PLASMONIC PROPERTIES OF METALLIC NANOPARTICLES

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Abstract

In this study, the scattering properties of three different gold nano-particles have been studied. The proposed nano-particles are spherical, conical and cylindrical. The simulation results indicate that as the parameter of these nano-particles are changed so different LSPR peaks and shifts achieved in the scattering spectra. So this shows that the resonance modes are strongly reliant on the parameters of the proposed nano-particles. Moreover we have compared the scattering spectra of all the three nano-particles on the basis of their volume. The spherical nano-particle got wide spectral width, shift and high amplitude in the scattering spectra due to which it can be used for biomedical applications.

Key words: Plasmon, spherical, conical, cylindrical, LSPR.

Introduction

Numerous studies have been made on the extraordinary and matchless properties of nano size gold particles. The very hasty and tremendous development has been adopted to chemically synthesis and modeling has been done on computational basis on various gold made nanostructures having multiple ranges like nanorods [1, 2] and nanostars [1, 3, 4] ,core shell nano shell [5, 6] and nano egg [7]. When the conduction electrons collectively oscillates on the surface of metallic nanoparticle is called surface Plasmon. When the external field is applied on these shining localized surface plasmons and the phase at which the frequency of the applied incident field and these localized surface plasmon become match so resonance phenomenon occurs and this is called localized surface plasmon resonance ,the frequency at which resonance take place is called resonance frequency[8-10]. These LSPR are strongly dependent on the nano particles size , shape and their local environment [9, 11]. Which can be used for various applications like surface enhanced Raman spectroscopy [12] , bio imaging [8] , and photo voltaics [13].

In this article, we observed the scattering properties of the three different gold made nano-particles i.e. spherical, conical and cylindrical. We found that the proposed nanoparticles are highly sensitive to the parameters of the nano-particles because different resonant modes are achieved and enhanced. Moreover we have done comparison of the proposed nano-particles on the basis of their volume while taking the volume of aspherical nanoparticle as a reference. So we found that the sphere nanoparticle exhibits large and enhanced resonant mode in the scattering spectra which can used for bio-sensing and bio-imagining applications.

Nanoparticle Geometry and their Numerical Methodology

Figure 1 shows the geometry of the proposed nano-particles. The spherical nanoparticle has only one parameter called radius ‘r’, while the cylindrical and conical nano-particles have two parameters i.e. radius ‘r’ and height ‘h’. The polarization is considered to be along x-axis and propagation is along z-axis. The software we used for simulations is COMSOL multi-physics, the technique which we used in our simulation is finite element method (FEM) for calculating nano-particles spectra.

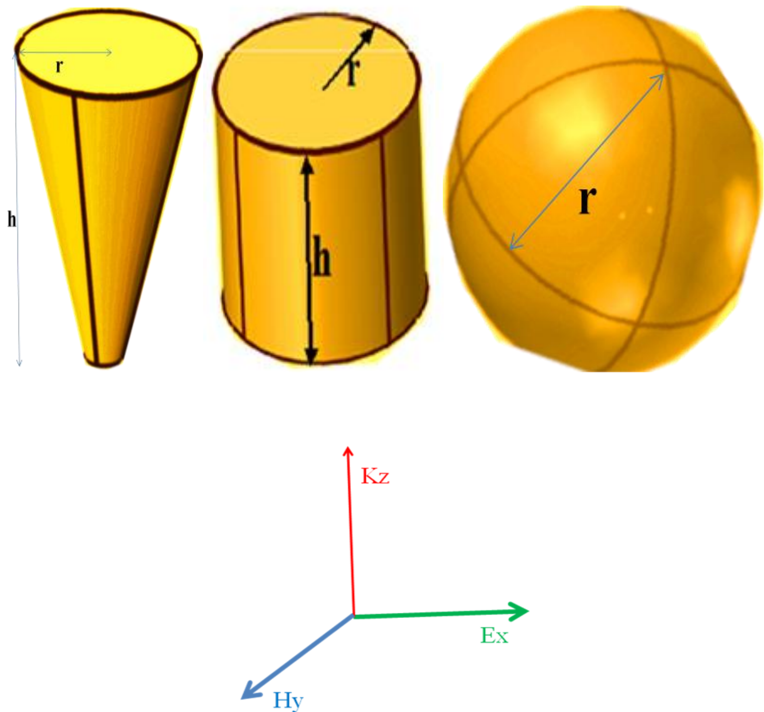


Figure 1 Spherical, Conical and Cylindrical nanostructures with polarization along X-axis

Figure 2 shows the 3 dimensional space we defined for the simulations are consist of the proposed nano-particles resonators , far field sphere enclosing the resonators and the perfect match layer (PML) enfolded all the spheres and nano-particles [14] . The PML provided an absorbing media for all the outgoing waves which can be not be reflected back. Furthermore we are interested to calculate far field scattering spectra on the far field sphere using the following equation

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

Where $R_f$shows the radius of the far field sphere, $E_{far}$is the far field computed Stratton-Chu formulation. E_{ins} shows the amplitude of the incident electric field and r defines the radius of the nanoparticle. We used the Johnson and Christy data model for the dielectric constant of gold [14].

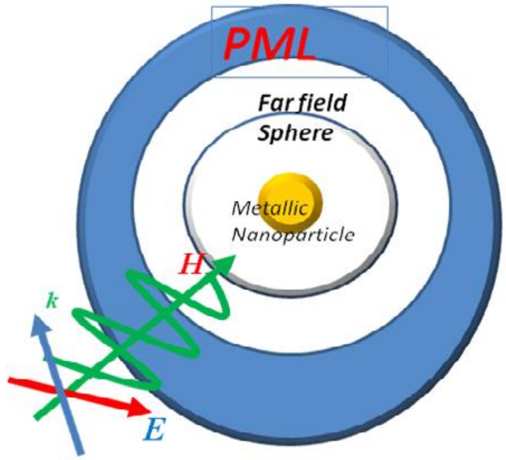
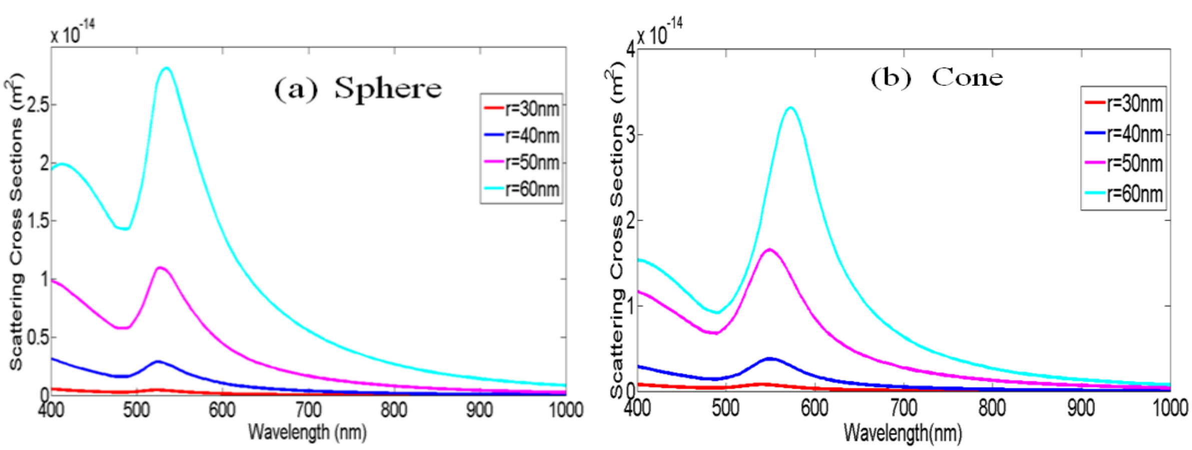


Figure 2. Perfect Match Layer with far field sphere and nanoparticle

Results and Discussion

Figure 3 (a) shows the scattering spectra of spherical nanoparticle having parameter radius. We computed the scattering spectra for the polarization is along x-axis. These results are achieved by tuning the radius of the spherical nanoparticle at initially r=30nm. It shows that by gradually increasing the radius of the spherical nanoparticle, the amplitude and the spectral width of the plasmon mode increases but there is no shift occur in the spectrum because the incident field have same effect on the all directions of the sphere. All theses peaks represents LSPR modes and that is dipole mode because the fundamental mode exhibit by the plasmonic nanoparticle is dipolar mode[15]. The higher order modes can be excited by the symmetry breaking of the nanoparticle[11, 16]. But in these all cases the higher order modes are dark, so by changing the radius of the spherical nanoparticle LSPR modes can easily be tuned. Figure 3(b) shows the scattering spectra for conical nanoparticle which is obtained by changing the radius of the nanoparticle. As the radius increases a red shift occur of the LSPR modes are observed in the scattering spectra. Whose spectral width and amplitude also increases. Figure 3(c) shows the scattering spectra for cylindrical nanoparticle. These results are obtained by changing the radius of cylindrical nanoparticle. By increasing the value of r, red shifts of the resonance mode are appeared in the scattering spectra, whose spectral width and amplitude also increases accordingly.



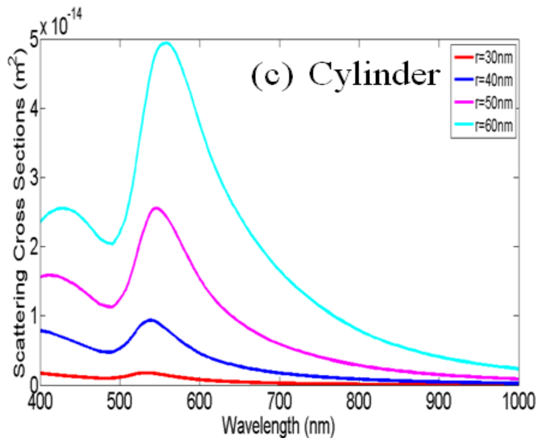


Figure 3.Scattering spectra of proposed nanoparticle for different value of radius (a) for spherical nanoparticle (b) for conical nanoparticle (c) for cylindrical nanoparticle

We next alter the height of the proposed nano-particles and study its effect on the scattering spectra. Figure 4a shows the scattering cross sections for the same polarization as like previous case in the x-direction. Which is achieved by the changing the height of the conical nanoparticle. By changing the height, a very small blue shift of the LSPR modes is appeared in the scattering cross section. Whose spectral width and amplitude of the resonate modes remain almost same. Figure 4b shows the scattering spectra by varying the height of the cylindrical nanoparticle. By changing height increases the LSPR modes can be tuned in the spectrum. As the height increases a small blue shift observed in the resonate mode of scattering spectra .the spectral width and amplitude of the LSPR modes are also almost same.

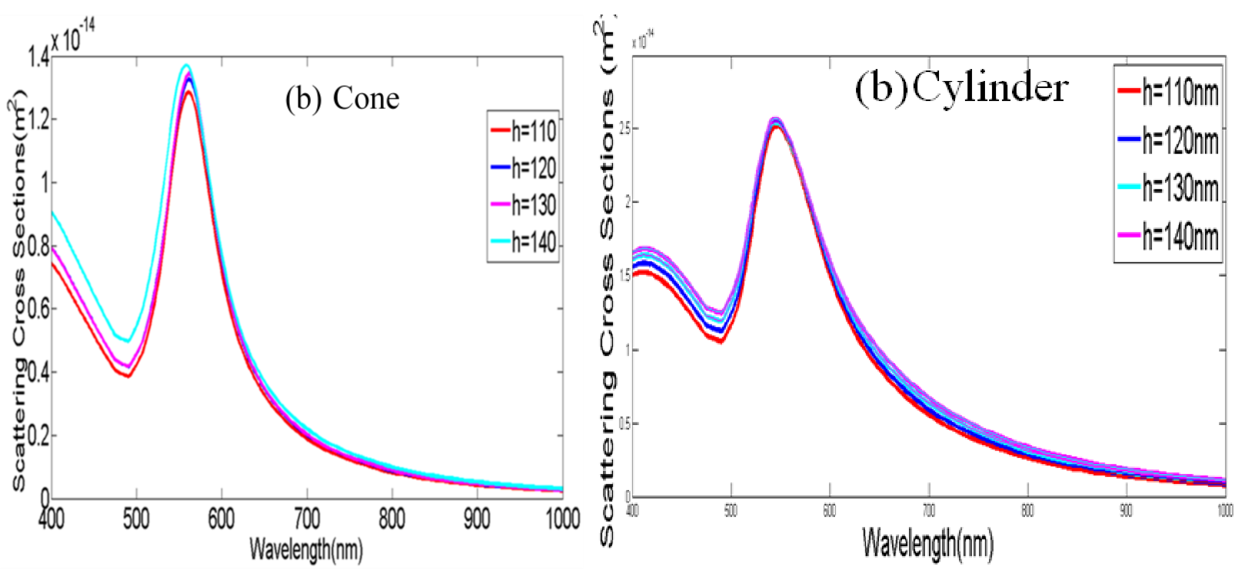


Figure 4a. Scattering Spectra of the proposed nano-particles for different values of height (a) Conical nanoparticle (b) Cylindrical nanoparticle

Finally we have achieved the result shown in figure 5 by the comparison of the three proposed nano-particles. We calculated the volume of the sphere taking the sphere as a reference by using the formula for the volume of sphere $V = {}^{4}/_{3}\,\pi r^{3}$. That value of radius r has chosen which is having the highest amplitude in the scattering spectra. Then next using this known volume of spherical nanoparticle, we find the volume for the conical nanoparticle using the conical volume formula$V = {}^{\pi}/_{3}\, r^2 h$ and finally we find the volume of cylindrical nanoparticle using the spherical known volume by using the volume formula for the cylinder $V = \pi r^2 h$. The result obtained from simulation showed that the spherical nanoparticle exhibits large amplitude and wide spectral width and shift in the scattering spectra.

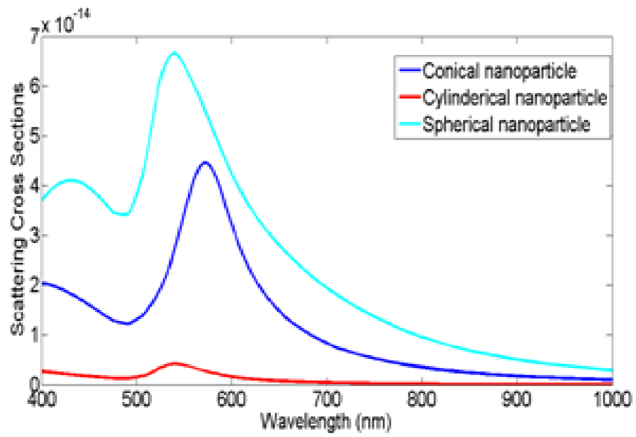


Figure 5. Scattering Spectra of the spherical, conical and cylindrical nanoparticle on the basis of their volume comparison.

Conclusion

We theoretically investigated the scattering properties of the spherical, conical and cylindrical nano-particles while considering the polarization along x-axis, it was observed that the LSPR modes can easily be tuned by changing the parameter of the nano-particles. The spherical nanoparticle exhibits large LSPR shifts and have large spectral width and amplitude. therefore, it can be used for biomedical applications.

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