Determination of Extinction, Absorption and Scattering Coefficients of Gold Nanoparticles

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Abstract. Optical properties of nano particles and their dependence on particle size effect have been investigated through Mie's Scattering theory. The absorption spectrum of gold nanoparticles of size 4-12nm has a maximum peak in the range 540-550nm, which is related to the surface plasmon resonance(SPR). Our main task is to calculate the extinction, absorption and scattering coefficients of gold nanoparticle of various sizes using Mie's theory with available simulations. Observed results reveals as the size of the nanoparticles increases from 4 to 50nm, extinction efficiency at resonant peak is also increases, along with SPR shifts from 520nm to 570nm.

Keywords: Extinction, Absorption, Scatterring, Gold nanoparticles.

INTRODUCTION

Nanoscience and nanotechnology are recent revolutionary developments of science and technology that are evolving at a very fast pace since a decade. Materials in the nanometer size regime show behavior which is intermediate between that of a macroscopic solid and an atomic or molecular system because of high surface to volume ratio, quantum size effect and electro dynamical interactions [1].

Nanoparticles show plasmon excitation[2], when the radius of a nanoparticle is large compared with the wavelength of light, due to their strong absorption of green light at about 545nm, corresponding to the frequency at which a plasmon resonance occurs with the gold [3]. An absorption band results when the incident photon frequency is resonant with the collective oscillation of the conduction band electrons and is known as the surface plasmon resonance (SPR).

Metal nanoparticles are of great current interest due to their applications as chemical catalysts, adsorbents, biological stains, sensors, catalysis, medical diagnostics, information storage, quantum computation, optical, electronic, and magnetic devices. As the size of the particle decreases to the 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 [5] that describes the extinction spectra (Extinction efficiency = scattering efficiency + absorption efficiency) of spherical particles of various size.

EXPERIMENTAL

Gold Nanoparticles(AuNP's) are synthesized via the reduction of $HAuCl_4$ with trimeric alanine-based phosphine (Thpal) as a reducing agent, Further to prevent aggregations of AuNP's Gum arabic (glycoprotein) is capped and it makes the AuNP's are stable even up to 6 months duration. SEM, TEM pictures of AuNP's of size 4-12nm are shown in Fig 2.

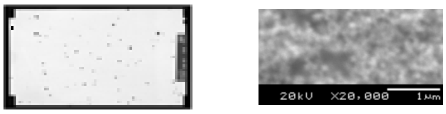

FIGURE 2(a). TEM (b) SEM image of gold nanoparticles

THEORETICAL STUDIES

Optical properties of isolated colloidal gold nanoparticle and their dependence on particle size have been investigated through Mie's [5] scattering theory.

The effect of particular size of the nanoparticles on the peak resonant wave length results from two different mechanisms depending on the particle size range. In the limit of $2R \ll \lambda$ (where R is the radius of the particles and λ is the wave length of the light in media), only the electric dipole term contributes significantly [1, 3, 5] to the extinction cross section (σ_{ext}) is,

$$\sigma_{ext} = 9\frac{\omega}{c}\varepsilon_m^{3/2}V\frac{\varepsilon_2(\omega)}{[\varepsilon_1(\omega)+2\varepsilon_m]^2+[\varepsilon_2(\omega)]^2} \quad (1)$$

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

$$\sigma_{abs} = \sigma_{ext} - \sigma_{sca} \quad (2)$$

ω is the angular frequency of the exciting light, c is the velocity of light, ε_m and $\varepsilon(\omega)$ [$\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega)$] are the dielectric frictions of the surrounding medium and the material itself respectively.

RESULTS AND DISCUSSION

In the present case the absorption spectrum is maximum in the range 520-550nm observed from Ocean Optics HR4000 high resolution spectrometer and peak at 545nm, which is related to the SPR formed due to the nano sized (4-12nm) gold particles (Fig 1).

Extinction coefficient is sum of absorption and scattering coefficients (Table 1). Scattering arises when charged particles accelerated by a field and reradiate. Absorption (Fig 3) 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 equation 1. The extinction efficiency spectrum for several nanoparticle radii can be seen in (Fig 4). The wavelength corresponding to maximum extinction shifts to longer wavelengths (red shift) as the particle radius increases. The peak seen at 521nm 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,

The dielectric constant (ε) of the medium is related to refractive index of the medium[6], i.e., $(n_{eff} + ik_{eff})^2 = \varepsilon_{eff}$ (ε_{eff} is the effective dielectric constant of the nanocomposite, n_{eff} is the real part of the effective complex refractive index for the nanocomposite, k_{eff} is the imaginary part of the effective complex index of refraction). Simulation results for gold nanoparticles for various sizes 10-50nm particles using Mie's theory, which matches with the bands in terms of the SPR wavelength as experimentally observed.

Fig 3 to 5 show the calculated spectra of the efficiency of absorption, scattering and extinction for gold nanoparticles having radii in the range 10-50nm.

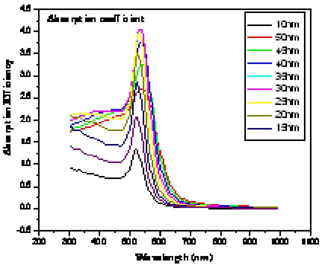

FIGURE 3. Absorption coefficient of gold nanoparticles of various sizes in the range 10-50nm.

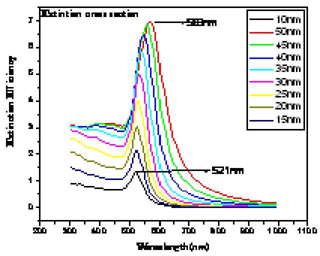

FIGURE 4. Extinction cross section of gold nanoparticles of various sizes in the range 10-50nm

The dimensionless efficiencies can be converted to the corresponding cross-sections σ_{abs}, σ_{ext} and σ_{sca} have units of m^2 as they represent an equivalent cross-sectional area of the particle that contributes to the absorption, scattering and extinction of the incident light.

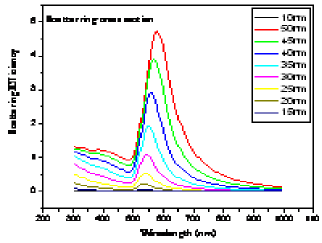

FIGURE 5. Scattering cross section of gold nanoparticles of various sizes in the range 10-50nm

TABLE 1. Observed Extinction, Absorption and Scattering efficiency of gold nanoparticles of various sizes in the surrounding water medium.

Radius of the nano particle (nm)	Peak λ_{max} (nm)	Extinction efficiency	Absorption efficiency	Scattering efficiency
10	521	1.349	1.339	0.019
15	527	2.121	2.066	0.055
20	527	3.041	2.681	0.368
25	527	4.004	2.842	1.162
30	533	5.010	3.263	1.847
35	539	5.856	3.523	2.331
40	551	6.459	3.782	2.777
45	556	6.825	3.976	3.921
50	568	6.949	4.048	4.719

CONCLUSION

The optical properties of spherical gold nanoparticles are extremely important and play a vital role in the intensity and placement of the plasmon resonance. 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 and RI properties.

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