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Electromagnetic Simulation on Silver Nanoparticle Based Biosensors

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Abstract

In this paper, we have theoretically investigated the biosensing capability and silver nanoparticle. We study the optical properties of the electromagnetic simulation of silver nanoparticle in far field and near fields. Silver nanoparticles have unique optical and electronic properties which make them suitable for biosensing applications. The interaction of light with silver nanoparticle produces a collective oscillation of conduction band electron known as localized surface plasmon resonance. Plasmon resonance occurs when the frequency (wavelength) of the source is equal to the target frequency. Around this peak wavelength, we can detect the presence of desired target. To simulate the extinction cross section of silver nanoparticle in the Plasmonic resonance peaks in far and near fields, Finite Difference Time Domain (FDTD) method is applied. In our investigations the optical properties of plasmon resonance peak position occur in the visible and near infrared light (400 nm to 800 nm). Using FDTD method, the Plasmonic resonance enhanced light extinctions has been determined for nanodisk shaped silver nanoparticles with radius range from 10 nm to 60 nm. The electromagnetic sources are used based on the frequency- domain field and power design, including completely customizable uniaxial- perfectly matched layer (UPML) to simulates the real open system.

Key word: silver nanoparticle, Biosensors, localized surface plasmon, Plasmon resonance, FDTD

1. Introduction

The term biosensor is an abbreviation to mean biological sensor. It is an analytical device used for the detection of bio chemical substance. It gives the information the bio-composition, structure and function and a biomolecule substance converting a biological response into an electrical signal [1]. Biosensors function by coupling a biological sensing element with a detector system using a transducer. The analytical devices composed of a biological recognition element directly interfaced to a signal transducer which together relates the concentration of an analytic to a measurable response. Biosensors give exciting opportunity for high-impact applications benefiting from “nano” attributes [2]. An optical biosensor is a compact analytical device containing a biorecognition sensing element integrated with an optical transducer system [3]. The basic characteristics of biosensors are linearity, sensitivity, selectivity and the response of time. The importance of these to the fundamental expansion of biosensors has been recognized. In particular, nano-materials such as gold nanoparticle, carbon nanotubes, magnetic nanoparticle and quantum dots have been being actively investigated for their applications in biosensors, which have developed a new interdisciplinary border between biological detection and material science [4]. Biosensors can be used for the detection of various substances [5] like metabolites, pollutants, microbial load, control parameters etc. Silver nanoparticles are one of the most commonly utilized nanomaterial’s due to their anti-microbial properties, high electrical conductivity, and optical properties [6].

Silver nanoparticles can have different shapes (spheres, rods, wires, and triangles), coatings (citrate, polymer, peptide, sugars,) and of different sizes from 1nm to 100 nm [7]. Nanoparticle can be defined as objects ranging in size from 1-100 nm that due to their size may differ from the bulk material [8]. Nanoparticle has a very large surface area compared to their volume, and then they are often able to react very quickly. Optical plasmonic nanoantennas are important for advanced optical sensing and imaging applications including localized surface plasmonic resonance, surface-enhanced fluorescence, chemiluminescence, and Raman scattering [9].

Silver nanoparticles have unique optical, electronic, and antibacterial properties [10], and are widely used in areas such as biosensing, photonics, electronics, and antimicrobial applications. The most used in biosensing and detection exploit the optical properties of silver nanoparticles, as conferred by the localized surface Plasmon resonance effect. That means, the specific wavelength (frequency) of incident light can induce collective oscillation of the surface electrons of silver nanoparticles. The wavelength of the localized surface Plasmon resonance is dependent on the silver nanoparticle size, shape, and agglomeration state. The simulated to the extinction cross section plasmonic resonance peak of silver nanoparticle in wavelength range from 400 nm to 800 nm.

Biosensors are characterized as simple measuring devices with a fast response suitable for measurement of wide spectrum of biological or chemical markers in different practical applications [11], for instance biochemical, medical, environmental, food, industrial, bio-security or pharmaceutical analysis and personal diagnostics which are based on connection of biological element or molecule with biological activity toward measured analytic on to surface of the used transducer [12]. For the simulation of the plasmon resonance of gold film completely dismisses the film the thicknesses from 1 nm to 10 nm but, the thickness greater than 10 nm there is the plasmon resonance peaks [13].The researcher studied, in experimental and simulating the novel metal nanoparticles and the extinction of the plasmonic resonance peaks sharply located. However, we studied in this paper about the simulation of nanoparticle for plasmonic resonance peaks optimized by using silver nanoparticle (Ag).

2. Objective of the study

2.1. General objective

In this paper study, characterizing the electromagnetic simulation on silver nanoparticle with different shape plasmonic based biosensors nanoantenna.

2.2. Specific objectives

- To simulate the plasmonic resonance peaks of silver nanoparticle in near field and far fields.
- To study the electromagnetic simulation of silver nanoparticle with different shape.

3. Methodology of the study

3.1. Theory of Finite Difference Time Domain

We study this paper electromagnetic simulation on silver nanoparticle based biosensors by using Finite Difference Time Domain (FDTD) simulation. The FDTD method approximates Maxwell’s equations in the differential form by a central distinction operator in both time and space [14]. FDTD method (named after the Chinese American applied mathematician Kane S. Yee, born 1934) is a numerical analysis technique used for modeling computational electrodynamics. FDTD is finding approximate solutions to the associated system of differential equations. FDTD is today's one of the most accepted method for the solution of electromagnetic problems. The method helps practitioners design antennas, wireless communications devices, high-speed digital and microwave circuits, and integrated optical devices with unsurpassed efficiency. There has been considerable improvement in FDTD computational technology over the past few years.

Computational electrodynamics or electromagnetic modifying is the process of modeling the interaction of electromagnetic fields with physical objects and the environment [15]. All design and simulation are done in FDTD tool. FDTD method is a numerical analysis method used for modeling differential equation. FDTD is time domain method with wide frequency range and treat nonlinear material property.

FDTD method simulation is easy to implement more than Discrete Dipole Approximation (DDA) and Finite Element Methods (FEM). Discrete Dipole Approximation (DDA) is a general method to compute scattering and absorption of electromagnetic waves by particles of arbitrary geometry and composition. Finite Element Method (FEM) is a numerical technique used to perform finite element analysis (FEA) of any given physical phenomenon. FDTD method is based on Maxwell equation. Widely used approach for modeling how light interacts with nano-scale structures [16]. Discretization of Maxwell equations can be adopted to solve the field distribution in different locations and at different points of time by the FDTD method in both time domain and space domain. In this paper, FDTD method is used to solve the scattering, absorption, and extinction spectrum of LSPR of silver NPs at the interface. The FDTD method was first introduced by Yee and is used to evaluate electric and magnetic field components based on a discrete mesh consisting of Yee cells. FDTD technique is used to computationally modify electromagnetic wave interactions with materials. It is used in various applications including, radar, high-speed analog, photonics, microscopy and nanotechnology. In order to clearly understand the usage of FDTD for modifying and simulation of plasmonic nano-particles, a brief review of FDTD and its various software packages are described in this section. The major significant of the FDTD method compared to other methods and its ability to provide a full spectrum in a single simulation by propagating in a short pulse in the time domain [17].

3.3. Software of FDTD simulation

There are a number of software packages available both as open source tools and as commercial tools which implement FDTD algorithms. Some of these tools have been optimized for parallel-processing systems [14]. The commercial packages available are FDTD Solutions by Lumerical, Electromagnetic Simulation Software, Electric field time domain solver and EMPro 3D

Electromagnetic Simulation Software. Meep is a free FDTD simulation tool developed at Massachusetts Institute of technology for computational modeling of electromagnetic systems. Meep supports simulation in one-dimension (1D), two-dimension (2D), three-dimension (3D) and cylindrical coordinates with support for distributed memory parallelism. The Angora package, based on FDTD, generates numerical solutions to electromagnetic radiation and scattering problems. Angora is flexible and provides full support for parallelism in 3D.

3.4. Working principle simulation of FDTD method

The working principle of the finite difference time domain method simulation; the parameterization is basic for the optimization. The parameterization can be consists of the position of the source and the monitors. The simulation region includes the geometry, boundary condition, simulation time to 400 fs and mesh accuracy to 1. The simulation of the source, structure, and monitor in the geometry of the wavelength have (x span, y span and z span) the same value, but use less mesh wavelength. The simulation of silver nanoparticle is simulating by using the circle and sphere simulation structures. The monitors including; the index monitor in x-y plane, set the field component to the electric field intensity, frequency domain field and power, and point of time monitor. The plane wave source makes sure it is large enough x span, y span and z- position of the wavelength of 600 nm. Using FDTD methods, the simulation of silver nanoparticles the wavelength range 400 nm to 800 nm and the propagation of direction to forward. Finally, check the memory requirement; check the material fits, save the simulation file under the name silver Ag.fsp. For the simulation the blue color row indicates that the polarization direction and the pink color row also indicate that the propagation of direction.

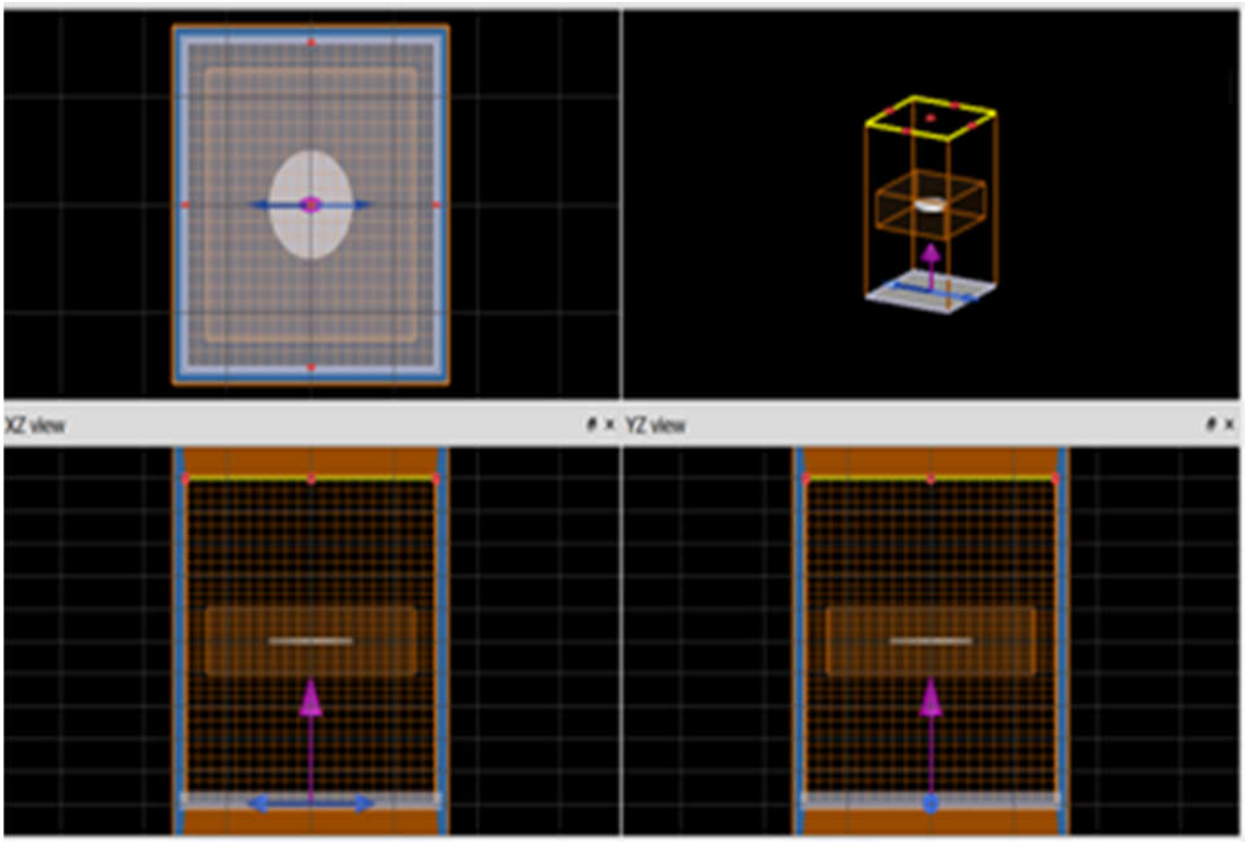


Figure 3.1: The schematic representation of the FDTD simulation work flow (screen shoot).

4. Result and Discussion

4.1. Simulated the extinction cross section and near field with FDTD

In this paper, we have characterized the simulation of silver nanoparticle by using the Finite difference time domain methods in different size and shape that obtained the plasmonic resonance peaks. We have used the structure of nanodisk, the source of the plane wave, the monitors of frequency-domain profile and power input to this simulation. Figure (4.1) shows that the thickness of all simulations have constant value (t = 25 nm), but radii of the colors are different values; that means the radius of pink color is 60 nm, red color is 50 nm, green color is

55 nm, and the radius of the blue color is 45 nm. Therefore, the pink and the blue colors were not the prefect plasmonic resonance peaks and the red color was good plasmonic resonance peak, and also the green color was the best plasmonic resonance peak at the wavelength of 650 nm. The electromagnetic spectrum simulation of the silver nanoparticle of the wavelength range from 400 nm up to 850 nm and the simulation time 400 fs. The silver nanodisk has one plasmonic resonance due to their symmetry, but the new resonances can appear when they are organized in small assembles and it depends on the symmetry of the assemblies. In far field, the detector put far way to the nanoparticle at distant in 500 nm. The position of the plasmonic resonance peak and the width of the peak could be used to approximation the radius of the silver nanoparticle.

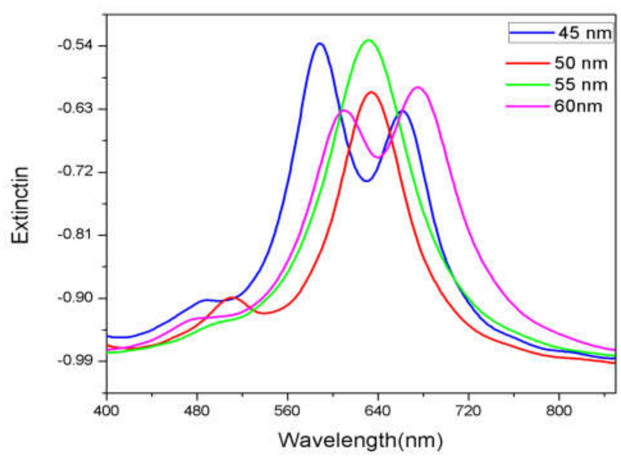


Figure 4.1: Simulated extinction spectra of silver nanodisk with various radii and t = 25 nm.

Figure (4.2) shows that the simulation of the extinction coefficient versus the wavelength of silver nanodisk with the radius (R = 50 nm) are constant value however, the thickness of the blue, green, red, and pink colors are different values ($t_1 = 20\,nm, t_2 = 35\,nm, t_3 = 45\,nm, t_4 = 60\,nm$) respectively. By using the same manner for the simulation of figure (4.1) however, the difference one was constant radius and they have different thickens then, the result of the plasmonic resonance peaks are vary. In this case, the best plasmonic resonance peak obtained that the red color at the wavelength of 650 nm than the pink, blue, and green colors. For a certain type of nanoparticles the spectral peaks can shift due to changes in the size, shape, aggregation state of the nanoparticles. We obtained the red shift of the plasmon resonance peaks that shift to longer wavelength. Therefore, the resonance of surface plasmon was strongly affected by the particle shape and the resonance intensity also increases with dielectric function of the medium. This means expected the performance for a forced oscillator.

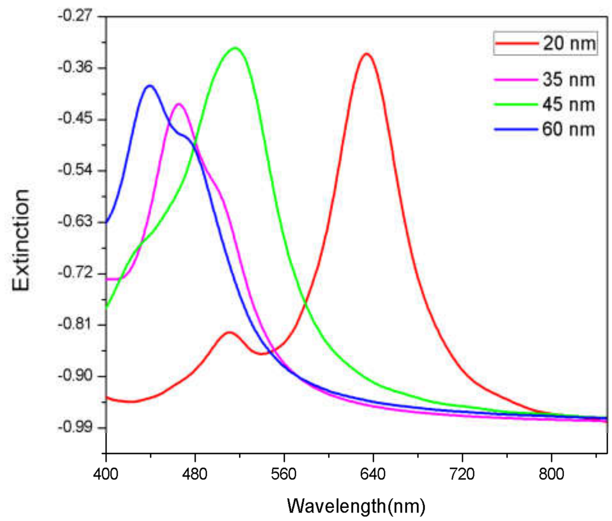


Figure 4.2: Simulated extinction spectra of silver nanoparticle with various thickness and R = 50 nm.

Figure (4.3) shows that the accumulation of the electric field distribution to simulating in silver nanoparticle with the different wavelength. In this thesis, we obtained the accumulated of electric field distribution is increasing, then the intensity also increasing. At 400 nm which has les confined of the near field in Figure (4.3a), because the plasmonic resonance sensing is less. Here we have obtained high accumulation of electric field distribution at the wavelength of 640 nm than other wavelengths of 400 nm, and 800 nm in figure (4.3b). Therefore, the maximum electric field distributions more accumulated at the wavelength of 640 nm. On the opposing, the diffraction pattern in the near field characteristically differs significantly from that observed at infinity and varies with distance from the source. However, near field, the detectors near to the target particle. At 800 nm of wavelength the accumulated of the electric field distribution less than the wavelength of 640 nm. The square of electric field is equal to intensity and units of wait per meter square (W/m^2).

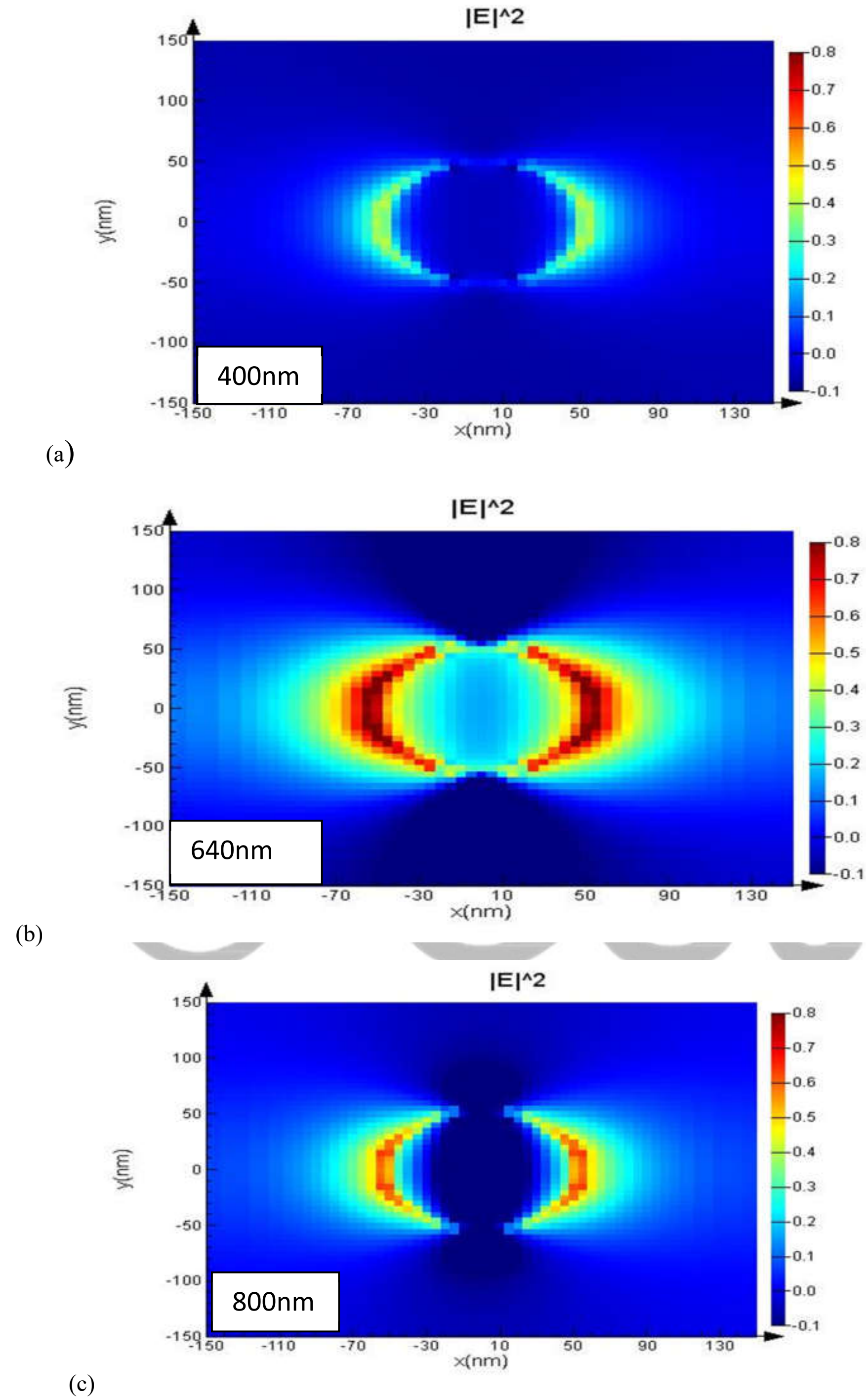


Figure 4.3: Simulated electric field distribution with different wavelength for silver nanoparticle the R = 50 nm and t = 20 nm.

Figure (4.4) shows that simulated of the extinction versus the wavelength of silver nanoparticle with the radius of 55 nm and the thickenes (t = 25 nm) in the wavelength range from 400 nm to 880 nm. At 640 nm wavelength that obtained the maximum extinction of plasmonic resonance peak of position. Therefore, we obtained the maximum accumulation of electric field distribution, which means highly plasmonic resonance sensing. Silver nanoparticles thus could be providing better sensitivity for malaria pigment diagnosis applications

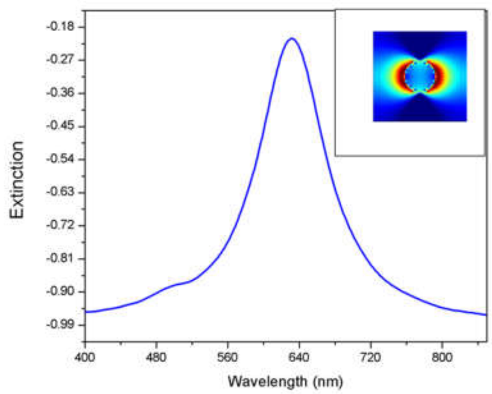


Figure 4.4: Simulated extinction of silver nanoparticle with radius R = 55nm and t = 25 nm

Figure (4.5) shows that the simulation of extinction versus the wavelength with the thickness is 20 nm and the different radii. In this case, the extinction coefficient occurred that the wavelength range from 400 nm to 800 nm. The extinction means the sum of all light that is not transmitted through the nanoparticle. In nanoparticles, the source can be removed the scattering event or through the absorption. The extinction was measured using UV-visible electromagnetic spectrum in the experiment. The Plasmon resonance peaks were the red shift to the larger wavelength. The maximum peak of the plasmonic resonance obtained at 600 nm, which is a red color, other resonance peaks also were occurred at the wavelength of 530 nm, 560 nm, and 580 nm. The proportion of the extinction due to the scattering or the absorption changes dramatically for different size of nanoparticles. When the radius of nanoparticle is increasing and also the plasmonic resonance peak is increasing. The width of the plasmonic resonance peak could be used to estimate the radius of silver nanoparticle.

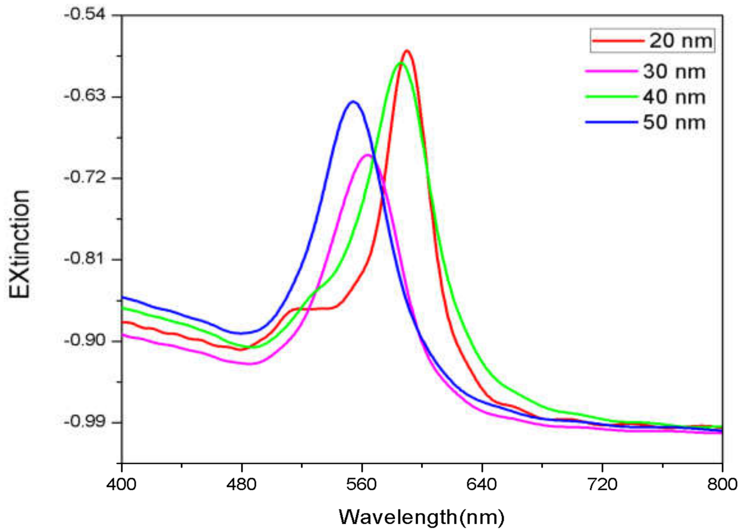


Figure 4.5: **The simulated representation of the silver nanodisk with different radii and t = 20 nm.**

Figure (4.6) shows that the extinction spectral of the silver nanoparticle to simulating in a constant radius of 50 nm and the different thickness ($t_1 = 20\,nm, t_2 = 30\,nm, t_3 = 40\,nm, t_4 = 50\,nm$) in the colors of green, pink, red, and blue respectively. We obtained the simulated red shift of the plasmonic resonance peak to increasing the wavelength. If the aspect ratio of the silver nanodisk is increasing then, the extinction wavelength red shifts from 400nm to 800nm. In this figure, the maximum resonance peak of the extinction coefficient of the silver nanodisk around 620 nm. The plasmon resonances required the application of mesh constraints to ensure the convergence of the simulation in the visible and near infrared (400 nm to 800 nm) [72]. In this thesis, the plasmonic resonance occurred at the convergence of autoshoot time simulation of nanodisk in the wavelength range from visible light. The optical properties of the near and far field of the nanodisk are determined numerically in the frequency domain using the extinction field formulation.

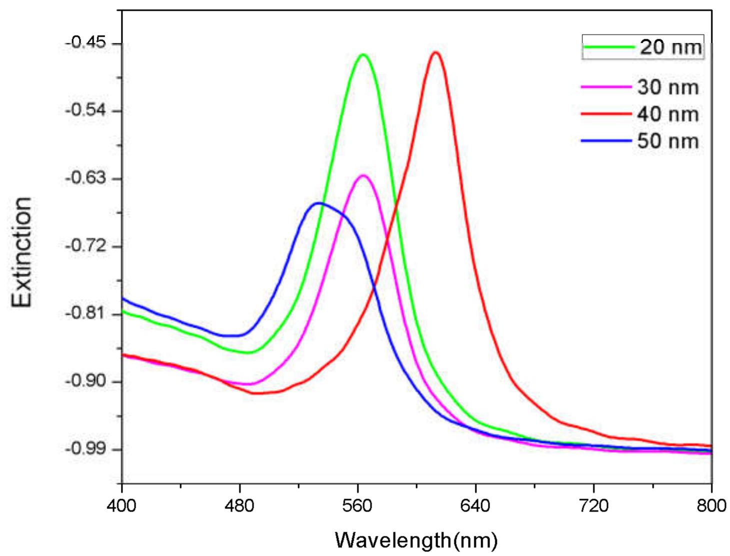
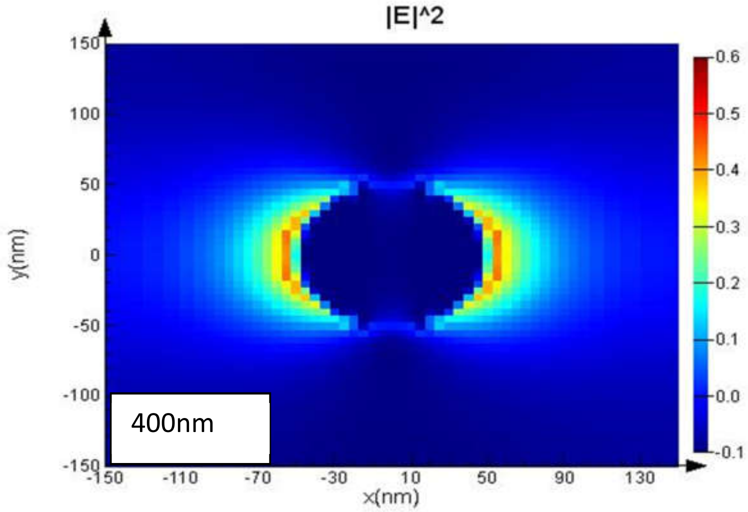
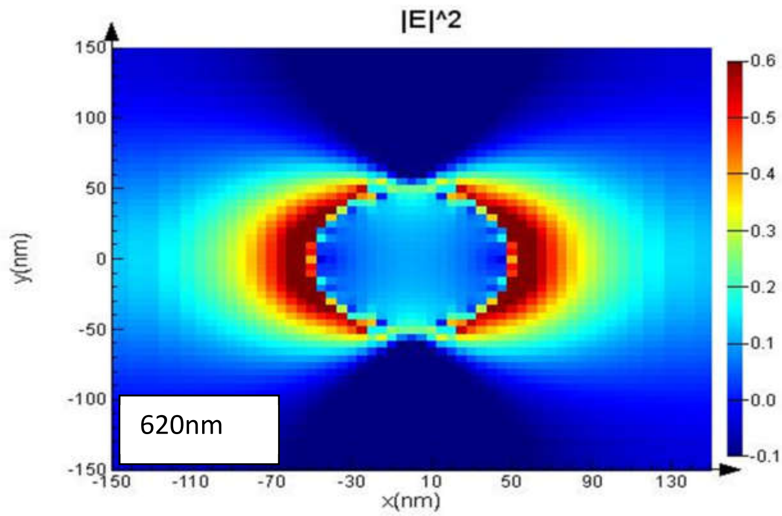


Figure 4.6: The simulated representation of the silver nanodisk with different thickness and R = 50nm.

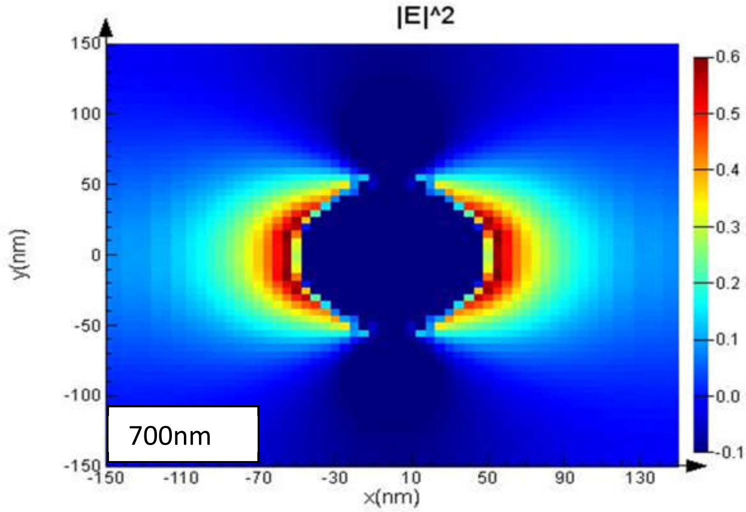
Figure (4.7) shows that the simulated in silver nanoparticle that obtained the accumulations of electric field distribution with the specific wavelength in near fields. In the near field, the electromagnetic waves are characterized by a single polarization type; that means horizontal, vertically, circularly, and elliptical this polarization types can represents in the near field. In this thesis, at 620 nm wavelength of the simulated the silver nanoparticle that obtained the minimum electric field intensity distribution in figure (4.7a). At 620 nm wavelength which has more accumulated the field intensity in near field as shown figure (4.7b). At 700nm which has less confined the near field as shown figure (4.7c). Therefore, in figure (4.7b) shows that more accumulated the electric field distribution of the wavelength at 620 nm. In figure (4.6c) the accumulation of electric field less than the electric field distribution in figure (4.7b).When the electric field was increasing, and its intensity also increased; that means the electric field is directly proportional to the intensity.


|E|^2
150
100
50
0
-50
-100
-150
y(nm)
-150
-110
-70
-30
10
50
90
130
x(nm)
0.6
0.5
0.4
0.3
0.2
0.1
0.0
-0.1
400nm

(a)


|E|^2
150
100
50
0
-50
-100
-150
y(nm)
-150
-110
-70
-30
10
50
90
130
x(nm)
0.6
0.5
0.4
0.3
0.2
0.1
0.0
-0.1
620nm

(b)



(c)

Figure 4.7: Simulated the electric field distribution with frequency- domain field profile for silver nanodisk R = 40 nm and t = 30 nm.

5. Conclusion

This paper, briefly deals about the optical properties, characterization and application of plasmonic based biosensors and silver nanoparticle. Biosensor based surface plasmon resonances have been obtained type of the optical sensor that utilized surface plasmon polariton waves. Then, to simulate the nanoanetnna by using these physical parameters was including; the structure, the source, the region/ mesh, and monitor using these parameters to construct the nanoantenna. Based on the finding of the study, we conclude that the simulation of the extinction cross section of the plasmonic resonance peak based silver nanoparticle, it depends on the radius and thickness of nanoparticle. We obtained the extinction cross section of the plasmonic resonance peak located at 640 nm, 600 nm, 470 nm used the silver nanoparticles in far field , the wavelength range from visible light to near infrared (400 nm to 800 nm). However, in the near field result shows the simulation of silver nanodisk particle that indicated the accumulation of the electric field distribution highly obtained at 640 nm, 620 nm, and 470 nm with the specific wavelength. In this thesis, the position of plasmon resonance peak and the width of the peak could be used to estimate the nanoparticle of radius and thickenes. So the result of this simulated of the plasmonic resonance peak based silver nanoparticle fits to the theoretical studies.

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