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Optical Properties of Different Shaped Metallic Nano particles

Zaid Yousaf[1], Hassan Wasim Khan[1], Imran Khan[1] and Haseeb Ahmad Khan[1,*]

[1]University of Engineering and Technology Mardan, Pakistan.
*Corresponding Author: Haseeb Ahmad Khan (haseebkhan@uetmardan.edu.pk)

Abstract- **In this paper Absorption, Scattering, and Extinction properties of different nanoparticles coated with gold and silver materials are studied. The simulated results show that by changing the proposed parameter for these nano-particles different LSPR (Localized surface plasmon resonance) peaks are activated in the spectra. The LSPR modes are dipole, quadrupole and octupole along with redshift. This study reveals that LSPR is strongly dependent on size. Moreover, the Extinction properties of gold-coated nanoparticles and silver-coated nanoparticles are compared. These observations and results may lead to new opportunities and applications in the field of bioimaging, biomedical and photovoltaics.**

Index Terms-- **Absorption, Scattering, Extinction, Structure Size, Structure Coating.**

I. INTRODUCTION

The study of nanoparticles brings a storm in the world by offering solutions to the problems which remains unsolved for the decades and brings innovations. A lot of work has been done on the plasmonic properties of different nanoparticles. The recent and tremendous development has been made on other structures of Nanoparticles such as nanorods [1,2] and Nano star [1-3], core-shell Nano shell [4-6], Nano eggs [7] and Nano cups. Cancer research has been expanded to a new level by including nanoparticle therapies [8, 9]. The field enhancements revolutionized the spectroscopic measurements, which are not available in laser facilities [10,11]. These nanoparticles also form the basis of inexpensive optical materials and bring a tremendous change in this field [12]. All these developments and changes depending upon the geometry of nanoparticles that is core-shell geometry which includes Nanoshells, Nano eggs and Nano cups.

The LSPR (Localized surface plasmon resonance) which mainly depends on the Nano particles size, geometry and shape. The motion of free electrons collectively on the nano-particles surface is called a surface plasmon. By applying an electric field on these surface plasmons and the frequency of both the localized plasmons and incident field matches, so resonance phenomenon occurs, and this is called LSPR [13-15]. A strong EM field is achieved near the surface of plasmonic nanostructures at a nanoscale when the energy for both excitation and localized plasmons matches. The peaks or LSPR modes position can be determined from the scattering and extinction spectra. The peaks in the graph show us the frequencies at which resonance occur. The Scattering properties of conical spherical and cylindrical gold made Nanoparticles was studied. It was observed that the proposed nanoparticles are strongly sensitive to the parameters of the Nanoparticles. It was also observed that the comparison between three different proposed nanoparticles based on volume taking the volume of a spherical Nanoparticle as a reference results into the large and enhanced resonant modes in the scattering spectra for spherical nanoparticles which can be used in applications like biosensing and bio imagining [16].

The nano-particles properties also change by the change in the symmetry of geometry as the interactions between plasmon modes changes. The near and far-field properties were examined by changing the geometry of nanoparticles that is Nano shell Nano egg and Nano cups. Nano shell has spherical shape core coated with silica inside the shell coated with gold. Offsets of a core within a shell give rise to Nano eggs and further offsetting the core, where the core forces the shell outside results in Nano cups [17-22].

Plasmonic structures with different metals such as Au, Ag and Cu etc nanoclusters having spheroidal or different shapes exhibits properties which can be utilized in different applications like nano imaging, nano photonics etc There is local electromagnetic field near plasmonic structure which is responsible for surface enhanced absorption.

In this paper, the author has investigated that

- The plasmonic properties of three different gold nanoparticles, i.e. spherical, conical and cylindrical shown in Fig.1.
- The author has shown that LSPR modes strongly depends on size. By changing the radius and height for spherical, conical and cylindrical shaped nanoparticles, different LSPR modes were observed in scattering spectra of proposed nanoparticles.
- It was observed that by changing these parameters, LSPR modes could be easily tuned.

In the case of spherical nanoparticle, the LSPR modes observed have massive shifts and large spectral width and amplitude, which can be used for biomedical applications.

LSPR modes are intensely sensitive to the geometry of the nanoparticles. The plasmon modes were tuned by modifying the geometry of the nanoparticles or proposing different geometries such as nanoshell, nanoeggs and nanocups. This type of tuning is done by changing the parameter D which is the core offset. The extinction spectra for these geometries shows that with 0<D<0.32 the spectrum is resembling that of nanoshell and further increase in D give rise several multipolar peaks with red shift.

The LSPR modes of gold nanocluster arrays on Si/SiO2 has been investigated. The study shows a strong dependency of LSPR modes position on distance between nanoclusters, size of the nanocluster and the SiO2 layer thickness.

The plasmonic properties of two gold nanocones placed adjacent have been studied. Two plasmon modes arises from the two nanocones couple with each other give rise Fano resonance. Recently fano resonance was observed in plasmonic dimer nanostructures [16]. Fano resonance is strongly dependent on shapes and refractive index of nanoparticles. Several geometries has been investigated for achieving fano resonance. Brown et al. Investigated the fano resonances for mismatched nano-particles pairs of different size and shapes [17]. The dimer nanostructures also depend on the polarization state of the incident light. The field enhancement and plasmon interactions are very weak in case of transversely polarized incident light and hence limited hybridization effects. No fano dip appears as compared to longitudinal polarized excited light [18].

II. GEOMETRY OF NANO-PARTICLES

Three different geometries have been shown where the spherical has only one variable 'r' while the cylindrical and conical have two parameters' r' and 'h'.

- Depends on size. By changing the radius and height for spherical, conical and cylindrical shaped nanoparticles different LSPR modes were observed in scattering spectra of proposed nanoparticles.

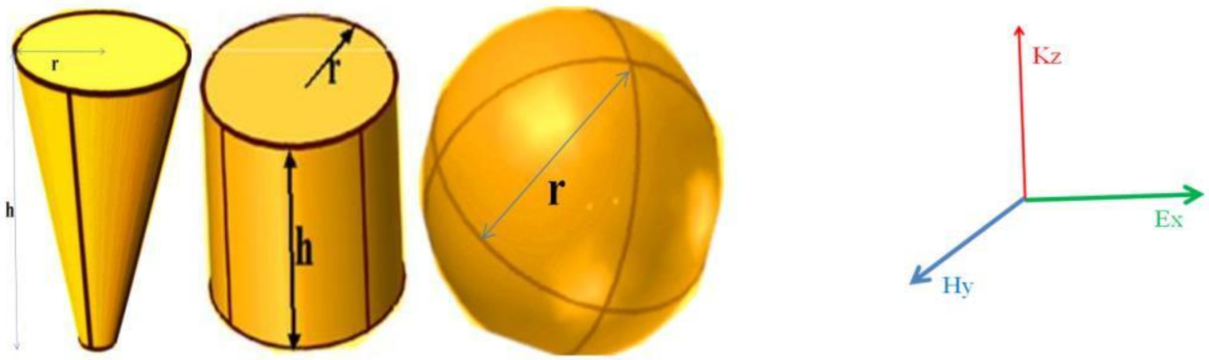


FIGURE 1: Spherical, Conical and Cylindrical nanostructures with polarization along X-axis

III. METHODOLOGY

COMSOL multi-physics software is used for the simulation and Finite element method (FEM) technique is used for calculating spectra of nanoparticles. The polarization and propagation is taken along x-axis and z-axis, respectively. All the nanoparticles are enfolded by perfectly matched layer (PML) providing an absorbing media for the waves which should not be reflected back. The PML material embedded was air. The near and far-field properties of the three nanoparticles were solved in the frequency domain using the formulation of scattered field. The simulation environment was composed of spherical nanoparticle coated with gold with embedded medium and PML surrounded it. Same is done for silver-coated different shaped nanoparticles. The scattering and absorption spectra were evaluated by the volume and surface integration in comsol. The extinction spectra of far-field are calculated by adding the far-field absorption (Qabs) and scattering (Qscat) efficiencies. Scattering spectra was obtained using Eq.1.

$$Q_{scat} = \frac{1}{\pi r^2 E_{inc}^2 R_f^2} \int \left| E_{far} \right|^2 R_f^2 d\Omega \quad \text{.........................} (1)$$

R_f is the radius of the boundary for calculation of far-field transform, E_{far} represents the far field component of the scattered field obtained from COMSOL. E_{inc} is the amplitude of electric field and r is the radius of the nanoparticle. Johnson and christy model was used for the dielectric constant of gold and silver [16].

And absorption spectra were obtained using Eq.2.

$$Q_{abs} = \frac{1}{\pi r_2^2} \frac{2}{\sqrt{\frac{\varepsilon_0}{\mu_0}} E_{inc}^2} \int (U_{av}) dV \quad \text{..................................} (2)$$

where U_{av} is the time-averaged resistive heating.

IV. RESULTS AND DISCUSSION

The scattering, absorption and extinction spectra for the gold and silver-coated spherical, conical and cylindrical shaped nanoparticles are computed. Different results are achieved by changing the radius of nanoparticles. First, the results of gold-coated plasmonic nanoparticle will be discussed and then the silver.

Figure 2 shows the scattering and absorption spectra for the spherical nanoparticle coated with gold. Initial radius is taken as 30nm and gradually increasing the radius to 80nm the scattering spectra show that with increasing radius, the amplitude and width of the LSPR modes increase with a small redshift. All these LSPR modes are dipole modes. Similarly, the absorption spectra also show the increase in amplitude and width with the increase in radius but no shift and dipole modes. The fundamental mode exhibited by the nanoparticle is called dipolar mode.

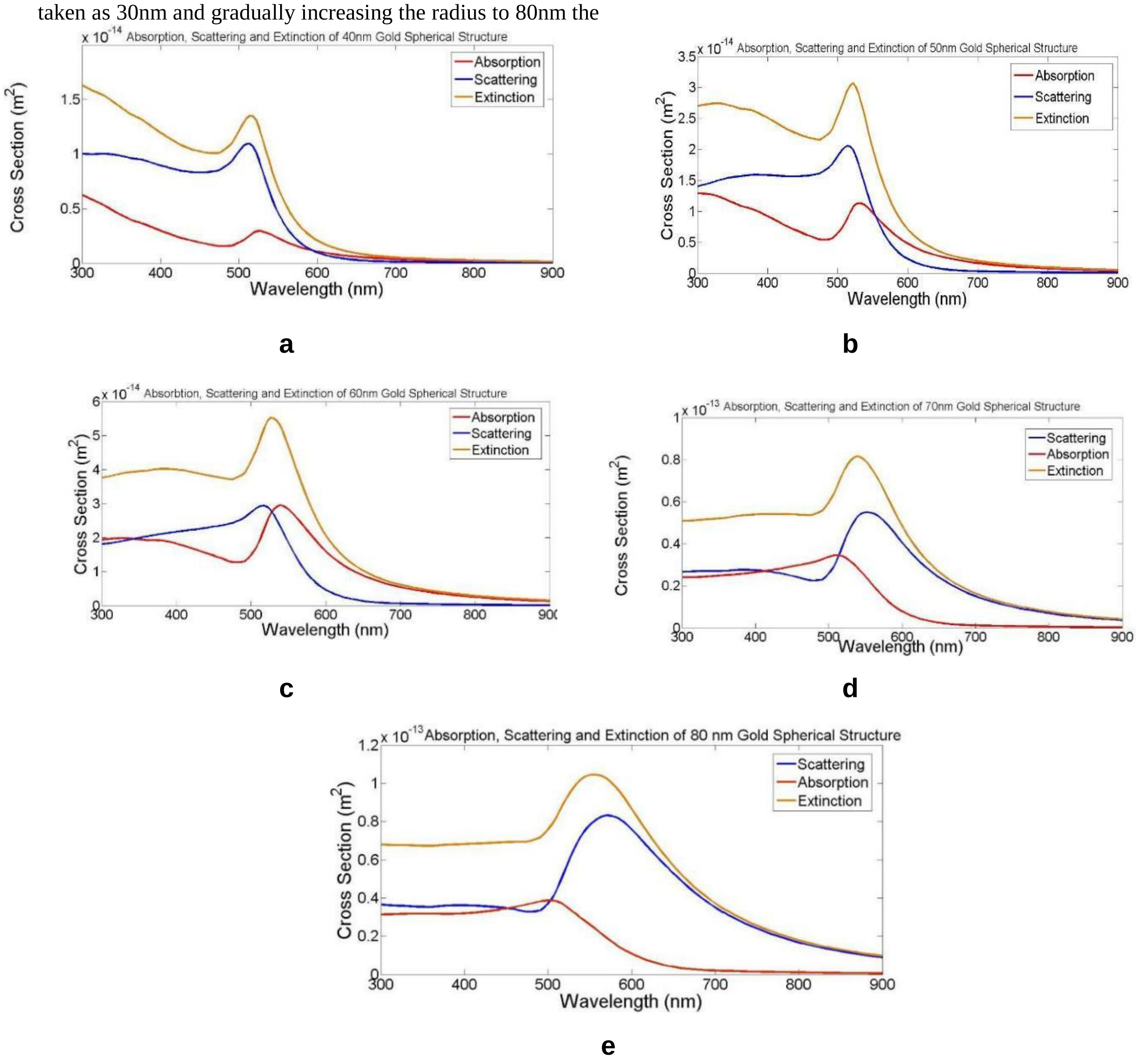
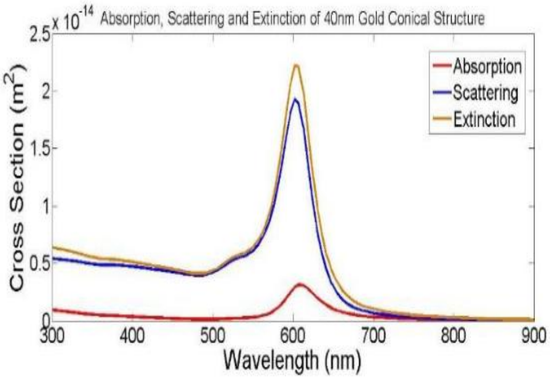
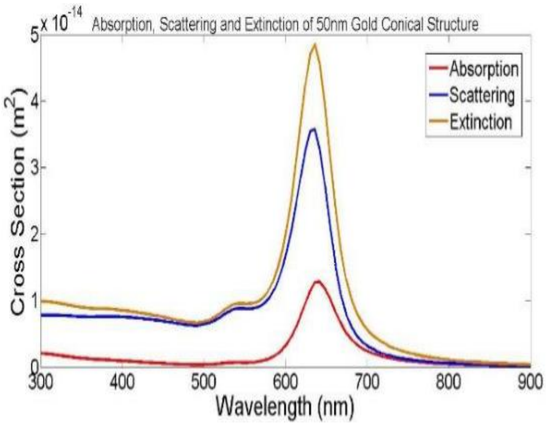


FIGURE 2: Absorption, Scattering and Extinction spectra for Spherical nanoparticle with 'r' a 40nm b 50nm c 60nm d 70nm e 80nm

Figure 3 shows the scattering and absorption spectra for the cone nanoparticle coated with gold. Cone has two parameters i-e radius and height but in this study, only the radius has been changed from 40nm to 80nm. The scattering and absorption spectra show that, as the radius increases the amplitude and width of the LSPR modes also increases with new mode also arises. For the cone there are two LSPR modes and red shift.



a



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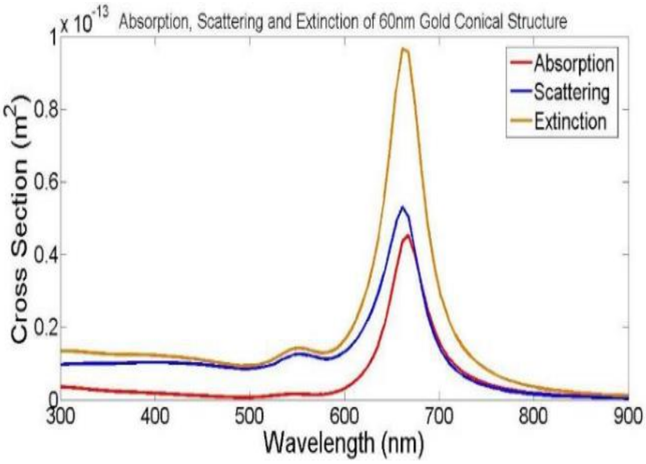

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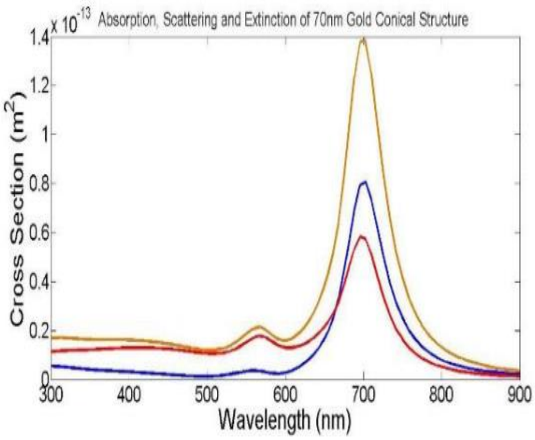

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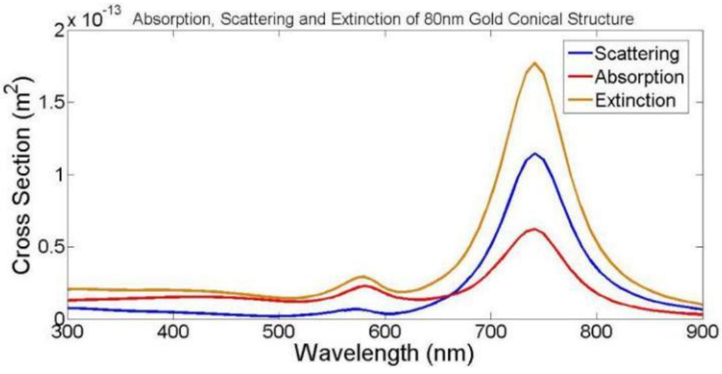


e

FIGURE 3: Absorption. Scattering and Extinction spectra for Conical nanoparticle with 'r' a 40nm b 50nm c 60nm d 70nm e 80nm

Figure 4 shows the scattering and absorption spectra for the cylindrical-shaped nanoparticle. The scattering and absorption spectra show that by gradually increasing the radius from 30 nm to 80nm the amplitude and width of the plasmon modes increases with redshift and dipole mode.

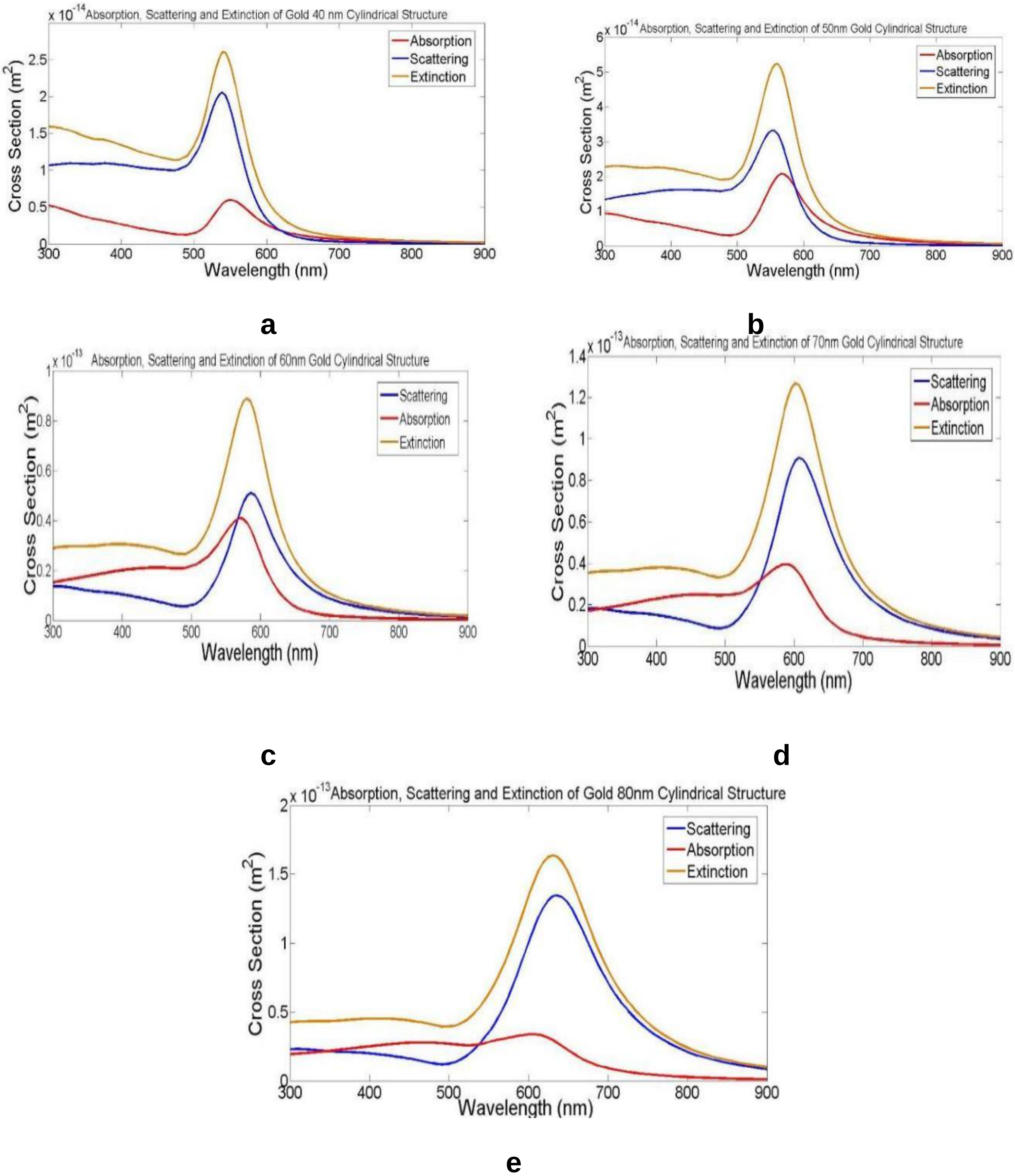


FIGURE 4: Absorption, Scattering and Extinction spectra for Cylindrical nanoparticle with 'r' a 40nm b 50nm c 60nm d 70nm e 80nm

Figure 5 shows the scattering and absorption spectra of Spherical shape nanoparticle having a radius ranging from 40nm to 80nm. The scattering spectra show that with an increasing radius the earlier mode gradually vanished and a new one arises Simultaneously. Similarly, the absorption spectra show the same result but here the LSPR modes are very weak as compared to the modes in the scattering spectra. The new modes are at lower wavelength as compared to the earlier ones.

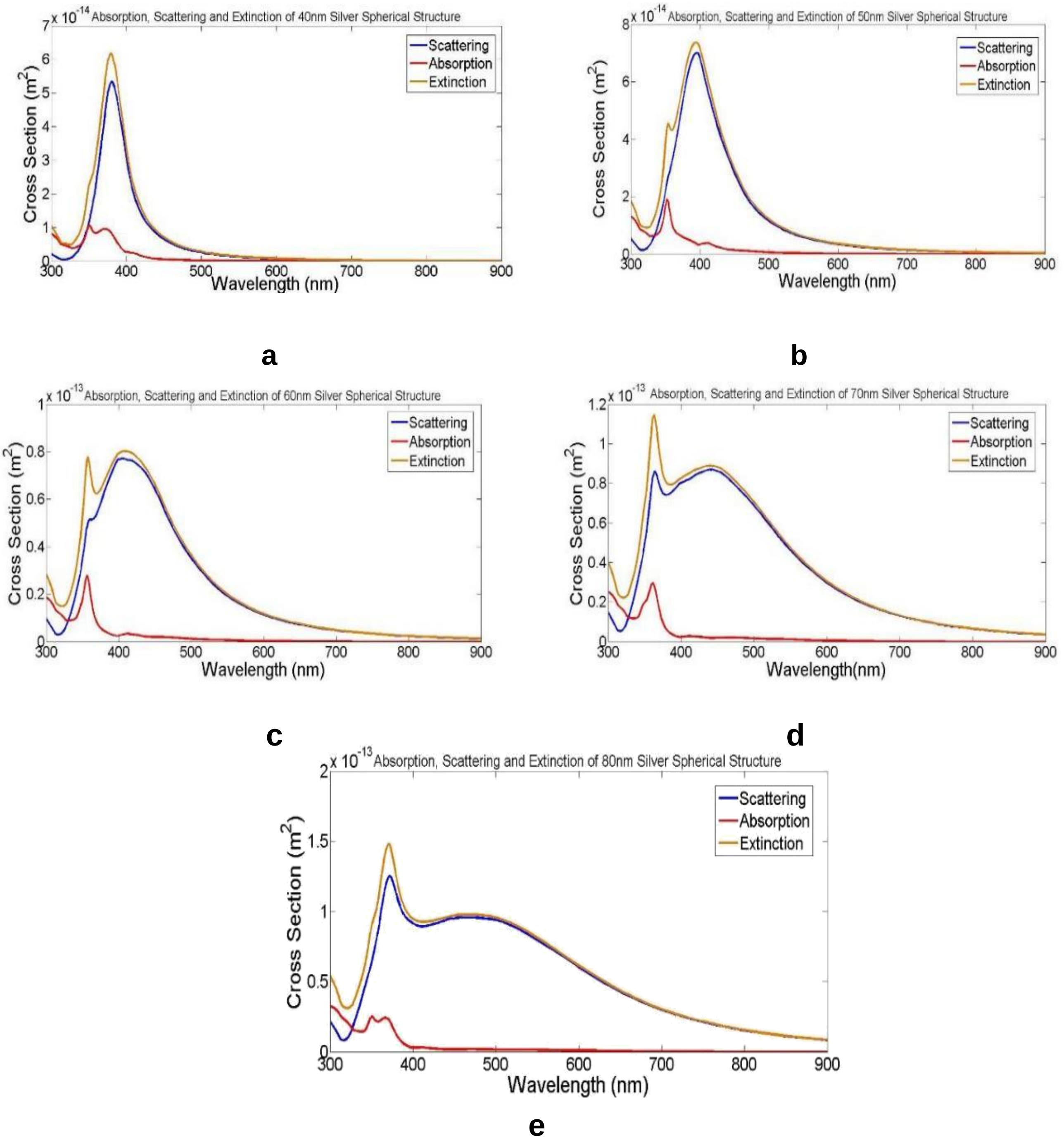


FIGURE 5: Absorption, Scattering and Extinction spectra for Spherical nanoparticle with 'r' a 40nm b 50nm c 60nm d 70nm e 80nm

Figure 6 shows the scattering and absorption spectra of conical shaped nanoparticle. Initially at r=40nm the scattering spectra have three modes with very weak mode at the left and high amplitude mode at right. The amplitude and width of the modes increase with the change in the radius of the nanoparticle along with a red shift. The nanoparticle with 80nm radius have highest amplitude and largest width mode at the right.

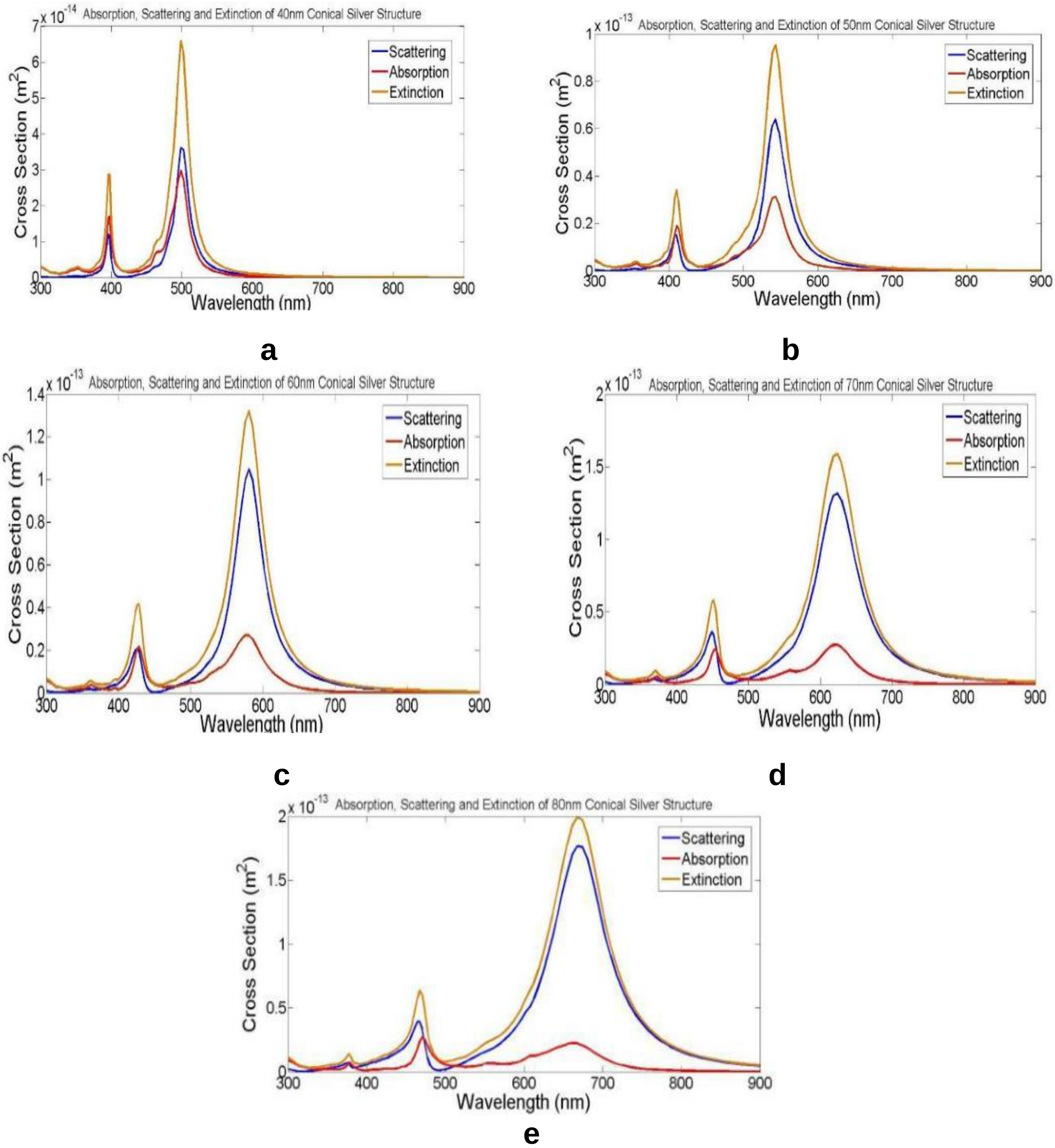


FIGURE 6: Absorption, Scattering and Extinction spectra for Conical nanoparticle with 'r' a 40nm b 50nm c 60nm d 70nm e 80nm

The absorption spectra show the same results but here the first mode get decreases gradually with increase in radius.

Figure 7 shows the scattering and absorption spectra of cylindrical shaped nanoparticle for different radius ranging from 40nm to 80nm. Initially at r=40nm the spectra have two modes one is large in amplitude and the other is very small. The smaller mode becomes disappear by increasing the 'r' and the larger one becomes wider and shows a red shift.

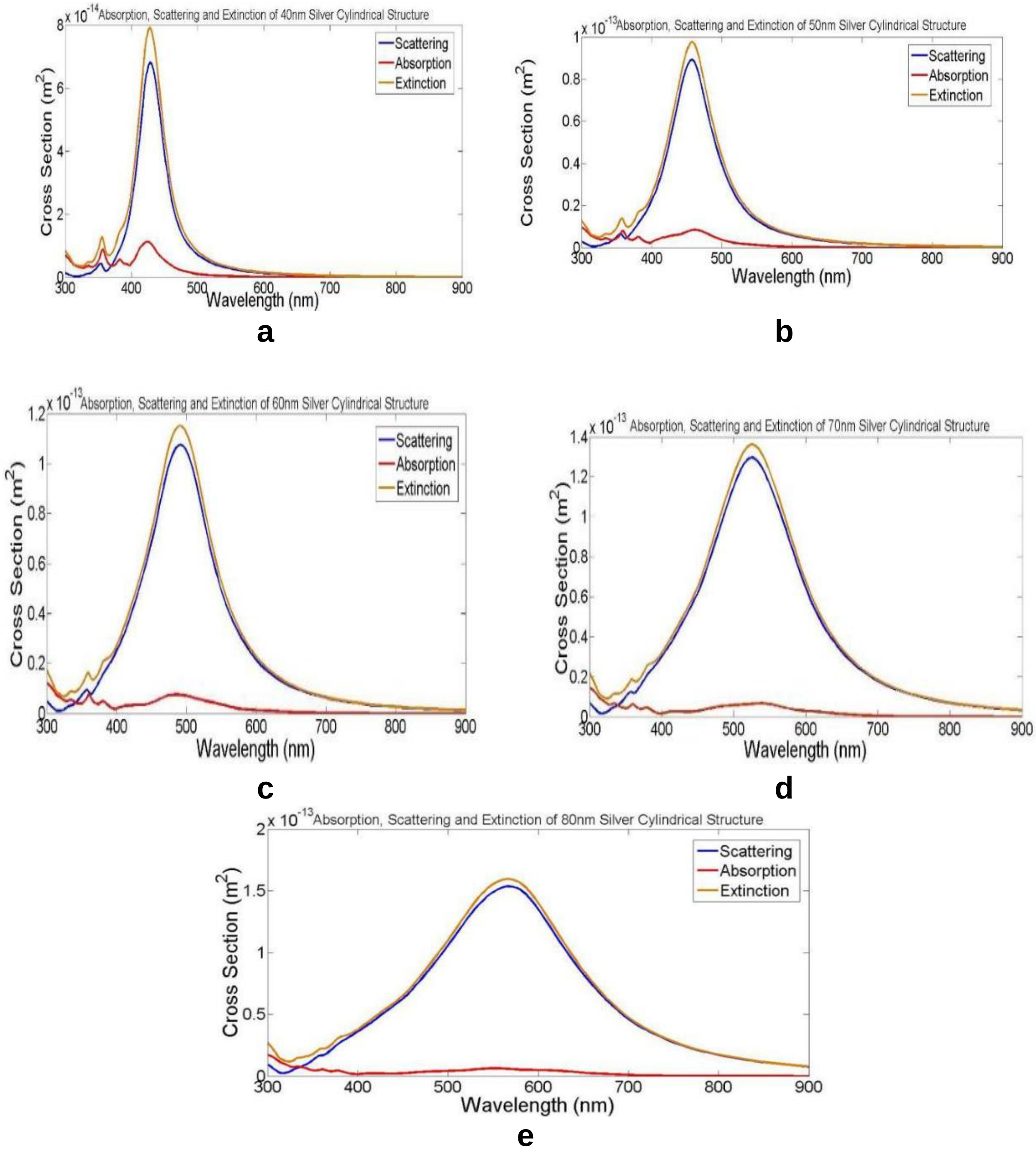
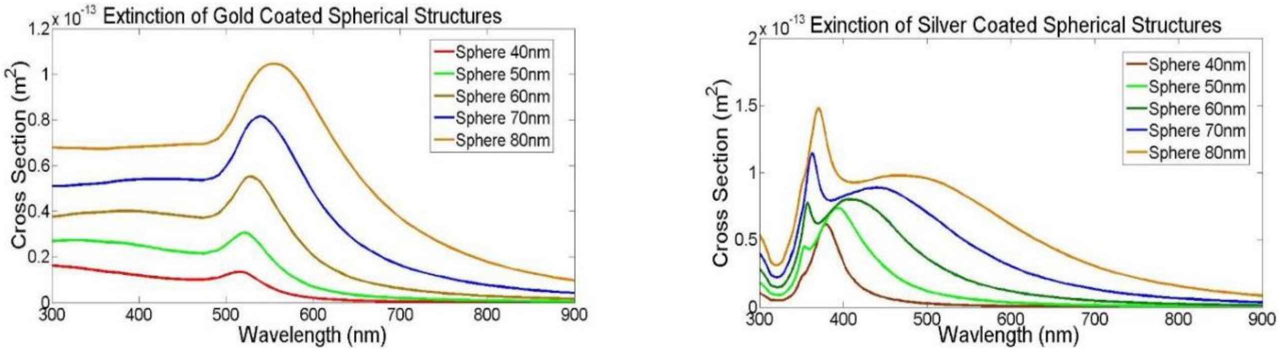


FIGURE 7: Absorption, Scattering and Extinction spectra for Cylindrical nanoparticle with 'r' a 40nm b 50nm c 60nm d 70nm e 80nm

The absorption spectra show that at r=40nm the spectra have three plasmon modes but are very small in amplitude. The modes gradually vanish with increase in radius of the proposed nanoparticle.

Here in this study the extinction spectra of different shaped nanoparticles coated with gold and silver separately will be compared. First the extinction spectra of gold and silver coated spherical nanoparticle for radius ranging from 40nm to 80nm will be compared.

Figure 8(a) shows the extinction spectra of gold coated spherical nanoparticle. The spectra show only one LSPR mode whose amplitude and width increases with the increase in 'r' and a small red shift.

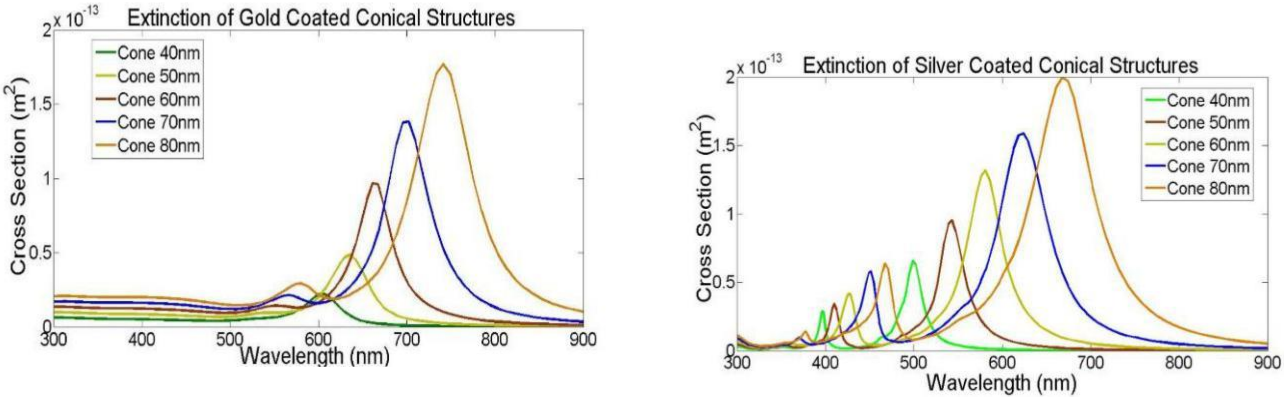


a **b**

FIGURE 8: Extinction spectra for spherical nanoparticle a. Gold coated b. Silver coated

Figure 8(b) shows the extinction spectra of silver coated spherical nanoparticle. Initially at r=40nm the spectra have two modes one is smaller and the other is larger but with increasing 'r' the larger mode gradually disappears and amplitude of smaller mode increases at lower wavelength.

Here compare the extinction spectra of gold and silver coated conical nanoparticle will be compared. Figure 9(a) shows the extinction spectra of gold conical nanoparticle having only one plasmonic mode at r=40nm and with increase in 'r' the amplitude and width of the first mode increases with a strong red shift and arising of second mode as shown for r=80nm.

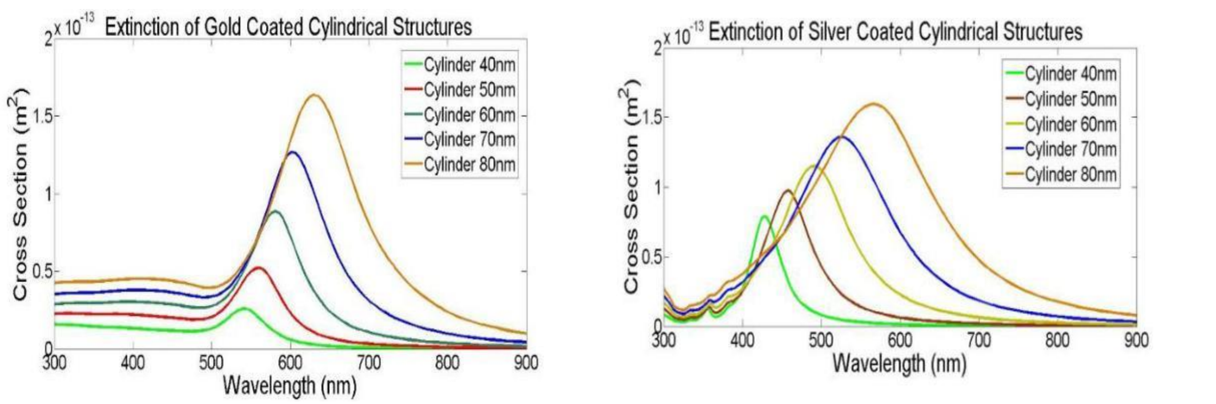


a **b**

FIGURE 9: Extinction spectra for conical nanoparticle a. Gold coated b. Silver coated

Figure 9(b) shows the extinction spectra of silver coated plasmonic nanoparticle which have two modes at r=40nm. Initially at r=40nm the spectra have two modes but by gradually increasing 'r' a third mode arises with increase in the amplitude and width of the former LSPR modes and a strong red shift is observed in all the plasmonic modes.

Now, the extinction spectra of gold and silver coated cylindrical nanoparticle will be studied. Figure 10(a) shows the extinction spectra of gold cylindrical plasmonic nanoparticle for different radius ranging from 40nm to 80nm. The spectra show that by gradually increasing 'r' the LSPR modes amplitude and width increases with a red shift observed.



a **b**

Fig. 10 Extinction spectra for Cylindrical nanoparticle a. Gold coated b. Silver coated

Fig.10(b) shows the extinction spectra of silver coated cylindrical nanoparticle for different radius. The spectra show that with increasing 'r' the amplitude and spectral width of the LSPR modes increases with red shift and small other modes arises.

V. CONCLUSION

In this paper, the scattering, absorption and extinction properties of three different shaped nano-particles i-e spherical, conical and cylindrical were investigated by taking polarization along x-axis. From the above study, it is concluded that the LSPR modes strongly depend upon the size. The gold-coated nanoparticle shows a dipolar mode except for conical shaped nanoparticle while silver-coated nanoparticle exhibits quadrupole and octopole mode.

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