# Electromagnetic Behavior Studies of Various Size Silver Nanoparticles using Simulation method

Dr Vadiraj.B.Tangod*
** Associate Professor, Sri JagadguruThontadarya Government First Grade College, Mundargi-582118, Karnataka, India.*

*Abstract*

In recent years, a surge of research accomplishments has been realized in the synthesis and characterization of noble metals like Nano gold and Nano silver particles in the field of physics and chemistry, but calculations like absorption, extinction and scattering coefficients using mathematical simulations by Mie's theory playing important role in the field of basic sciences, since materials in the nanometer regime display delightful size-dependent optical, electronic, magnetic, chemical and medicinal properties, which are remarkably different from its bulk behavior. There are copious possible applications for such Nano scale materials in developing industrial and medical fields, due to its unique property of high surface area and exceptional surface activity. These nanoparticles with different sizes show the different extinction, absorption and scattering coefficients. These coefficients can be easily evaluated with the help of mathematical Mie's scattering theory.

Keywords: **Extinction, Absorption, Scattering, Silver nanoparticles.**

## 1. INTRODUCTION

Nanoscience and nanotechnology are recent revolutionary developments of science and technology that are evolving at a very fast pace since a decade. They are driven by the desire to fabricate materials with novel and improved properties that are likely to impact virtually in all areas of physics, chemistry, biology, medicine and other interdisciplinary fields of science and technology. Particles with sizes in the range of 1-100nm are called nanoparticles, whether they are dispersed in gaseous, liquid or solid media. Nanoparticles are a number of atoms or molecules bonded together (about $10^6$ atoms) and are intermediate in size between individual atoms and

aggregates large enough to be called bulk material. Because the nanoparticles are larger than individual atoms and molecules but are smaller than the bulk solid, materials in the nanometer size regime show behavior that is intermediate between macroscopic solid and that of an atomic or molecular system. There are three major factors [1-5] that are responsible for these differences:

1. High surface to volume ratio.
2. Quantum size effect.
3. Electro dynamical interactions.

Metallic nanoparticles possess unique optical, electronic, chemical and magnetic properties that are strikingly different from those of the individual atoms as well as their bulk counterparts. Nano ($10^{-9}$m) sized metal particles exhibit optical properties of great aesthetic, technological and intellectual value. Colloidal solutions of the noble metals namely, silver and gold show characteristic colors that have received considerable attention to researchers.

Metal nanoparticles, especially gold and silver; have attracted considerable attention recently because of their many interesting properties [6] and innumerable technological and medical applications. The optical properties of isolated gold and silver nanoparticles have been extensively studied. Bulk gold has a familiar yellow color, and silver has peculiar silver color, caused by a reduction in reflectivity for light at the end of the spectrum. Whenever gold or silver is sub divided into smaller and smaller particles, the ratio of the radius to the wavelength becomes important, and when the particle is smaller than the wavelength, the Rayleigh approximation (i.e., no retardation) holds and the mathematics becomes simple. Mie [7] has shown that Plasmon excitation is present when the radius is large compared with the wavelength of light, and in that case, the retardation effect should be included to get the correct results. When the particles of gold are small enough, their color is ruby red, due to their strong absorption of green light at about 545nm, corresponding to the frequency at which a Plasmon resonance occurs with the gold [8]. When the dimensions of the conductor are reduced, boundary and surface effects become very important, and for this reason, the optical properties [9] of small metal nanoparticles are dominated by collective oscillation of conduction electrons. An absorption band results when the incident photon frequency is resonant with the collective oscillation of the conduction band electrons and is known (Fig 1) as the Surface Plasmon Resonance (SPR).

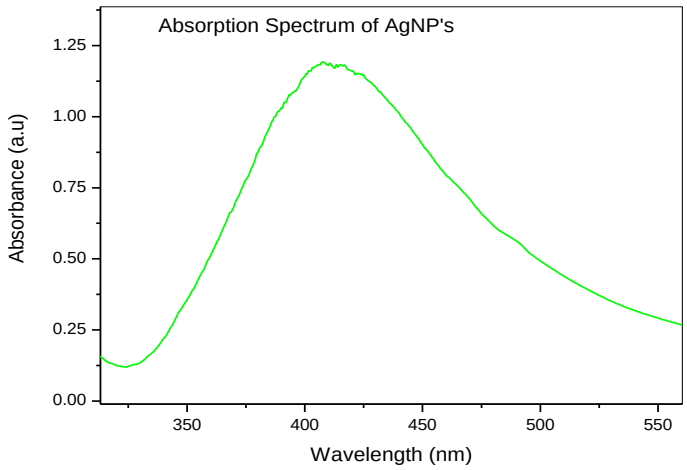


Figure 1. Plasmon resonance absorption spectrum of AgNP's in aqueous solution.

Metal nanoparticles are of great current interest due to their functions as chemical catalysts, adsorbents, biological stains, and elements of novel nanometer scale optical, electronic, and magnetic devices, as the size of the particle decreases to 1-100nm range, it is well-known that the electronic, optical, catalytic and thermodynamic properties of metal particles deviate from bulk properties. Mie presented a solution to Maxwell's equations [10-12] that describes the extinction spectra (Extinction efficiency = scattering efficiency + absorption efficiency) of spherical particles of various size. Mathematical Mie's solution remains of great interest to this day, but the modern generation of metal nanoparticle science, including applications to medical diagnostics and Nano optics has provided new challenges for theory. In this paper, we highlight recent advances in theoretical research in this area, emphasizing especially the linear optical properties (extinction, absorption, scattering) of isolated silver nanoparticles of various shapes in nanometer regime.

### 2.3. Experimental and Simulation Arrangements:

Optical absorption and fluorescence were recorded using Ocean Optics HR4000 high resolution spectrometer. Computational electrodynamics calculations like absorption, scattering and extinction efficiencies are calculated using nanohub.org simulations. Graphical representations are done through Origin 6.1 software.

Synthesis and analysis of silver nanoparticles was done using computational electrodynamic calculations and are available in the nanohub.org simulation software. The tool we will be used in the present study is "Nanospehere Optics Lab", and is based on the Mie's theory.

**3. Theoretical Studies:**

Optical properties of isolated colloidal particles in particular, their dependence on particle size have been intensively investigated through mathematical Mie's scattering theory. In particular Mie's theory [10, 19-20] is a mathematical and physical description of the scattering of electromagnetic radiation by spherical particles immersed in a continuous medium. The Mie scattering solution begins with Maxwell's equations. Using the complex representation of electric field E and the magnetic field H, the Maxwell's equations are of the form,

$$\nabla \cdot E = 0 \quad 3.1$$

$$\nabla \cdot H = 0 \quad 3.2$$

$$\nabla \times E = i\omega\mu H \quad 3.3$$

$$\nabla \times H = -i\omega\varepsilon E \quad 3.4$$

The configuration of an incident electromagnetic field with two components, the electric field E and the magnetic field H can be described by the Helmholtz's relation [19-20] as

$$\nabla^2 E + k^2 E = 0 \quad 3.5$$

$$\nabla^2 H + k^2 H = 0 \quad 3.6$$

In which k is the wave number defined by

$$k^2 = \omega^2 \varepsilon\mu \quad 3.7$$

The effect of the particular size on the peak resonant wave length results from two different mechanisms depending on the particle size range. In the limit of $2R << \lambda$ (where R is the radius of the particles and $\lambda$ is the wave length of the light in media), only the electric dipole term contributes significantly [1,7,10,21] to the extinction cross section ($\sigma_{ext}$) is,

$$\sigma_{ext} = 9\frac{\omega}{c}\varepsilon_m^{3/2} V \frac{\varepsilon_2(\omega)}{\left[\varepsilon_1(\omega) + 2\varepsilon_m\right]^2 + \left[\varepsilon_2(\omega)\right]^2} \quad 3.8$$

Where $V = \left(\frac{4\pi}{3}\right) R^3$ is volume of the spherical particle.

$$\sigma_{abs} = \sigma_{ext} - \sigma_{sca} \qquad 3.9$$

ω is the angular frequency of the exciting light, c is the velocity of light, $\varepsilon_m$ and ε(ω) [ε(ω)= $\varepsilon_1(\omega)$+ i$\varepsilon_2(\omega)$] are the dielectric frictions of the surrounding medium and the material itself respectively. The resonance condition is fulfilled when $\varepsilon_1(\omega) = -2\ \varepsilon_m$ provided $\varepsilon_2$ is small or weakly dependent on ω.

The ability to assemble nanoparticles of controllable sizes and shapes is increasingly important because many frontier areas of research, such as sensors, catalysis, medical diagnostics, information storage, and quantum computation, require the precise control of nanomaterial architecture and component miniaturization. In nanotechnology, the assembly of metal nanoparticles has resulted in novel materials with interesting properties, i.e., extremely high extinction coefficients and the strongly distance-dependent.

## 4. RESULTS AND DISCUSSION

In the present case the absorption spectrum of AuNP's has a maximum in the range 480-490nm peaking at 485nm, which is related to the Plasmon resonance formed due to the Nano sized (4-12nm) silver particles. This absorption band results from interactions of free electrons confined to small metallic spherical objects with incident electromagnetic radiation. The observed Plasmon resonance band (Fig 1) shows that the silver nanoparticles are spherical in shape.

Extinction coefficient is sum of absorption and scattering coefficients (Table 1). Scattering arises when charged particles accelerated by a field and reradiate. Absorption (Fig 2) occurs when the particle takes energy out of the beam and converts it to other forms. Mie's expression for Extinction efficiency is given by Eqn 3.8, the extinction efficiency spectrum for several nanoparticle radii can be seen in (Fig 3). The wavelength corresponding to maximum extinction shifts to longer wavelengths (red shift) as the particle radius increases. The peak seen at 485nm corresponds to the resonance condition for small spheres specifically when $\varepsilon_1(\omega) = -2\ \varepsilon_m$. A large shift of the dipole peak and a much more complex spectrum occur when the particle radius is increased further.

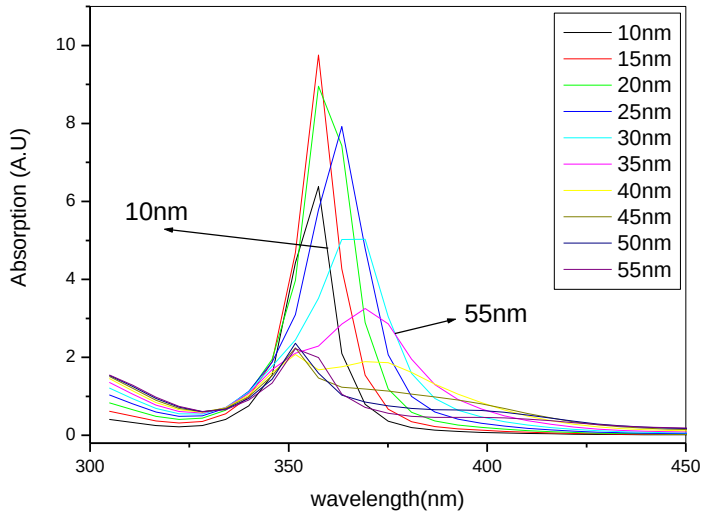


Figure 2. Absorption coefficient of silver nanoparticles of various sizes from 10-55nm.

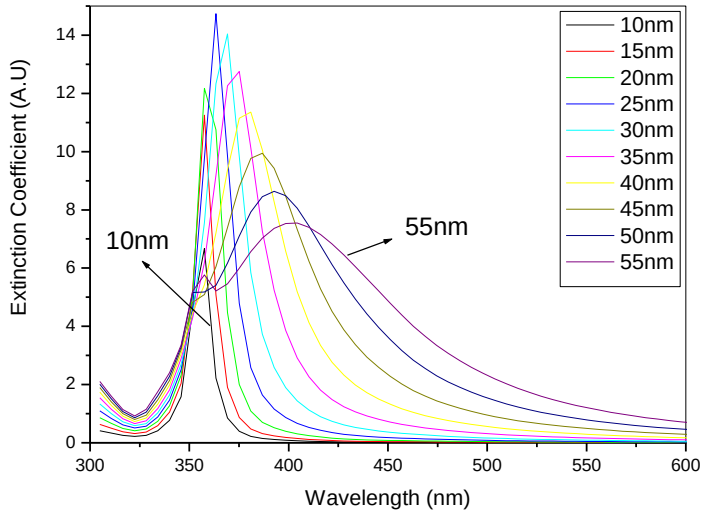


Figure 3.Extinction cross section of silver nanoparticles of various sizes from 10-55nm.

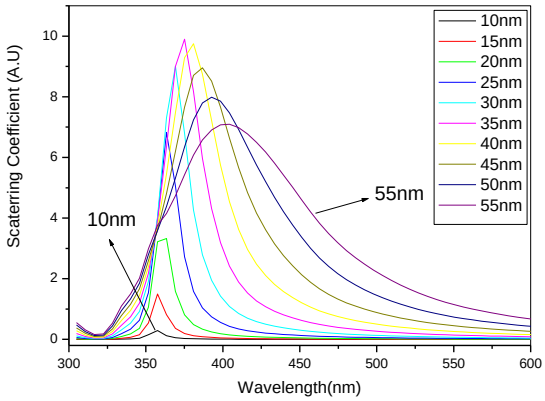


Figure 4. Scattering cross section of silver nanoparticles of various sizes from 10-55nm.

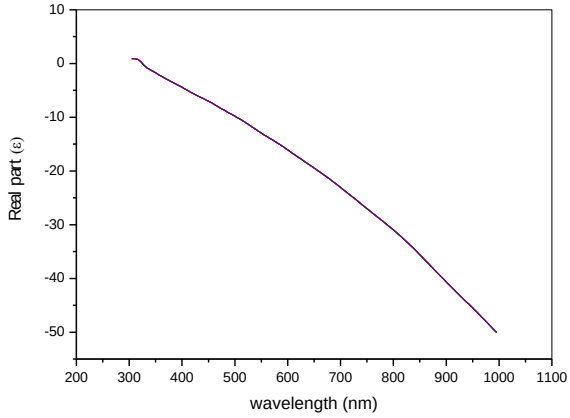


Figure 5. Real part of dielectric constant of silver nanoparticles.

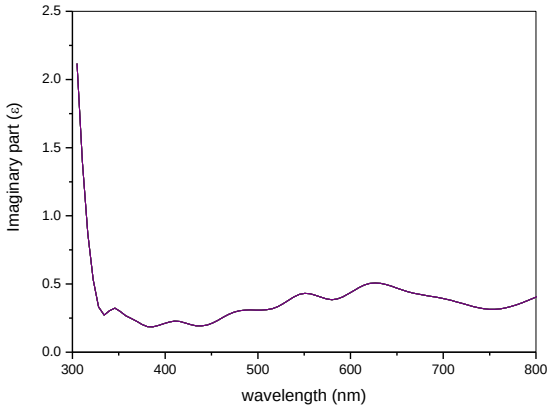


Figure 6. Imaginary part of dielectric constant of silver nanoparticles.

Since the dielectric medium constant (ε ) is related to refractive index, [ 9-11, 22] i.e., $(n_{eff} + ik_{eff})^2 = \varepsilon_{eff}$ ($\varepsilon_{eff}$ is the effective dielectric constant of the nanocomposite, $n_{eff}$ is the real part of the effective complex index of refraction for the nanocomposite, $k_{eff}$ is the imaginary part of the effective complex index of refraction), we show here that the evolution of the SPR band at the longer wavelength region can be considered a result of the increase in effective refractive index for nanoparticles in the assembly, in the assembly process, the size of individual silver nanoparticles in the solution should remain largely constant, whereas the inter particle distance changes, which leads to changes in the inter particle dielectric medium constant or refractive index. Refractive index n will be used to represent the $n_{eff}$. Interestingly, the change in n was found to exhibit an approximate linear relationship with $\lambda_{max}$. Simulation results for silver nanoparticles for various sizes 10-55nm particles using Mie's theory, which matches with the bands in terms of the SPR wavelength as observed. On the basis of the documented principle that the Plasmon red shift increases with refractive index change, a basic assumption for applying the Mie's theory simulation to this system is that the nanoparticles within the assembly environment have a refractive index higher than that in the water environment. This assumption is qualitatively supported by the trend of refractive index changes reported in previous studies for similar assemblies of metal nanoparticles in different systems. The effect of electromagnetic retardation in larger sized nanoparticles makes the observed red shift in the Plasmon resonance.

Fig 2 to 6 shows the calculated spectra of the efficiency of absorption, scattering and extinction for silver nanoparticles of radius 10-55nm in size. The dimensionless efficiencies can be converted to the corresponding cross-sections $\sigma_{abs}$ , $\sigma_{ext}$ and $\sigma_{sca}$ have units of $m^2$ because they represent an equivalent cross-sectional area of the particle that contributes to the absorption, scattering and extinction of the incident light.

**TABLE 1.** Observed Extinction, Absorption and Scattering efficiencies of silver nanoparticles of various sizes in the surrounding water medium.

| Radius of the nanoparticle (nm) | Position of $\lambda_{max}$ (nm) | Extinction efficiency | Absorption efficiency | Scattering efficiency |
|---|---|---|---|---|
| 10 | 357.53 | 6.673 | 6.380 | 0.293 |
| 15 | 357.33 | 11.256 | 9.757 | 1.499 |
| 20 | 357.53 | 12.172 | 8.953 | 3.323 |
| 25 | 363.38 | 14.739 | 7.923 | 6.816 |
| 30 | 369.23 | 14.039 | 5.032 | 9.007 |
| 35 | 375.08 | 12.757 | 2.860 | 9.897 |
| 40 | 380.93 | 11.358 | 1.613 | 9.745 |
| 45 | 386.78 | 9.941 | 0.983 | 8.958 |
| 50 | 392.63 | 8.637 | 0.654 | 7.983 |
| 55 | 404.33 | 7.545 | 0.448 | 7.096 |

## 5. CONCLUSION

The optical properties of spherical silver nanoparticles can be tuned by adjusting the physical dimensions. The dielectric properties of the material are extremely important and play a large role in the intensity and placement of the Plasmon resonances. As spherical nanoparticles get larger, the peaks broaden and shift to longer (red shift) wavelengths. This shift of the SPR of the band position and intensity of the nanoparticle assembly can be related to the change in dielectric medium of RI properties, which provides a means to produce optical signals for up taking or releasing of molecular species in the nanoparticle assembly. This type of inter particle property also has potential applications in controlled drug delivery, in regard to the exploitation of these Nano materials for application in electrical sensors, the electrical response of nanoparticle assemblies to vapor sorption serve as an excellent example illustrating the correlation of the electrical properties with inter particle dielectric medium properties, The understanding of the precise control of the inter particle properties will benefit these nanostructured sensing applications. These mathematical simulations carried out during the present work is useful to tunable the properties of central development in Nano science and nanotechnology. In view of this we have highlighted some recent progress towards the development of basic physics and chemistry in the field of Nano science and nanotechnology which opens up the new avenues towards latest advances in the field of mathematics and physics.

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