

Master's Thesis

Scattering Properties of
Nanoantennas

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Abstract

The concept of antennas at optical frequency has recently opened up new fields of experimental and theoretical research in nanotechnology and antenna science. The growing interest in optical antennas and nanoscale metals can be attributed to their ability to support plasmon resonances that interact with optical fields. The remarkable advances of nanotechnology experienced in recent years have increased the interest in optical antennas as devices for efficiently manipulating light by means of their optical properties such as concentration, absorption and radiation of light at nanoscale. In particular, much research has recently been done on this topic, suggesting how different materials and geometries of nanoparticles may be employed as nanoantennas with possible applications in medicine, physics, wireless communications, chemistry, biology, etc. However, this technology is in its early stage and has a lot to be investigated.

The optical properties of a nanoantenna are highly dependent on its size, geometry and material. This work is an approach to the effect of size, shape and material on the resonance characteristics of nanoantennas. In addition, the anomalous behavior of plasmonic materials that is associated with their dispersive permittivity, is investigated. The dispersion of metals at optical frequencies is described by the Drude-Lorentz model which considers both free electrons contribution and harmonic oscillators contribution.

The total interactions of the incident electromagnetic plane wave and the nanoantenna are obtained from frequency dependent cross sections. Using the optical theorem that relates the imaginary part of forward scattering amplitude, the extinction cross section (sum of scattering and absorption cross sections) is determined from scattering dyadic in the forward direction. According to the forward scattering sum rule the integrated extinction cross section over all wave lengths can be determined by the total polarizability (sum of electric and magnetic polarizability) of the

nanoantenna.

It is also shown that the dispersive material data of a nanoantenna determines its resonance characteristics. In addition, the total polarizability of the nanoantenna determines the total area under the curve of extinction cross section therefore the so called Full Width at Half Maximum (FWHM) is obtainable. The resonance characteristics of a nanoantenna, is highly dependent on its size, and the integrated extinction efficiency (the ratio of extinction cross section to the physical cross section of the nanoantenna) over all normalized wavelengths by its longest dimension, is identical for any size of it.

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Introduction

1.1 Nanoantennas

The complex and interesting optical properties of metal nanostructures have recently opened a new field of research in antenna technology [3,4]. At optical frequencies under specific conditions, these structures especially noble metals like gold and silver with certain geometries, are able to show peculiar electromagnetic resonances, when being excited by an incident light. These electromagnetic resonances called *surface plasmon polariton resonances* (SPPRs) are intuitively associated with the jump of conduction electrons to the upper valence electron layers which generates a strong light scattering and absorption causing local electromagnetic field enhancement. In other words SPPs transport electromagnetic energy at the interface of the metal and a dielectric [5].

Nanoantennas as a part of plasmonic structures are often known as optical antennas since, they work in the optical regime. They can be considered as the counterpart of conventional antennas working at radio frequencies [6]. However, contrary to RF antennas where their geometry can be used to shrink their size, in nanoantennas their dispersive permittivity allows for shrinking their size.

When it comes to plasmonic nanoparticles, the *scattering properties* become more interesting compared to the conventional antenna responses. Typically, the scattering spectrum of a plasmonic material has a peak at a certain resonance wavelength. This resonance wavelength can be affected by the optical parameters, the geometry and the size of the particle [1].

Recently, the possibility of observing optical characteristics of plasmonic nanoparticles has attracted considerable interest in nanotechnology and it should be associated with the increasing mass of the research done on the topics of nanoparticles scattering properties [3,7,8]. In some cases a dipole source is modelled by a single molecule excited by a plane wave so

that the impact of the plasmonic nanoparticles can be studied [4,9]. Furthermore, plasmonic nanoparticles as simple radiating structures, have been explored in detail, both experimentally and theoretically to maximize the power generated by sub wavelength radiators [10]. In addition, the conducted numerical and experimental investigations in nanoantenna technology based on plasmonic resonant nanoparticles, have made it possible to improve the radiation pattern and directivity of nanoantennas [11–18].

In contrast to the conventional antennas operating at radio frequencies (RF) and microwave domains, the anomalous characteristics of metals (dispersive permittivity and finite conductivity) at optical frequencies should be taken into account as a significant parameter in design and characterization of nanoantennas [19]. In this sense, depending on the material and operating frequency of the nanoantenna, its plasmonic features and/or harmonic oscillators contribution, play a key role in its scattering properties since, the optical properties of most metal structures are significantly affected by the existence of surface plasmon polariton resonances and /or free electrons contribution (SPPRs).

Additionally, the nanoscale feature size of optical antennas, limits the ability to design, manufacture and characterize their resonant behavior. The antenna size reduction may affect its performance e.g., efficiency, bandwidth etc. in the optical regime, as different groups of research, have recently proposed these limitations both theoretically and experimentally (see [20–23]).

The frequency dependent complex permittivity of plasmonic materials is one of the most critical parameters in their resonant characteristics. This work shows how the optical responses of some nanoantennas such as gold (Au), silver (Ag), copper (Cu) and Aluminum (AL), are affected by their size, shape and their frequency dependent optical functions. The optical functions of these metals are described by the Drude-Lorentz model which considers both the free electrons contributions and harmonic oscillator (SPPRs) contributions. The extinction cross section of optical antennas is determined by using the optical theorem from forward scattering dyadic. According to the forward scattering sum rule, the integration of the extinction cross section over all wavelengths is obtained from the total polarizability of the nanoantennas therefore, full width at half maximum (FWHM) can be obtained. For different nanoantennas with different sizes and shapes the total extinction efficiencies as well as the resonance behavior in terms of frequency and the corresponding FWHM are compared with each other. Eventually, the local field enhancement of a nanodipole with different nanoloads at the gap region is investigated.

Optical Antenna Applications and Properties

2.1 Optical Antenna Applications

The advent of antenna concepts in the optical regime has introduced a new vision of antennas and their capability in many applications. The research on plasmonic-based techniques is considerably active due to the high potential of plasmonic structures in various applications such as: infrared and multi-spectral imaging, near-field optics, and optical antenna sensors (these three applications are explained below).

2.1.1 Infrared and Multi-Spectral Imaging

Using optical antennas has recently caused a significant progress in the technology of infrared detectors. The initial challenge is to couple the same kind of antenna used at radio frequency e.g., dipole, bow-tie antenna, spiral, micro patch, micro strip or arrays of them, to the conventional infrared multi-spectral imaging devices [24].

2.1.2 Near-Field Optics

Near-field optics (NFO) has recently become a focus of research and development in the field of optical microscopy. In this technology the optical properties of nanoparticles with a size on the order of less than 100 nm is proposed [25–27]. The surface plasmon polariton resonances (SPPRs) play a dominant role at optical frequencies to induce the antenna currents within the wires and thus to propagate the signals. In the optical regime, the bound electrons (conduction electrons) of metals in the lower valence band may jump to higher bands. This phenomenon contribute to their

dispersive permittivity and finite conductivity [28]. Although the excitation of SPPs weakens the conductivity of most metals at optical frequencies, it allows for the design and manufacturing of frequency dependent nanoscale components made of metal that are suitable for optical frequencies. In this sense the antenna resonances and surface polariton resonances contribute to a great localized field enhancement [7].

Scanning near-field optical microscopy (SNOM) is a technique to image by exciting and collecting diffraction in the near field. In this method, due to the diffraction limited optical microscopy, the spatial resolution of an image is limited by the wavelength of the incident light and by the numerical apertures of the condenser and objective lens systems [29]. Furthermore, the structure sizes, apertures and scattering particles, are on the order of less than 100 nm have been used for nanostructure investigation and optical imaging that solves the far field resolution issues by exploiting the properties of evanescent waves [29].

2.1.3 Optical Antenna Sensors

Scientific advances in nanotechnology, have recently made it possible to efficiently manipulate the light by using plasmonic sensing materials in nanoscale volumes. Moreover, the generation of sensitive geometries in nanoscience technology has made it possible to sense even minute refractive index change of surrounding materials. In this case, the electromagnetic field enhancement near the surface of the resonant nanometallic structures, commonly noble metals, dominates sensing. The basis for the use of noble metal nanoparticles as sensitive sensors in nanosphere lithography lies in the detection of chemically bound molecules and observing their induced change in the electron density on their surface which shifts the position of the maximum absorption of the surface plasmon resonance. This method has generated a great deal of attention in nanotechnology due to its low cost and easy design and fabrication [30].

Plasmonic metal nanoparticles, due to their strong scattering or absorption, have the capability to easily monitor the light signal. Their sensitive spectral response to the local environment of the nanostructure surface has been recently used in a variety of new chemical and biological sensor applications. Furthermore, since optical antennas have the ability to detect polarization, they can be easily used in new generations of sensors for spectroscopic applications.

It should be noted that sensing can not only be allocated to dielectric substances but also to non-resonant metallic structures which are either too small to have a significant scattering resonances or the strong plas-

monic resonances are prevented by the inherent damping of the metal like the optical detection of hydrogen in palladium [30].

2.2 Optical Properties of Nanoparticles

The interactions of incident light with nanoparticles result in reflected and refracted light by the particles that contribute to scattering and absorption, respectively. At optical frequencies the scattering and absorption properties of nanoparticles are of primary importance compared to other quantities like reflection and transmission [1]. However, when the nanoparticle systems account for a macroscopic body, composed by an almost infinite number of nanoparticles, called a cluster of nanoparticles, the quantities of reflectance and transmittance are still defined.

The scattering and absorption properties, can be highly affected by several parameters such as the particle size and shape as well as the optical material constants of the nanoparticle and the polarizability of its surrounding medium. In other words, the changes in size, shape, and the distances between densely lumped nanoparticles result in characteristic changes of the optical properties [1].

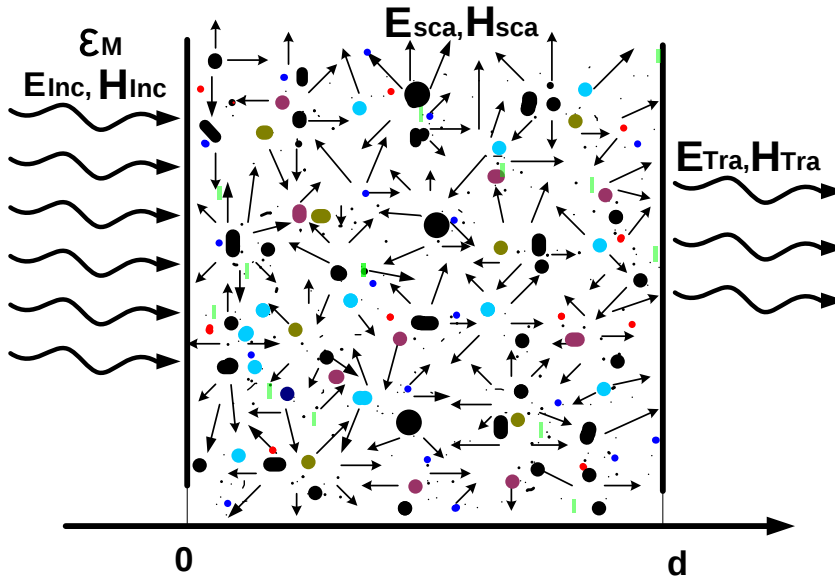


Figure 2.1: Scattering and absorption in a cluster of nanoparticles [1].

Figure 2.1, shows a cluster of nanoparticles illuminated by an electromagnetic plane wave. The electromagnetic fields of incident light (E_{Inc} , H_{Inc}) interact with the nanoparticles thus the external light is absorbed and scattered by the particles or aggregate in the volume to a certain extent. The reflected and refracted light contribute to the so called scattering and absorption, respectively. Due to scattering and absorption process the transmitted light becomes weaker along the propagation direction of the incident light.

2.3 A Simple Model for An Optical Antenna Plasmon Excitation

The interesting interactions of an incident light with metal nanoparticles can be modelled simply by a single metal nanoparticle, whose size is less than 100 nm in all three dimensions excited by an external light field E_{ext} (see figure 2.2). Since, the size of the particle is comparable with the wavelength of light, the incident field can easily penetrate the particle and polarizes the electron density in the particle to one surface so that the internal field E_{int} opposite to the incident one is formed. As the light travels, the polarized electrons on the surface of the particle called SPPs start to oscillate. Since, the incident light is in resonance with the surface plasmon oscillation a standing oscillation takes place. This simple model of surface plasmon polaritons in a metal nanoparticle, illustrates an understandable perspective of an "optical antenna" [1].

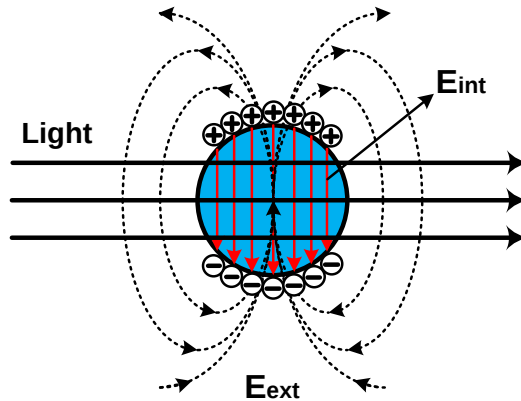


Figure 2.2: A simple model of an external light field excitation of a particle plasmon oscillation in a metal nanoparticle [1].

The attraction of the negative and the positive charges on the surface of the particle strengthen the oscillation caused by even a small exciting field. The resonance condition is mainly determined by the strength of the attraction force dependent on the separation of the surface charges, the particle size, shape, the polarizability of the material and the surrounding medium as well as the structural parameters of the nanoparticle system such as the condensation of nanoparticles. Since, the electromagnetic field density on the surface of the nanoparticle is highly related to the surface geometry determined by the shape and the size of it, a change in shape or size of the nanoparticle leads to a shift in the oscillation frequency of the polarized electrons and consequently, different cross sections (scattering and absorption cross sections) in the optical regime [1].

2.3.1 The Effect of Nanoparticle Size and Shape

The resonance feature of nanoparticles is generally determined from absorption and scattering which is referred to the surface plasmon polariton resonances that are located at the surface of the particle. It is observed that the ratio of the particle size to the wavelength of the incident light is a helpful parameter to classify nanostructures. Therefore, nanoparticles are classified in two groups: the *Rayleigh scattering regime* and the *Mie scattering regime*. At optical regime, the particles with sizes roughly less than 300 nm, meet the specifications of the former class which is simpler technique in light scattering phenomena. For the higher frequencies, the particles with larger sizes satisfy the conditions of the latter class which analyzes symmetric structures like spherical particles, whereas the scattering properties for smaller sizes of particles can be determined by the Rayleigh scattering regime compared to the Mie scattering regime. It is notable that if the particles size is 100 times less than the wavelength of the incident light, the particle is considered as homogeneous material and the optical properties of the nanoparticle is determined by a complex-valued dielectric function $\epsilon(\omega)$ [1].

In semiconductors the size of nanoparticles plays a significant role in their optical properties during light scattering. As the size of these nanoparticles becomes smaller than a certain threshold, quantum confinement of the electrons becomes important and the levels of energy are more quantized compared to the valence and conduction band in larger ones. Metal nanoparticles strongly absorb and scatter light at the plasmon resonance frequency, which leads to strong color in noble metals. It is found that the ratio of scattering to absorption, is highly sensitive to the changes in size. Large particles scatter light significantly, whereas the color of small

particles is mainly caused by absorption. In other words, in case of very small particles, absorption dominates over scattering and the weakness of transmitted light along the propagation direction of the incident light, is basically attributed to absorption. It is found that in metal particles with dimensions above 30 nm, scattering phenomena is of great importance [1]. This work investigates the scattering properties of nanoantennas with sizes larger than 50 nm to 2000 nm. Therefore, the optical responses of small antennas are highly dominated by absorption whereas for larger ones can be associated with scattering.

A particle size parameter $X_{p,s}$ is defined as a helpful classification parameter for a better approach to the extinction cross section of small spherical nanoparticles [1].

$$X_{p,s} = ka = \frac{\text{circumference}}{\text{wavelength}} \quad (2.1)$$

Where k is the wave number and the circumference of a spherical nanoparticle with the radius a is equal to $2\pi a$. This parameter is used in 4.1.1 on page 15, where the simulation results of the extinction efficiency for a PEC and a dielectric spherical nanoparticle with a radius of 50 nm, are plotted against ka .

In nanoscale sizes, the shape of the nanoparticles can be affected by the surface energy, and the proportion of the edges and corners which are no longer negligible. It is evident that, various characteristics of a nanoantenna like sensitivity, resonance frequency, bandwidth radiation properties etc., may be optimized by proper selection of shape and surface geometry [6]. The changes in oscillation frequency of the electrons are referred to the shifts in the electric field density on the surface of nanoparticles. One of the main reasons for this phenomenon can be a change in the nanoparticle shape and its surface geometry which is reflected in different cross-sections for the optical properties including absorption and scattering [6].

The shape of a nanoparticle is chemically referred to as the characteristics of its constituent atoms and molecules forming its edges, corners and surface topology. The edges and corners of a metal nanoparticle are often densely accumulated by electrons. Therefore, the origins of different optical properties in metal nanoparticles may be their different shapes in terms of edges and corners to a certain extend [6].

It is notable that there is a trade-off between the antenna size reduction and its performance e.g., efficiency and bandwidth, at optical regime, as different research groups have recently proposed these limitations [11,12, 20–23,28].

The Optical Material Function

3.1 Metal Nanoparticle Dielectric Functions

At infrared and optical frequencies where metals do not present high conductivity, the dispersion of metals becomes crucial. In this scenario, the dielectric function, $\epsilon(\omega)$, is determined by experimental methods or theoretical models like the Drude model, the Lorentz model, the Drude-Lorentz model, the Debye-Lorentz model etc. [1]. This is a common method done for semiconducting materials, metals, and often for dielectrics at optical frequencies, where strong resonances take place. In other words, the prediction of the optical properties of a nanoparticle system depends on its frequency dependent dielectric function and its surrounding medium characteristics.

The optical constants can be taken from various sources e.g., Drude-Lorentz model by Bora Ung [31], the values for dielectric function tabulated by Johnson-Christy [32] and Palik [33]. The Drude-Lorentz model is a more precise method to describe the dispersion of different metal nanoparticles compared to the two other ones since, it considers both the free electron contributions and harmonic oscillations caused by bound electrons. Therefore, in this work, the complex permittivity of the used metal nanoparticles, is described by the Drude-Lorentz model in [31].

3.1.1 Dispersion In Metals

Metals, due to the existence of both free electrons and bound electrons represent anomalous optical properties during light scattering and absorption [1]. In this sense, their dispersive permittivity which determines their resonance characteristics at optical frequencies, becomes vital. Therefore, in this work, the Drude-Lorentz model that considers both free electrons contribution and bound electrons (harmonic oscillators) contribution, is

used as an efficient and precise model to describe the dielectric functions of metals [1].

This work investigates important characteristics, e.g., extinction cross section, of plasmonic resonators such as, gold, silver, copper, and aluminum in the optical regime, where metals do not present high conductivity and thus their frequency dependent optical functions are of importance. The initial step in this work is an approach to scattering of spherical nanoparticles at the frequency range of 300-3000 THz. It should be mentioned that in order to investigate the frequency dependent radiation characteristics of the interested nanoantenna system, the dispersion of the plasmonic material (the frequency dependent dielectric function limits their conductivity) must be taken into account. Therefore, it is required to describe the frequency dependent complex permittivity of the interested metals at optical frequencies by means of a precise model like the classical Drude-Lorentz model (see [31]).

If $e^{-i\omega t}$ is considered for the time dependence of the electric field, the definition of the dielectric function is as $\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega)$. In Drude-Lorentz model, with the contribution of free electrons and harmonic oscillators the dielectric function can be defined as (3.1) (see [1]).

$$\varepsilon(\omega) = \varepsilon_\infty - \underbrace{\frac{\omega_p^2}{\omega^2 + i\omega\gamma_{fe}}}_{\text{free electrons}} + \sum_{j=1}^J \underbrace{\frac{\omega_{pj}^2}{\omega_j^2 - \omega^2 - i\omega\gamma_j}}_{\text{harmonic oscillators}} \quad (3.1)$$

Where ε_∞ is the relative permittivity at infinite frequency. In the free electrons term ω_p and γ_{fe} denote the plasma frequency and damping constant of the free electrons and in the harmonic oscillators term, ω_{pj} , ω_j and γ_j denote the plasma frequency, resonance frequency, and damping constant of the j th oscillator, respectively. In this model the small resonances observed in frequency response of the metals is described by exploiting J damped harmonic oscillators. The bound electrons in a metal nanoparticle contribute to harmonic oscillators and the dielectric function $\varepsilon(\omega)$ reflects both free electron contributions along with harmonic oscillator behavior.

The real part of the metal dielectric function can be negative due to either free electron contributions or close to the resonance frequency of a harmonic oscillator. The latter which is an inter band transition, happens when the bound electrons in deeper bands are likely to be promoted into the conduction band. This phenomenon compared to free electrons contributions, plays a dominant role in changing the sign of the real part of $\varepsilon(\omega)$ to negative as shifting to high frequencies close to the resonance frequency. It should also be mentioned that, at the resonance frequency of a plasmonic structure, the imaginary part of the metal complex permittivity

plays a dominant role in its absorption loss compared to other parameters such as the size and shape of the optical antenna [1].

The Drude model is basically a classical free electron model that can be used in free electron metals like gold and silver which have d electrons freely travelling through the material. Therefore, this model is used in case there is no harmonic oscillation in the particle and thus it can be described if the harmonic oscillators term in the general equation (3.1) is removed [1]. In a real metal at optical frequencies, the tightly bound electrons lying in the lower valence electron band may be promoted to upper layers by an external light field excitation. The presence of free charge carriers in such metals, semi-metals and semiconductors provides a polarizable medium which can be excited by incident light. For noble metals and the Drude metals, spheres smaller than 100 nm show prominently surface plasmon polariton resonances [1].

The Lorentz model which is a harmonic oscillator model, can be defined if in the general model in the equation (3.1) the free electrons contributions do not exist and thus, each atom represents more than one resonance frequency [1].

Figure 3.1 shows the complex permittivities of gold, silver, copper and aluminum which were taken from the Drude-Lorentz model in [31] within the frequency range of 25-6000 THz (the wavelength range of 0.05-12 μm). At very short wavelengths below 0.4 μm , the Lorentz resonances (harmonic oscillator resonances) are noticeable.

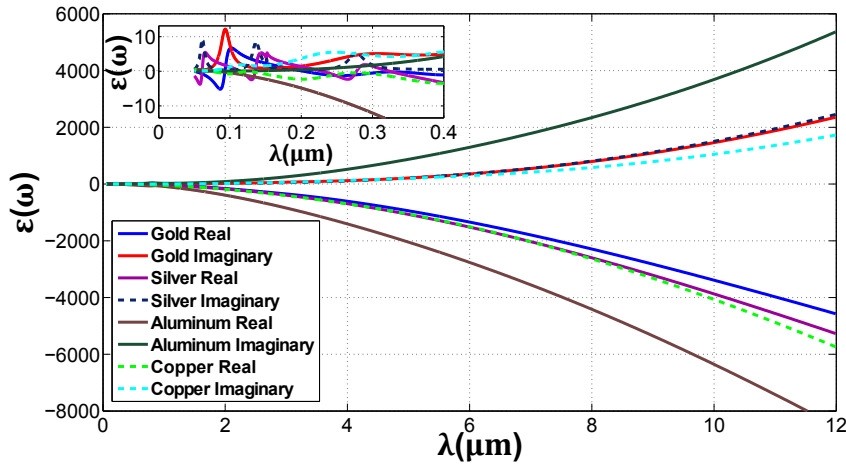


Figure 3.1: The dielectric functions for gold (Au), silver (Ag), copper (Cu) and aluminum (Al) at optical frequencies.

3.2 A Sum Rule for The Extinction Cross Section

At optical frequencies the optical response of a nanoantenna (scattering, absorption and extinction cross section) is described by frequency dependent cross section σ . Consider a linearly polarized electromagnetic plane wave $\mathbf{E}e^{ik\hat{\mathbf{k}}\cdot\mathbf{x}}$ with time dependence $e^{-i\omega t}$ that propagates in $\hat{\mathbf{k}}$ direction impinging the nanoantenna located in free space, can be described by frequency dependent cross-sections σ . The wave number k is defined as

$$k = \frac{2\pi}{\lambda} = \frac{\omega}{c_0} \quad (3.2)$$

Where c_0 denote the speed of light in free space, respectively. The scattered electric field $\mathbf{E}_{\text{sca}}$ corresponds to the scattering dyadic $\mathbf{S}$ which is independent of the incident electromagnetic plane wave [34].

$$\mathbf{S}(k; \hat{\mathbf{k}} \curvearrowright \hat{\mathbf{x}})\mathbf{E} = \lim_{x \rightarrow \infty} x e^{-ikx} \mathbf{E}_{\text{sca}}(k; \mathbf{x}) \quad (3.3)$$

Where

$$\hat{\mathbf{x}} = \frac{\mathbf{x}}{x} \quad (3.4)$$

Using the optical theorem that relates the imaginary part of the forward scattering amplitude to the total cross-section, the extinction cross section can be obtained from the scattering dyadic $\mathbf{S}$ in the forward direction which means $\hat{\mathbf{x}} = \hat{\mathbf{k}}$. This fact shows that $\mathbf{S}$ cannot be real in all directions, and in particular, $\mathbf{S}$ has a positive imaginary part in the forward direction [34, 35].

$$\sigma_{\text{ext}}(k; \hat{\mathbf{k}}, \hat{\mathbf{e}}) = \frac{4\pi}{k} \text{Im}\{\hat{\mathbf{e}}^* \cdot \mathbf{S}(k; \hat{\mathbf{k}} \curvearrowright \hat{\mathbf{k}}) \cdot \hat{\mathbf{e}}^*\} \quad (3.5)$$

This equation is also known as the optical theorem or forward scattering theorem [35, 36]. Where

$$\hat{\mathbf{e}} = \frac{\mathbf{E}}{|\mathbf{E}|} \quad (3.6)$$

is electric polarization that is here assumed to be linear, and $\mathbf{e}^*$ denotes the complex conjugate of the electric polarization.

According to the forward scattering sum rule, the integration of the total extinction cross section σ_{ext} (sum of scattering and absorption cross section) over all wavelengths can be determined by the total polarizability of the object [2, 34]. In general, the total polarizability (sum of electric and magnetic polarizability) can be mathematically determined (in this work by using the MATLAB code in [37]).

$$\frac{1}{\pi^2} \int_0^\infty \sigma_{ext}(\lambda; \hat{\mathbf{k}}, \hat{\mathbf{e}}) d\lambda = \{ \hat{\mathbf{e}}^* \cdot \gamma_e \cdot \hat{\mathbf{e}} + (\hat{\mathbf{k}} \times \hat{\mathbf{e}}^*) \cdot \gamma_m \cdot (\hat{\mathbf{k}} \times \hat{\mathbf{e}}) \} \quad (3.7)$$

Using the relation (3.2) will lead to:

$$\frac{2}{\pi} \int_0^\infty \frac{\sigma_{ext}(k; \hat{\mathbf{k}}, \hat{\mathbf{e}})}{k^2} dk = \{ \hat{\mathbf{e}}^* \cdot \gamma_e \cdot \hat{\mathbf{e}} + (\hat{\mathbf{k}} \times \hat{\mathbf{e}}^*) \cdot \gamma_m \cdot (\hat{\mathbf{k}} \times \hat{\mathbf{e}}) \} \quad (3.8)$$

Where γ_e and γ_m denote the electric and magnetic polarizability dyadics respectively [2, 34]. It should be pointed that the left-hand side of the relation (3.9), determines the extinction cross section (sum of scattering and absorption properties) of the object, which is the total interaction of the incident electromagnetic plane wave with the object. Furthermore, the larger scattering and/or absorption cross section requires the greater electric and/or magnetic polarizability dyadic. Thus a large value for the integral on the left-hand side of the relation (3.9) results from large scattering or/and absorption effects [2, 34].

The total scattering properties are determined by the scattering cross section σ_{sca} , which is the total power scattered in all directions divided by the incident power flux. The absorbed power in the obstacle is related to absorption cross section σ_{abs} . The extinction cross section σ_{ext} is defined as the sum of the scattering and absorption cross sections which is independent of the strength of the incident electromagnetic fields [1].

$$\sigma_{ext} = \sigma_{sca} + \sigma_{abs} \quad (3.9)$$

In general, the cross sections are normalized to the actual geometrical cross section of the particle (πa^2 for spherical particles with radius a) to give the so called efficiencies Q_{ext} , Q_{sca} and Q_{abs} which are dimensionless efficiencies called Q [1].

$$Q_{ext} = Q_{sca} + Q_{abs} \quad (3.10)$$

4.1 Metal Spherical Nanoparticle Scattering Properties

In this part, the scattering and absorption properties of nanoantennas excited by an electromagnetic plane wave, are investigated. In order to verify the simulation results from CST Microwave Studio as an initial step a simple structured nanoantenna, a nanosphere, made of PEC and a dielectric is investigated. After verification of the simulation result, the optical properties of gold, silver, copper and aluminum nanospheres are determined and compared with the theoretical result based on Mie series approach [2]. The next step is an approach to extinction efficiency and the resonant characteristics of spheroid nanodipoles made of the same metals with different sizes and with the same size of 100 nm are studied. Afterwards, the nanodipoles with the total length of 100 nm are loaded with different materials at their gap region with the gap length of 5 nm and the corresponding optical properties of the nanoantennas in each case are compared with each other. Finally, the local electromagnetic field enhancement of gold spheroid nanodipole without a gap and with a gap loaded by air and silver are studied. Additionally, the value of full width at half maximum (FWHM) and the value of $Q_{ext,res}$ for the nanoantennas in some parts are investigated.

4.1.1 CST Microwave Studio General Setting

The best evolved and understandable model for light scattering and absorption can be simply described by symmetrical shapes like spherical particles [1]. In order to excite the nanoparticle a linearly polarized electromagnetic plane wave is exploited and to generate the structure of the

sphere, the template for antennas in free space is used. The frequency unit is set to terahertz and the frequency range is 800 to 6500 THz. The background material is defined as vacuum, and the boundary conditions are set to "expanded open". The excitation is determined as an external plane wave propagating in -z direction and in order to obtain the far field properties, a probe of "E-field (far field)" is located at a distance beyond the well known Rayleigh far field distance (here 3000 nm is chosen, from the center of the sphere located at the origin. This distance can be simply determined by the well known far field criterion formula, i.e $2d^2/\lambda$, where d is the largest dimension of the antenna and λ is the operational wavelength of interest. The probe information is stored in the folder "Probe" in the navigation tree, where the corresponding plot mode has to be chosen to get the visualization of the E-field (far-field) properties. The excitation signal of the plane wave is listed in the folder "1D Results" as well. The solver is time domain solver, where the mesh type is "Hexahedral" and the steady state energy accuracy level is set to -80 dB to get as precise result as possible. As the first step, PEC and dielectric $\epsilon = 2$ spherical nanoantennas with a radius $a=50$ nm, are simulated and then the data from the probe in CST is exported to MATLAB for post processing. Figure 4.1 summarizes the extinction efficiency of PEC and the dielectric sphere against the size parameter $X_{P,S} = ka$ within the frequency range of 800 to 6500 THz. It

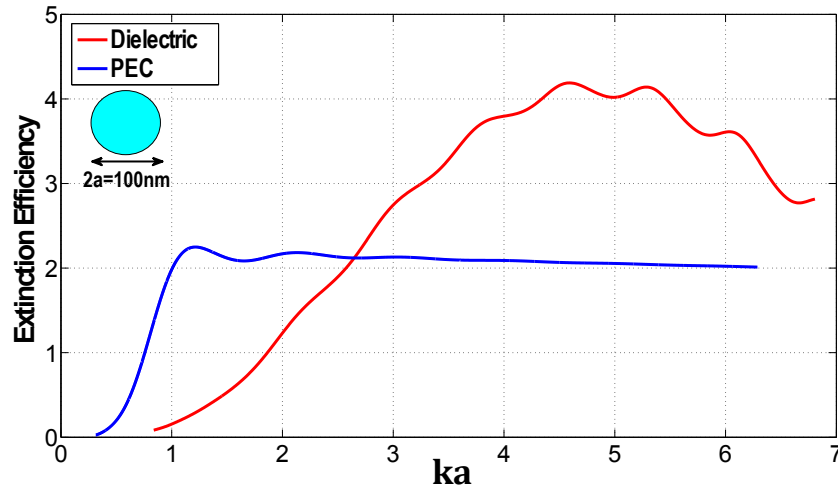


Figure 4.1: The extinction efficiency spectra of dielectric with permittivity of $\epsilon = 2$ and PEC spherical nanoparticles.

is notable that the extinction efficiency denotes the extinction cross section normalized by the geometrical cross section of the nanoparticle, and k is the wave number. In this figure, the Rayleigh scattering regime is attributed to longer wavelengths corresponding to $ka \lesssim 1$, whereas the Mie scattering regime is associated with $ka \gtrsim 1$. The CST simulation results for PEC and dielectric spherical nanoparticle are the same as the corresponding theoretical results from a MATLAB script that is based on Mie series approach. Thus, the verification of the result from CST allowed for investigation of the scattering properties of the other nanometals with different shape and sizes.

4.1.2 Au, Ag, Cu, and Al Spherical Nanoparticles

In this part, an aluminum nanosphere was the first choice to investigate its scattering properties. Using the Drude-Lorentz model from [31], the complex permittivity of aluminum at the frequency range of 300 to 3000 THz is described by the Drude-Lorentz model in [31] and loaded to CST Microwave Studio. In order to achieve as accurate results as possible, there are several settings in CST that should be appropriately managed before running the solver. The polar data of the far field probe from simulation in CST Microwave Studio were exported to MATLAB for post processing. The results for the extinction efficiency of aluminum nanosphere in different steps of setting in "Boundary Conditions" and "Mesh Properties" of simulation in CST is shown in figure 4.2(a) and also the comparison between the final simulation result and the theoretical result based on Mie series approach (see [2], part 4, figure 5) are depicted in figure 4.2(b). Due to the lack of appropriate setting in "Boundary Conditions" and "Mesh Properties" The initial results were far away from the theoretical result. The high precision of the final simulation result for aluminum spherical nanoparticle compared to the theoretical one based on Mie series approach in [2], allows to evaluate the extinction efficiency of other interesting metals. In order to obtain the scattering properties of gold, silver and copper, the complex values of permittivities for the corresponding metals from the MATLAB code of Drude-Lorentz model in [38], were loaded to the CST "material library".

Figure 4.3 summarizes Au, Ag, Cu and Al nanosphere with a radius of $a=50$ nm. The nanospheres exhibit their extinction bands peaked several times around their harmonic resonance wavelengths, which is associated with both the surface plasmon polariton resonances and harmonic oscillators in the corresponding nanometals. Here, the forward scattering sum rule simply estimates the overall behavior of the extinction cross section in

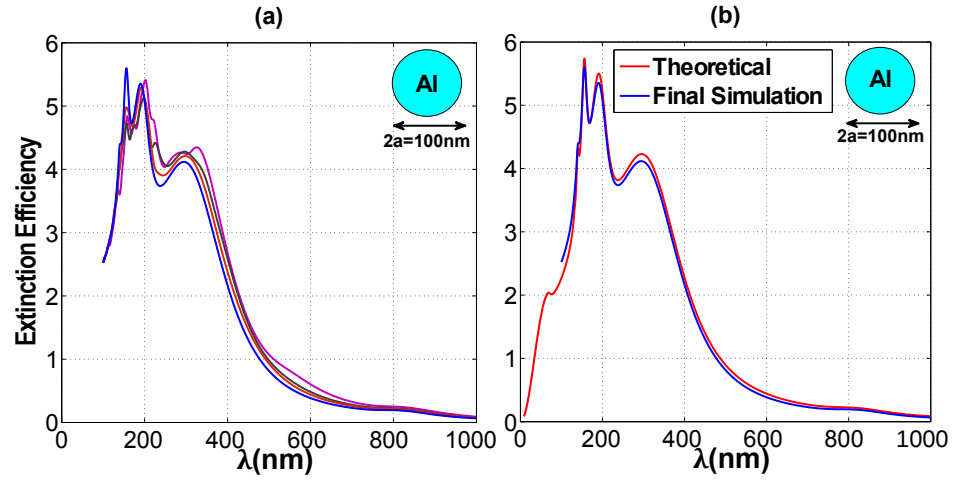


Figure 4.2: (a): Different simulation results of the extinction efficiency spectra of an aluminum spherical nanoparticle with low accuracy. (b): A comparison between the theoretical result based on Mie series approach in [2] and final simulation result for an aluminum spherical nanoparticle with a radius of $a=50\text{ nm}$.

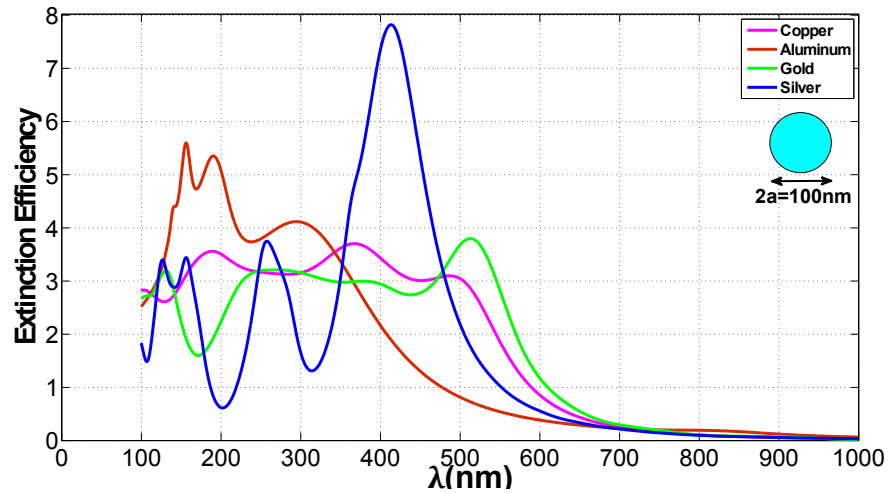


Figure 4.3: The extinction efficiency spectra of Au, Ag, Cu and Al nanospheres with a radius of $a=50\text{ nm}$.

a way that the dispersive characteristics of the metals determine the resonances and the total polarizability of the nano spheres determine the areas below the curves.

In noble metals, the changes in the observed color are attributed to the changes in shape of nanoparticles to some extent. Typically, during light scattering, silver spheres have a characteristic yellow color, whereas gold spheres are red. The main cause of the colors in noble metal nanoparticles is the collective oscillation of the electrons in the conduction band. Their oscillation frequency is usually located in the visible region thus, they usually represent strong surface plasmon resonance absorption [38].

4.2 The Scattering Properties of Au, Ag, Cu and Al spheroid Nanodipoles

Consider a metal nanospheroid (a spheroid nanodipole without a gap) embedded in a transparent background with permittivity ϵ_0 and permeability μ_0 . At optical frequencies the nanoantenna works as a scatterer illuminated by a uniform plane wave travelling along the negative z direction with the electric field polarized along dipole axis, in this work x axis.

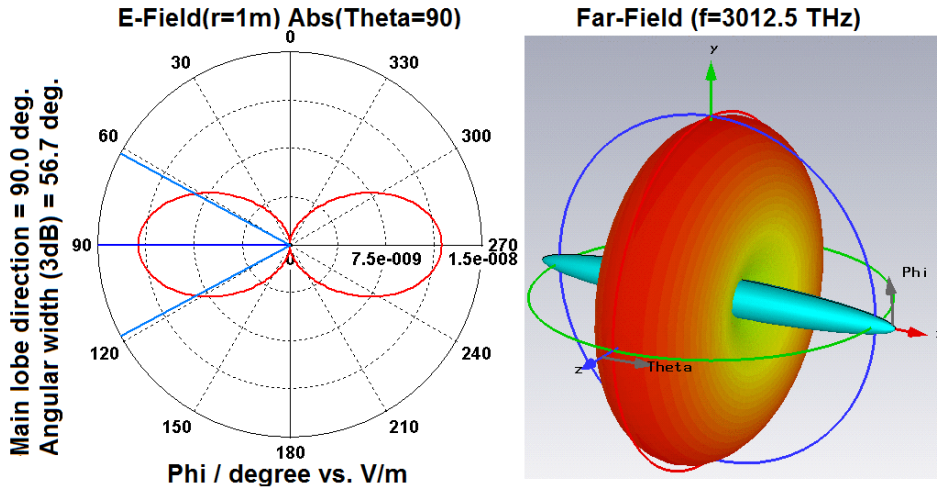


Figure 4.4: The far-field distribution of gold spheroid nanodipole with a length of $L = 100$ nm and a diameter (in the center of the two arms) of $D = 10$ nm.

Using the optical theorem in [35], the extinction cross sections can be obtained from the scattered far-fields in the forward direction. Typically, in sub wavelength sizes, the dipole fields are dominant when conventional materials are used, and the nanoantenna is conveniently described in terms of its electric and magnetic polarizabilities. In this case, the far field distribution is similar to the standard "donut" shape of a conventional dipole pattern, which is azimuthally uniform around the direction of polarization, with a null along the polarization axis (see figure 4.4). The frequency range is set to 25-6000 THz, and all the simulation settings in CST are done as the same process as previous part. It should be underlined that the increase in sizes of gold and silver spheroid nanodipole leads to higher resonance wavelength, and also a convergence in the value of λ_{res}/L to that of a half wavelength PEC spheroid nanodipole. Furthermore, the extinction spectra for different length of PEC nanodipoles are exactly mapped on each other, which means the two dipoles perform as half wavelength spheroid nanodipole. Additionally, the areas below the curves for the same metal, gold or silver, but different sizes, must be exactly the same since, the extinction cross section is normalized with the geometrical cross section of the spheroid nanodipole, A , (for a spheroid nanodipole the geometrical cross section is equal to $\pi L D/4$) and the wavelength is normalized by the length of the corresponding dipole L , which result in dimensionless plots. Therefore, if the relation (3.9) is normalized by $L \cdot A$ (the length times the geometrical cross section), it will result in equal scalar (dimensionless) values for both sides of the relation.

$$\frac{1}{\pi^2 L A} \int_0^\infty \sigma_{ext}(\lambda; \hat{\mathbf{k}}, \hat{\mathbf{e}}) d\lambda = \frac{1}{L A} \{ \hat{\mathbf{e}}^* \cdot \gamma_e \cdot \hat{\mathbf{e}} + (\hat{\mathbf{k}} \times \hat{\mathbf{e}}^*) \cdot \gamma_m \cdot (\hat{\mathbf{k}} \times \hat{\mathbf{e}}) \} \quad (4.1)$$

The left hand side of the relation (4.1) denotes the total surface below each curve (in figures 4.5 and 4.6) which can be mathematically determined. On the other side of the relation (4.1), since, γ_m is negligible and the value of $(\hat{\mathbf{e}}^* \cdot \gamma_e \cdot \hat{\mathbf{e}})$ for each spheroid nanodipole is obtainable using the MATLAB script in [37], the right hand side of the relation boils down to $(\hat{\mathbf{e}}^* \cdot \gamma_e \cdot \hat{\mathbf{e}})/(L A)$. It is notable that γ_e itself is dependent on the size and shape of the nanodipoles regardless of the material, whereas the fraction of $(\hat{\mathbf{e}}^* \cdot \gamma_e \cdot \hat{\mathbf{e}})/(L A)$ is equal to 3.286 for both gold and silver spheroid nanodipoles and it is independent of the size, shape and material of the nanodipoles. However, for PEC, γ_m has a negative value which causing a slightly less value for the left hand side of the relation (4.1). Therefore, the comparison between the value of $(\hat{\mathbf{e}}^* \cdot \gamma_e \cdot \hat{\mathbf{e}})/(L A)$ and the left hand side of the equation (4.1) can be helpful to investigate the precision of the simulation results depicted in figures 4.5, 4.6, 4.11, 4.12, 4.13 and 4.14.

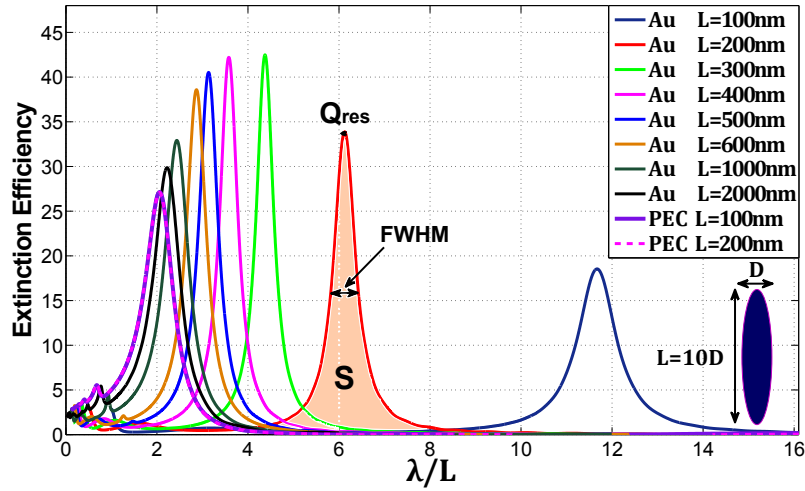


Figure 4.5: The extinction efficiency spectra of Au and PEC spheroid nanodipole with different lengths L increasing from right to left.

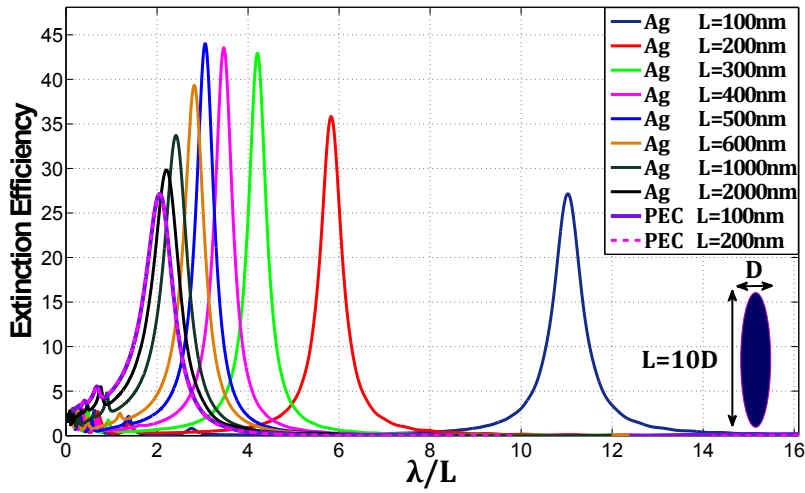


Figure 4.6: The extinction efficiency spectra of Ag and PEC spheroid nanodipole with different length L increasing from right to left.

It is notable that the peak position, the resonance wavelength and the FWHM (where the extinction efficiency becomes half of its maximum at λ_{res}/L) is referred to the size, shape, material and the polarizability of the dipoles.

Due to the equal values for the surfaces below the curves, the greater the extinction efficiency is, the less FWHM is (see also figure 4.5, 4.6 and the corresponding tables 4.1 and 4.2, respectively as well as figure 4.16).

The results for gold and silver spheroid nanodipoles with different lengths corresponding to figures 4.5, 4.6 are summarized in tables 4.1 and 4.2, respectively. In these tables $(\hat{\mathbf{e}}^* \cdot \gamma_e \cdot \hat{\mathbf{e}})/(LA)$ is identical for different sizes and shapes of the dipoles are noticeable.

According to the tables 4.1 and 4.2 that summarizes the size effect on the scattering properties of gold and silver spheroid nanodipoles, the increase in size of the dipoles, shifts the peaks to longer wavelengths, decreasing the value of λ_{res}/L which converges to that of half wavelength PEC spheroid nanodipoles.

In addition, as the size of gold and silver spheroid dipoles increases the resonance frequencies for the same size of the dipoles are very close to each other, whereas in shorter dipoles with the same length, for example $L=100$ nm, the corresponding resonance frequencies are clearly different. Furthermore, the surface below each curve in figures 4.5, 4.6 is almost equal to the constant value of $(\hat{\mathbf{e}}^* \cdot \gamma_e \cdot \hat{\mathbf{e}})/(LA)$ for the two dipoles with different sizes and thus the higher values of $Q_{ext,res}$ leads to less values for FWHM. It should be mentioned that there is about 2% error, since the frequency range of the simulation does not cover all frequencies from zero to ∞ moreover, there is some CST simulation error as well.

Table 4.1: The Optical Properties of Gold Spheroid Nanodipole with Different Lengths.

L [nm]	f_{res} [THz]	λ_{res}/L	S	$\hat{\mathbf{e}}^* \cdot \boldsymbol{\gamma}_e \cdot \hat{\mathbf{e}}/(LA)$	$S/(\gamma_e/LA)$	$Q_{ext,res}$	$FWHM$	$Q_{ext,res} \cdot FWHM$
100	256.87	11.67	3.216	3.286	0.979	18.537	1.0200	18.9
200	244.76	6.124	3.251	3.286	0.989	33.862	0.5700	19.3
300	228.39	4.376	3.251	3.286	0.989	42.493	0.4615	19.6
400	209.39	3.579	3.258	3.286	0.991	42.208	0.4780	20.2
500	191.25	3.135	3.258	3.286	0.991	40.524	0.5085	20.6
600	174.17	2.869	3.255	3.286	0.990	38.591	0.5366	20.7
1000	122.99	2.438	3.273	3.286	0.996	32.917	0.6450	21.2
2000	67.423	2.223	3.240	3.286	0.986	29.868	0.7210	21.5

Table 4.2: The Optical Properties of Silver Spheroid Nanodipole with Different Lengths.

$L [nm]$	$f_{res} [THz]$	λ_{res}/L	S	$\epsilon^* \cdot \gamma_e \cdot \epsilon / (LA)$	$S / (\gamma_e / LA)$	$Q_{ext,res}$	$FWHM$	$Q_{ext,res} \cdot FWHM$
100	271.900	11.03	3.201	3.286	0.974	27.149	0.730	19.8
200	257.308	5.826	3.324	3.286	1.011	35.829	0.556	19.9
300	237.591	4.206	3.249	3.286	0.989	42.946	0.474	20.3
400	216.200	3.467	3.292	3.286	1.002	43.551	0.462	20.1
500	196.034	3.059	3.280	3.286	0.998	44.013	0.473	20.8
600	177.243	2.819	3.282	3.286	0.999	39.323	0.533	20.9
1000	124.066	2.416	3.262	3.286	0.993	33.708	0.630	21.2
2000	67.8706	2.209	3.225	3.286	0.981	29.836	0.720	21.5

At optical frequencies in most metals, due to free electron contributions called inter band transition, the real part of $\epsilon(\omega)$ is changed to negative causing these resonance structures. Figure 4.7 shows how the changes in size impact the resonance wavelength and compares the dielectric functions of gold and silver spheroid nanodipoles with different lengths increasing from left to right, at their resonance wavelengths.

When it comes to noble metals such as gold and silver, the resonance wavelength is increased for larger sizes of the nanodipoles. While the imaginary parts of the dielectric function for gold and silver are almost similar, gold has a larger real part of the dielectric function than silver.

According to the figure 4.7, for the same size of gold and silver spheroid nanodipoles, since gold has lower plasma frequency than silver, it has higher resonance wavelength (lower resonance frequency) compared to that of silver. This difference becomes more apparent as the size of the

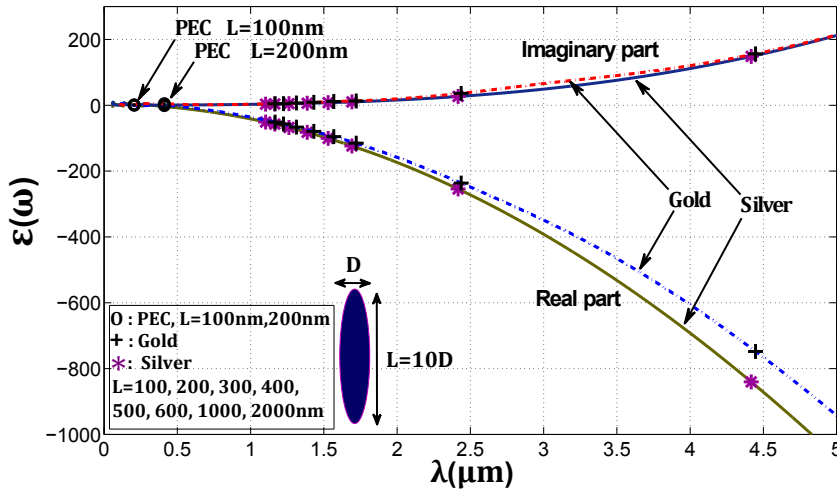


Figure 4.7: The complex permittivity $\epsilon_{\lambda_{res}}$ at the resonance wavelengths of gold and silver spheroid nanodipoles with different lengths of L increasing from left to right.

dipoles decreases from right to left in figure 4.7 particularly for the nanodipoles with the length of 100 nm, where the resonance wavelength of the gold spheroid nanodipole is remarkably larger than that of silver spheroid dipole.

Figure 4.8 also shows that as the size of nano spheroid dipoles increases to 1 μm and 2 μm the two dipoles with different materials but the same size represent almost the same resonance characteristics.

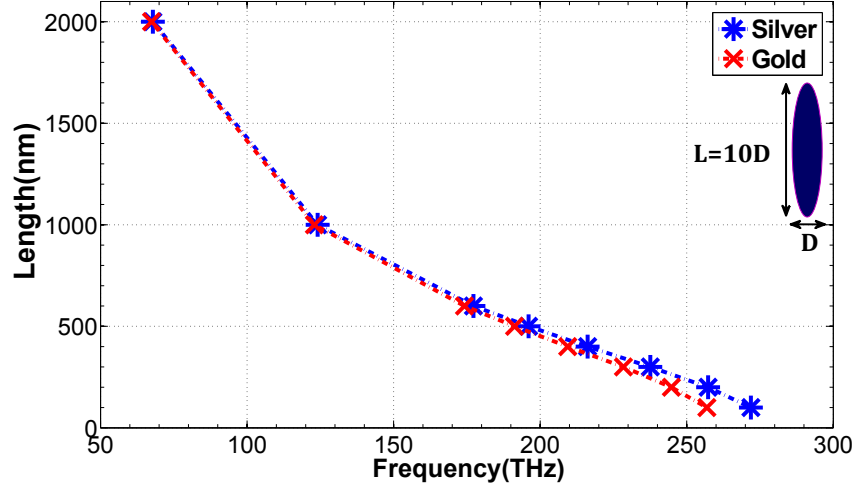


Figure 4.8: The resonance frequency of gold and silver spheroid nanodipoles with different lengths. The length increases from 100 nm to 2000 nm (from right to left).

In terms of energy, the shorter the resonance wavelength is, the higher the photon energy is. In other words the photon energy is proportional to frequency f and moving to higher frequencies at which the surface Plasmon occurs, results in larger amount of photon energy.

$$E_{ph} = hf = \frac{hc_0}{\lambda} \quad (4.2)$$

Where E_{ph} is the photon energy in joules and $h = 6.626069 \cdot 10^{-34} \text{ J} \cdot \text{s}$ is Plank's constant. Commonly, the unit of energy for nanoparticles is the electron-volt (eV) rather than the Joule (J), where $1\text{eV} = 1.602 \cdot 10^{-19} \text{ J}$. Figures 4.9 and 4.10 studies the size effect on the extinction efficiency against photon energy for gold and silver spheroid nanodipoles with different lengths.

It is obvious that, as the size of the nanodipoles increase from right to left, the peak position is shifted to longer wavelengths corresponding to the lower photon energy. This fact can also be studied in detail in figure 4.7. It should be mentioned that in this sense since, the x-axis is defined as photon energy, the plots are not any more dimensionless therefore, the surface below the curves are not equal here.

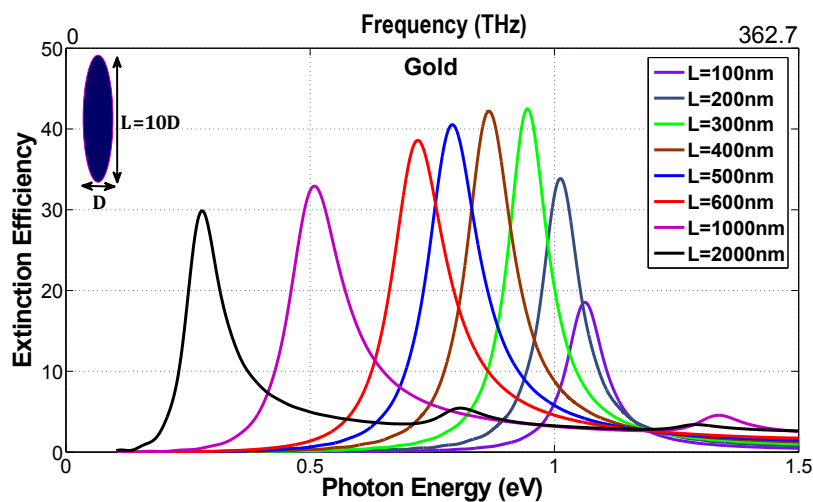


Figure 4.9: The extinction efficiency spectra against photon energy for gold spheroid nanodipole with different length L increasing from right to left. The plots are not dimensionless therefore, the surface below the curves are not equal here.

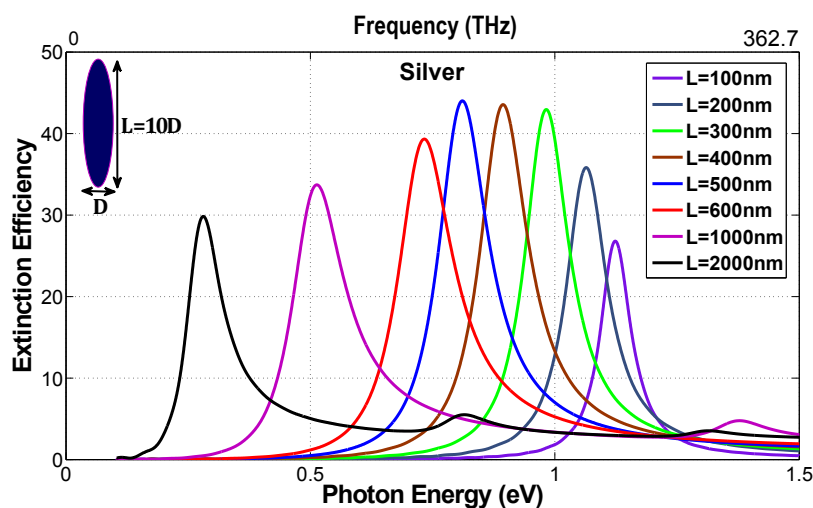


Figure 4.10: The extinction efficiency spectra against photon energy for silver spheroid nanodipole with different length L increasing from right to left. The plots are not dimensionless therefore, the surface below the curves are not equal here.

The principals of the photon energy is used in many applications e.g., light emitting devices, photovoltaics and spectroscopy applications, where an electron and hole pair are combined, separated, or polarized by incident light field which leads to photon emission (in LED), photon absorption (in photovoltaics), or both photon emission and absorption simultaneously (in spectroscopy), respectively.

Figure 4.11 illustrates the effect of material on the extinction efficiency spectra of Au, Ag, Cu, and Al spheroid nanodipole with the length of 100 nm against wavelength. Consider figure 3.1 which illustrates the dielectric functions of gold, silver, copper, and aluminum at optical frequency.

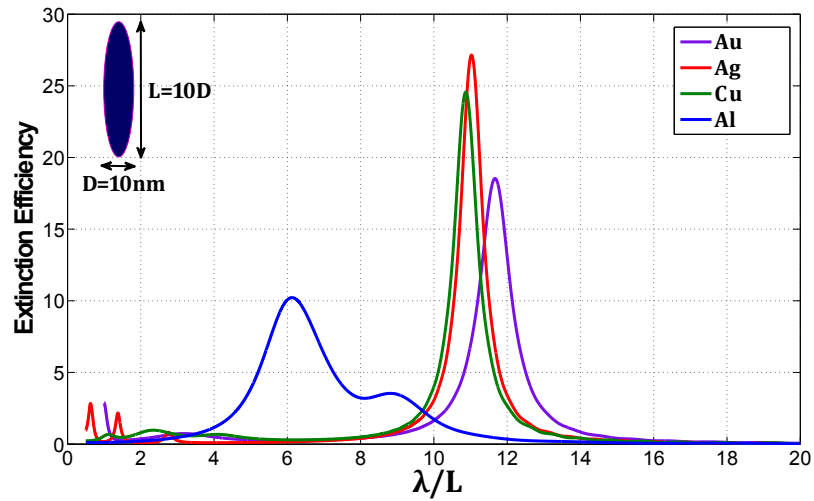


Figure 4.11: The extinction efficiency spectra of Au, Ag, Cu, and Al spheroid nanodipole dipoles with the same length of $L = 100$ nm. The plots are dimensionless thus the areas below them are equal.

This figure conveys plenty of information, first of all, while the imaginary parts of gold and silver complex permittivities are almost similar, gold has a larger real part than silver. It is predictable that, the resonance frequency for gold nanodipole is lower than that of silver, since gold has a lower plasma frequency compared to silver.

It is notable that for the same size of the dipoles the lower resonance frequencies leads to larger values for λ_{res}/L . On the other hand, copper has smaller imaginary part compared to gold, and due to a bit higher plasma frequency its resonance frequency is slightly higher compared to silver. Eventually, for aluminum due to an even higher plasma frequency, the

resonance frequency is shifted to a quite higher frequency, while it has remarkably large imaginary part than gold and silver. This fact is obviously summarized in figure 4.7 (for gold, and silver spheroid nanodipoles with different length L) and figure 4.11 (for gold, silver, copper, and aluminum spheroid nanodipoles with the length of 100 nm).

4.3 Metal Spheroid Nanodipole With Different Loading Materials At The Gap Region

In this section, the geometry of the problem is the same as in the previous part and the only difference is the existence of a gap between the two arms of the dipole. The gap thickness G is 5 nm and the center of the gap has diameter of $D = 10$ nm. The total length of the dipole L including the gap is 100 nm. For the simulation in CST Microwave Studio, a plane wave polarized along the dipole axis x , impinging the optical spheroid nanodipole made of gold, silver, copper and aluminum. Here also the permittivity of the metals at the frequency range of interest (i.e., 25-6000 THz) is taken from the classical Drude-Lorentz model in [38].

Here, the two dipole arms are capacitively or inductively, depending on the loading nanoparticles at the gap, coupled. Typically a nanodipole excited by external light field has the ability of generating a considerable field enhancement within its nano-gap region. The incident plane wave causes an electromagnetic field inside the dipole polarizing the charges on the surface of the two dipole arms. The collective negative and positive charges on the surfaces of the dipole arms facing the gap, form a capacitor or inductor. This capacitor or inductor and the two arms of the dipole form an electric network that can be in resonance with the excitation of even a small plane wave field [6].

The plane wave excitation of the dipole creates alternating surface charges causing the dipole oscillation. The resonance frequency depends on the gap size and the polarizability of the material constituting the gap and also the size of the dipole. The coupling between the two arms of the nanodipole is determined by the gap size since it has a key role in the dipole far field responses shifting its resonances.

In this scenario, the nanogap is loaded either with air or with a nanodisk made of a material with a positive (negative) real part permittivity, ϵ_{load} , that acts as an optical lumped element, a nanocapacitor (nanoinductor) [6]. In addition, depending on the operating frequency the incident plane wave penetrates deeper into the nanodipole displacing the electrons in the atoms so that each atom acts as an electric dipole [1].

Initially, the nanogap is loaded by air and the antenna is excited by an external plane wave field the same as previous part. Based on this aspect, the simulation results of the extinction efficiency for gold, silver, copper and aluminum spheroid nanodipole with the total length of $L = 10D = 100$ nm and the air gap of $G = 5$ nm is depicted in figure 4.12, where the effect of the material on the scattering properties of the dipoles is apparent.

Similar to figure 4.11, the material that the nanodipole is made of, dominantly determines the peak location. In this scenario, the areas below the plots in figure 4.12 are equal but due to the air gap, less than that of spheroid nanodipoles without gap in figure 4.11. Additionally, the air gap as a capacitive load has remarkably shifted the corresponding resonant wavelengths to lower values with less values for the extinction efficiency compared to figure 4.11. Therefore, it can be concluded that, the operation frequency of a nanodipole can be promoted to higher values by using insulating nanomaterials like air that functions as capacitive load. However, less values for the extinction efficiency is inevitable.

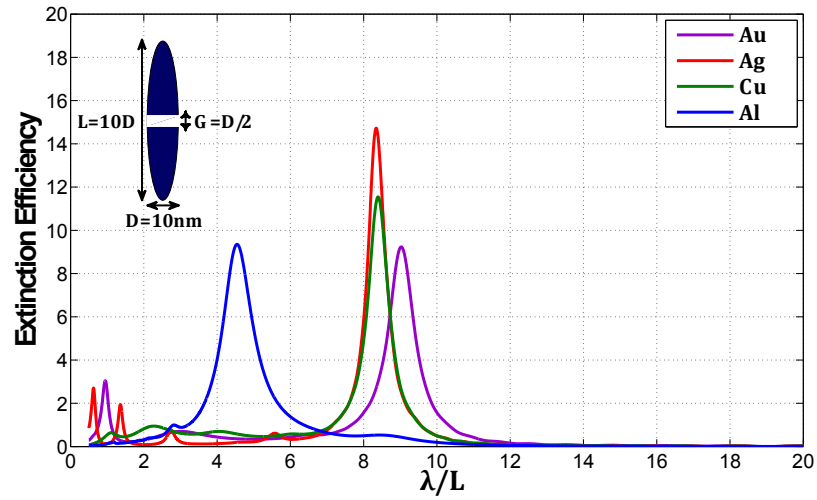


Figure 4.12: The extinction efficiency spectra of Au, Ag, Cu, and Al spheroid dipole with an air gap. The areas below the plots are equal but due to the air gap, less than that of spheroid nanodipoles without gap.

The gap region can be loaded with different materials with different complex permittivities of, either inductive load by using plasmonic materials or capacitive load by using insulating materials. The interaction of the nanoparticle atoms in the gap region with the impinging light can be

directly referred to the loading materials at the gap. In this case, the optical properties of the nanodipole, the sensitivity and the resonant frequency of the nanodipole, is highly associated with the complex permittivity of the loading material at the nanogap region [6].

Figures 4.13 and 4.14 report the simulation results of the extinction efficiency of gold and silver spheroid nanodipoles with different nanoloads at their gaps. These figures show the effect of the loading material at the nanogap region on the optical properties. The different loading materials at the gap region of a spheroid nanodipole with the same total length of 100 nm and gap length of $G=5$ nm, result in different values for the extinction efficiency and resonance characteristics since these materials act as optical lumped elements with different characteristics.

Since the two plots are dimensionless, the areas below the curves are equal except the vacuum case. Furthermore, in these two figures, for metal gap cases the areas below the plots are also equal to that of spheroid nanodipole without gap in figures 4.5, 4.6 and 4.11. It can also be inferred that the specific shape, size and material of these nanoantennas as well as the loading materials at the gap, guarantee a large concentration and specific orientation of the electric field at the gap location, interacting with the loading nanoparticles.

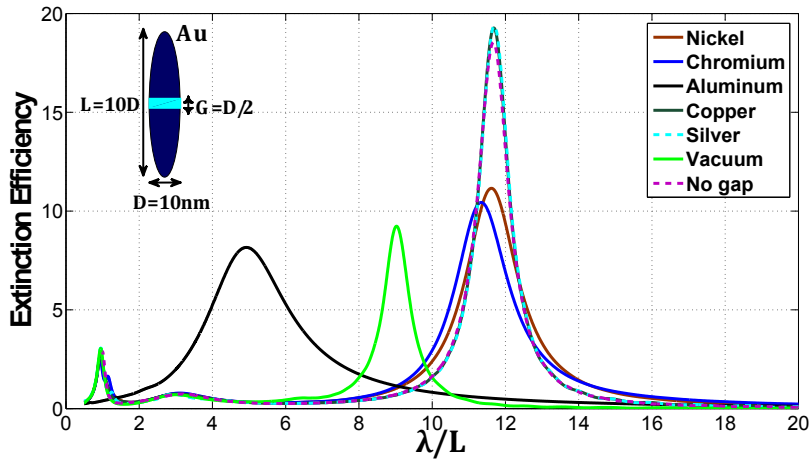


Figure 4.13: The extinction efficiency spectra of gold spheroid nanodipole with different nanoloads at the gap region. For the cases that the gap is loaded with metals, the areas below the plots are equal to each other and also to that of spheroid nanodipole without gap.

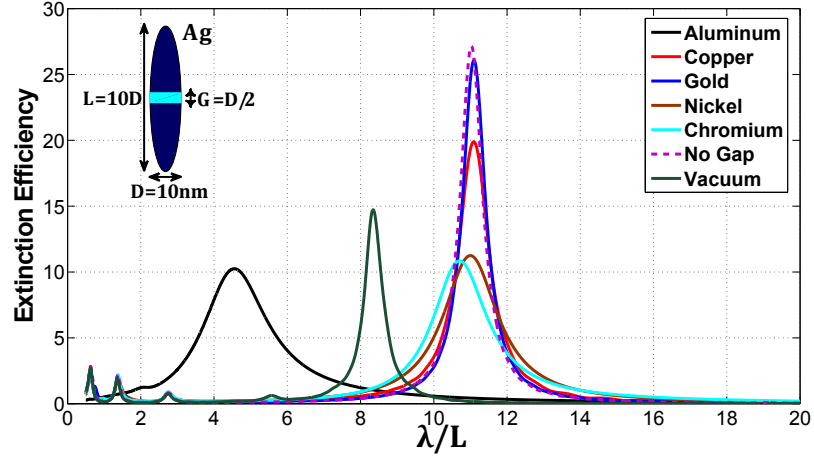


Figure 4.14: The extinction efficiency spectra of silver spheroid nanodipole with different nanoloads at the gap region. For the metal gap cases the areas below the plots are equal to each other and also to that of spheroid nanodipole without gap.

Figure 4.15 shows the electric field distribution and its absolute value for the gold spheroid nanodipole in figure 4.13 in three cases: (a): without a gap, (b): with a vacuum load at the gap and (c): with a silver load at the gap region, at their resonance frequencies $f = 257$ THz, $f = 256$ THz and $f = 332$ THz, corresponding to $(\lambda_{res}/L = 11.67)$, $(\lambda_{res}/L = 9.03)$ and $(\lambda_{res}/L = 11.71)$, respectively.

This informative figure shows how the field is locally confined at the end of the two nanodipole arms and its gap (if a gap exists). The left hand side figures correspond to the absolute value of the electric field and confirm the resonant characteristics of the nanodipole in the three cases, while the right hand side figures illustrate the spreading of displacement current in the three cases. It should be underlined that, the air gap in the case (b) couples the two arms of the nanodipole capacitively owing to the fact that it serves as capacitive nanogap, the electric field is locally enhanced at the gap region and the dipole arm ends. For the dipole in the case (c), the gap loaded with silver (a plasmonic material with very similar resonant characteristics to gold) couples the two dipole arms inductively. Therefore, a close resonance frequency to that of gold nanospheroid dipole takes place for the same size of silver spheroid nanodipole as gold one. This fact should be attributed to a higher resonance frequency in the case of the air gap compared to the two other cases.

Furthermore, the close resonance frequencies in the gold spheroid nanodipole without a gap and with a gap loaded with silver is referred to the similar characteristics of gold and silver in terms of SPPRs at the gap region since, they are both plasmonic noble metals and also the imaginary part of their complex permittivities are almost the same thus, they have similar loss at optical frequencies. In this sense, the field confinement and enhancement at the both dipole tips in (a) without a gap and (c) with a silver loading material at the gap region, is noticeable.

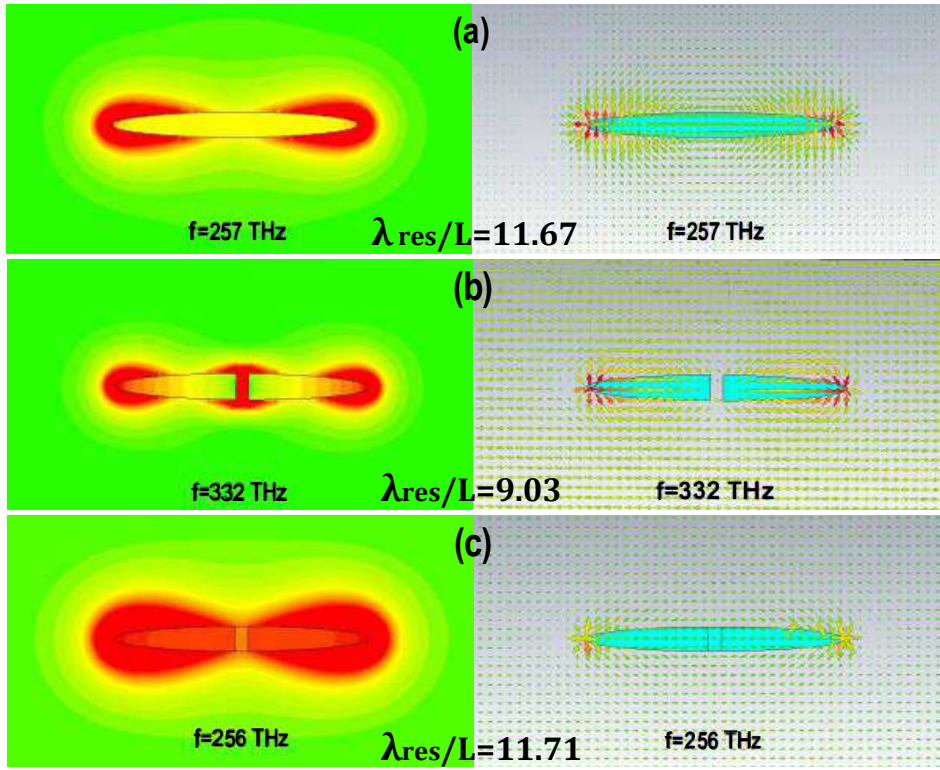


Figure 4.15: The snapshot of electric field distribution and its absolute value on the XY plane of gold spheroid nanodipole with different loading material at the gap region. The total length of the dipole is 100 nm. (a): the dipole with no gap at its resonance frequency $f_{(a)} = 257$ THz ($\lambda_{(a)}/L = 11.67$), (b) and (c): the gap with the length of 5 nm loaded with air and silver at the corresponding resonance frequencies $f_{(b)} = 332$ THz ($\lambda_{(b)}/L = 9.032$) and $f_{(c)} = 256$ THz ($\lambda_{(c)}/L = 11.71$), respectively.

The next step is to analyze and quantify the field confinement at the gap and the end of the two arms of a nanodipole. The *Full Width at Half Maximum* (FWHM) is a helpful parameter to describe the width of a curve or a function which hits a peak. This parameter is commonly defined as the distance between the two points on the curve at which the function reaches half of its maximum. In this work this parameter denotes the distance between the two points on the extinction efficiency spectrum where Q_{ext} becomes half of its maximum.

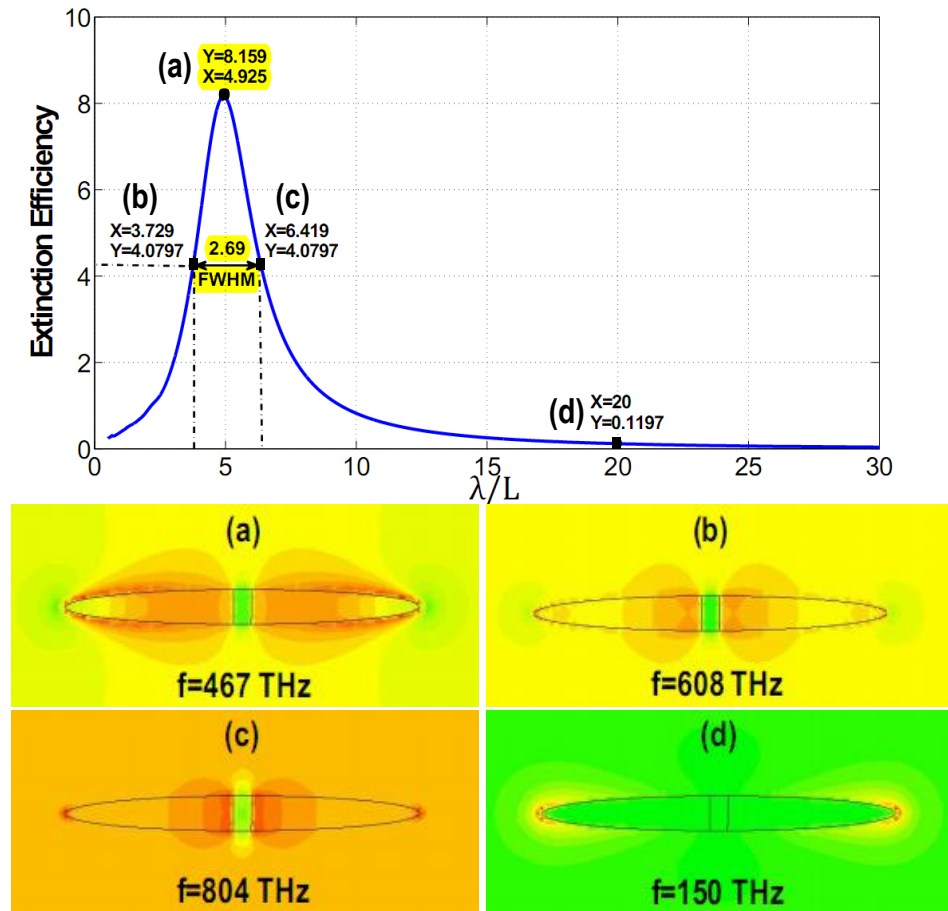


Figure 4.16: The extinction efficiency of gold spheroid nanodipole with the total length of 100 nm and the gap length of 5 nm loaded with aluminum (taken from figure 4.13) as well as the snapshot of absolute value of electric field distribution on the XY plane at four different points of (a), (b), (c) and (d).

Figure 4.16 compares the absolute values of the electric field distribution of gold spheroid nanodipole where the nanogap is loaded with aluminum (see figure 4.13), on the XY plane at four different points: (a) At the resonance frequency ($\lambda_{res}/L \approx 5$) where the extinction efficiency hits a peak $Q_{ext,res} \approx 8.16$. (b),(c) At full width at half maximum (FWHM) ($\lambda_{FWHM(a)}/L = 3.729$ and $\lambda_{FWHM(c)}/L \approx 6.42$) where the extinction efficiency becomes half of its maximum $Q_{FWHM(b)\&(c)} \approx 4.1$. (d) At an arbitrary point ($\lambda_{(d)}/L \approx 0.12$) that the corresponding extinction efficiency has a very low value $Q_d \approx 8.16$. In addition, the figure gives information about the interesting values of $FWHM = 2.69$ and $Q_{ext,res} \cdot FWHM \approx 21.95$ at the resonance frequency.

Conclusions

This master's thesis investigates the scattering properties of plasmonic structures (nanoantennas) at optical frequencies. The finite conductivity and dispersive permittivity of metals in the optical regime, are associated with the presence of both free electrons contribution and harmonic oscillators contribution. Therefore, the frequency dependent dielectric function of nanoantennas plays a significant role in their scattering properties.

The scattering properties of a nanoantenna are significantly affected by the size, shape, material and polarizability of the nanoantenna and its surrounding medium. While the dispersive permittivity of a nanoantenna determines its resonance characteristics, the total polarizability of the nanoantenna determines the total area under the curve of the integrated extinction cross section over all wavelengths.

It is notable that different sizes of a nanoantenna represent different polarizabilities and thus different resonance characteristics, and the integrated extinction efficiency over all normalized wavelengths by the longest dimension of the nanoantenna, is identical for any size of it, therefore the larger value for the extinction efficiency at the resonance frequency leads to less value for FWHM and vice versa.

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