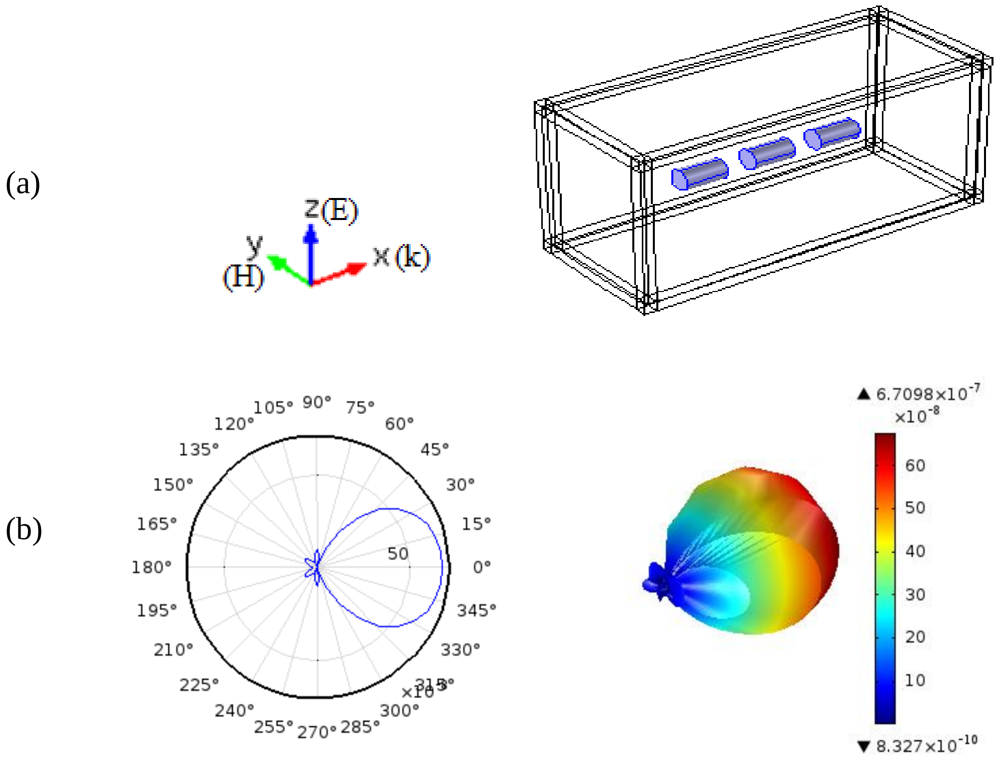

Figure 13: (a) design of nanochain when it is oriented along the direction of propagation. (b) 2D and 3D far field plots

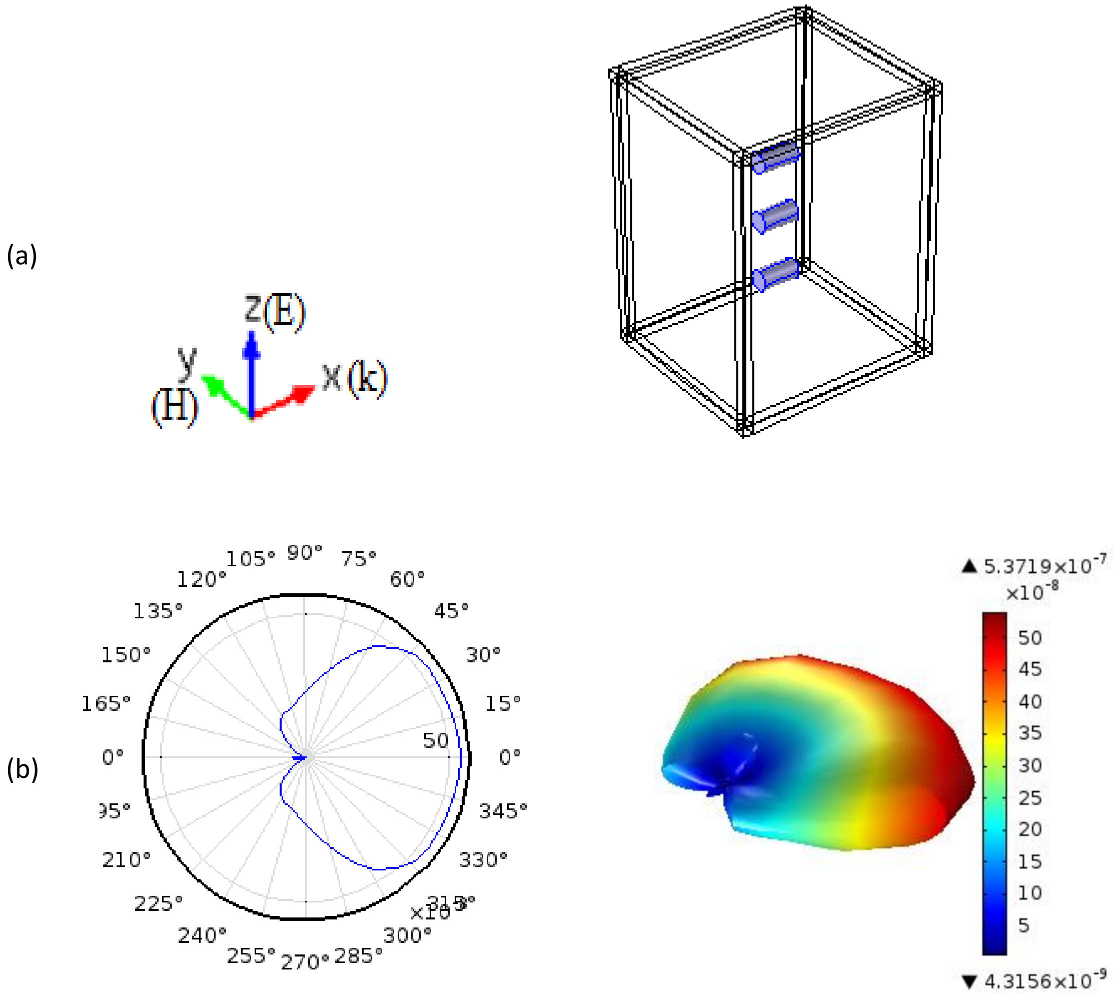

Figure 14: (a) design of the nanochain when it is oriented along the direction of the electric field. (b) 2D and 3D far field plots of the nanochain

In figure 14, the nanochain is oriented along the direction of electric field and the propagation of the incident radiation is along the length of the nanocylinder. The nanocylinders are oriented 300 nm apart. The directivity obtained in this case is 3.99. Although the the far field plot is having no backward scattering but the scattering pattern is very broad. Figure 15 (a) and (b) show the orientation of the nanoparticle chain along the direction of magnetic field or y axis. The far field polar plot has no backward scattering but with considerable side lobes. Side lobes are a sign of losses or the scattering along the side lobes is considered as wasted.

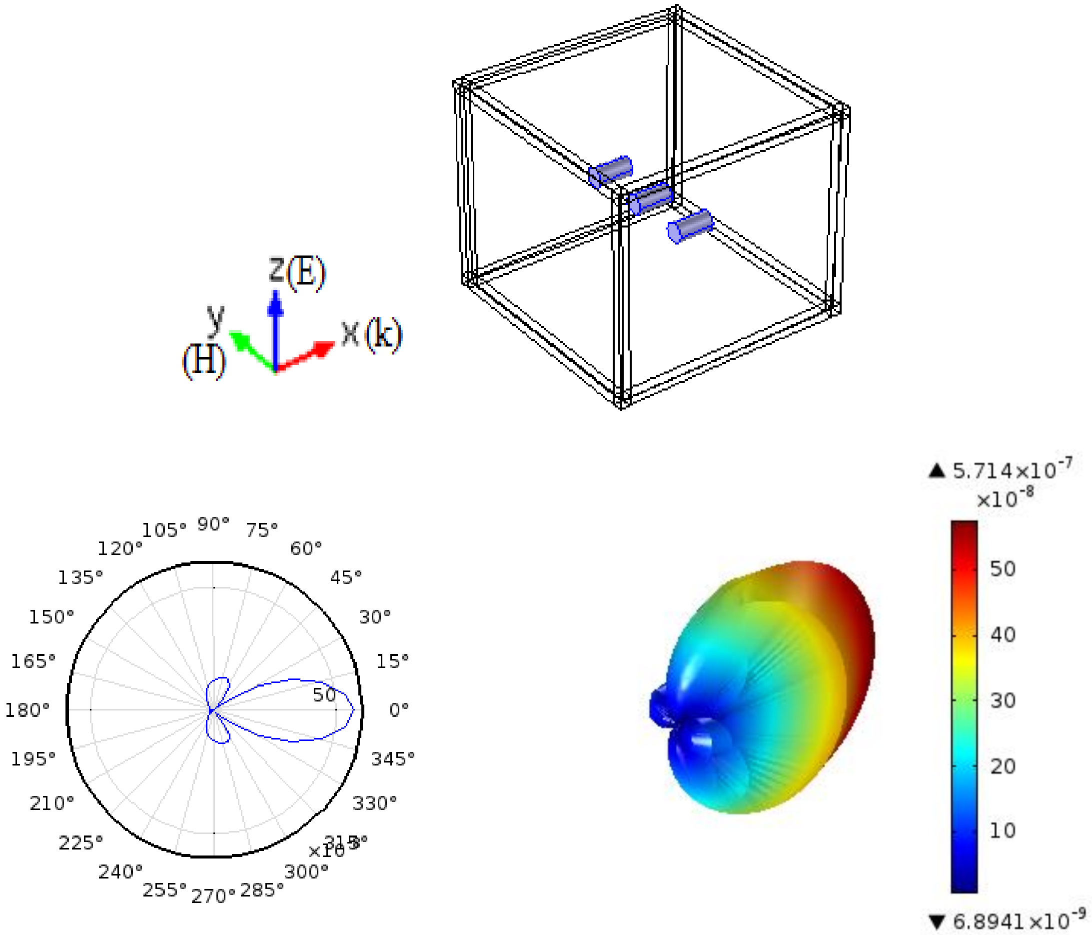

Figure 15: (a) orientation of nanoparticle chain. (b) 2D and 3D far field plots of the oriented chain.

ANALYSIS: All the three designs are studied with the help of far field plots. It can be inferred from the above study that when the chain of silicon cylindrical nanoparticles is oriented along the direction of propagation of the incident electromagnetic radiation, it is having no side lobes and also the scattering pattern is narrow and completely in the forward direction with nearly no backward scattering. The directivity obtained for this case is also high as compared to the rest of the two cases.

VARIATION OF DIRECTIVITY WITH THE ADDITION OF CHAIN ELEMENTS:

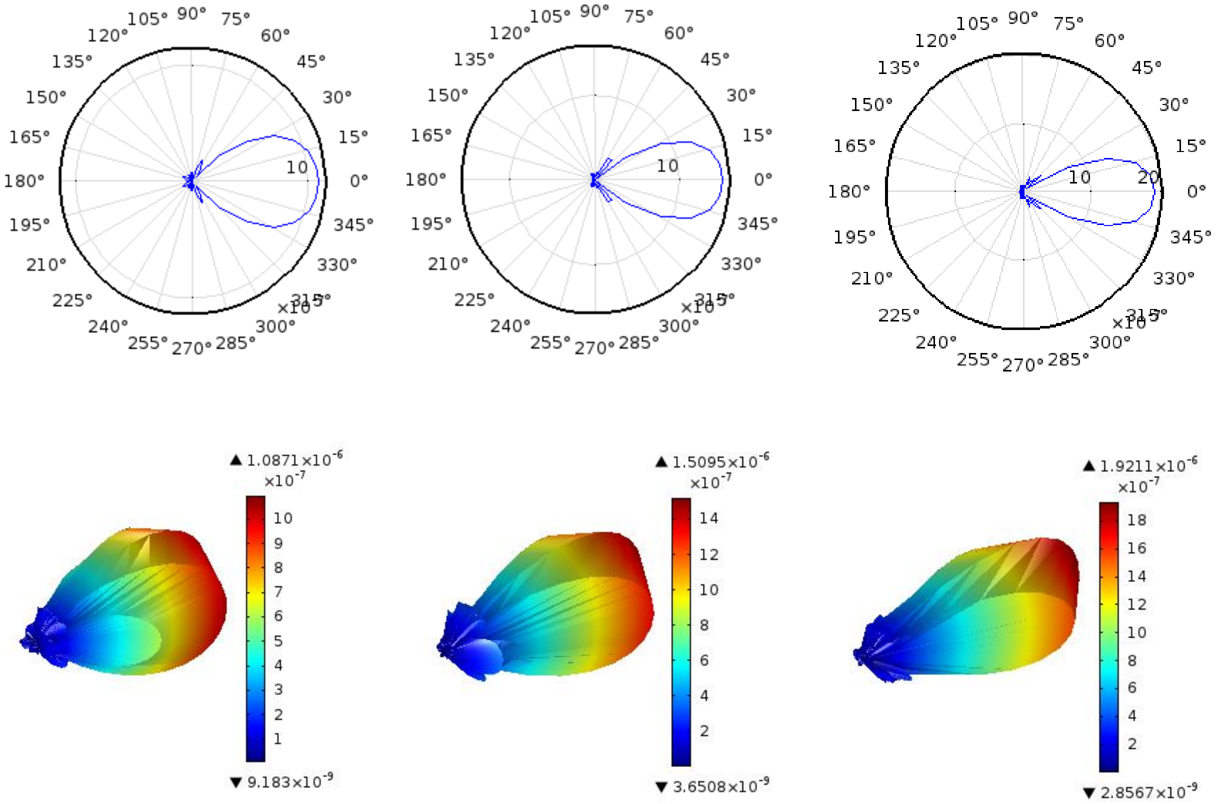

Figure 16: The far field plots for the chain of cylindrical nanoparticles with n=5, 7 and 9 respectively.

As discussed earlier, the chain designed and aligned in the direction of propagation of the incoming radiations showed highly efficient scattering in the forward direction (i.e. in the direction same as that of the incident electromagnetic radiations) as compared to the other two designs. Hence, we will study the effect of increasing the number of chain elements on the directivity of the chain.

Initially we created a chain of 3 nanocylinders placed 300 nm apart and obtained a directivity of 4.44 . With number of chain elements, denoted by ‘n’, increasing to 5, the directivity increases to 6.38 . Further, for n=7, the directivity becomes 8.56 and lastly for n=9, the directivity increases to 10.75 . The far field plots, shown above, clearly demonstrate narrowing of the scattering pattern with an increasing number of chain elements. Also, the scattering is highly in the forward direction with very small side and back lobes.

CHAPTER – 7

CONCLUSION AND FUTURE SCOPE

CONCLUSION: In this dissertation, directional forward scattering by linear chain of cylindrical nanoparticles is being studied. An important result regarding the orientation of the chain to obtain comparatively efficient forward scattering has been obtained. These results are important in the near-infrared and visible region of spectrum.

It is shown that for the orientation of the linear chain of silicon cylindrical nanoparticles along the direction of propagation of incident electromagnetic radiations, the scattering spectrum is along the forward direction with very small backward scattering (which can be neglected easily) and very small side lobes. That is, there is comparatively narrow scattering spectrum which further goes on becoming narrower on increasing the number of nanocylinders in the linear chain showing less wastage of energy.

Further, it is being reported that with an increase in the number of cylindrical nanoparticles in the linear chain, the directivity goes on increasing.

FUTURE SCOPE:

Many researches have been done in the field of dielectric nanoantennas and they find great scope in the field of science called nanophotonics. Nanoantenna is a device that converts freely propagating radiations to highly oriented ones in the subwavelength region. Directivity and efficiency are the two important characteristics of an antenna. Both the features are being enhanced by the linear chain of cylindrical nanoparticles which is being disgned in this dissertation. So the linear chain of cylindrical nanoparticles can be easily implemented for nanoantenna applications. Also, the scattering properties shown by this linear chain design in visible and infrared region makes it suitable for nanoantenna design.

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