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Numerical Analysis of Optical Properties of Silver Nanoparticle

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Abstract: *The plasmonic properties of metallic dielectric nanoparticles exhibit a highly sensitive dependence on geometry, due to the interaction between Primitive Plasmon modes associated with the surfaces of the nanoparticle. Changes in nanoparticle geometry that reduce symmetry alter the interactions between Plasmon modes and give rise to modified, and altogether new, plasmonic features. Plasmons are density waves of electrons created when light hits the surface of a nanoparticle under precise conditions. The wavelength of incident light is greater than size of particle. To overcome this problem we have examined the optical properties: near-field and far-field; scattering, absorption, extinction and field enhancement for block shape core shell nanoparticle for 200 frequency values. Size of the 3D block is {60; 60; 60} and the wavelength is 400-900nm.*

I. Introduction:

A rapidly expanding army of metallic dielectric nanoparticles has taken the world of Nano photonics by storm, offering solutions to decades-old problems and opening up new avenues of exploration. Cancer research has been expanded from a focus in pharmaceuticals and radiotherapy to include engineered nanoparticle therapies [1, 2]. Spectroscopic measurements have been revolutionized by field enhancements previously unavailable outside of specialized laser facilities [3]–[4]. Eventually, such nanoparticles may even form the basis of inexpensive optical metamaterials [5]. When external optics hit a metallic surface, so that resonance occurs, this oscillation of the free electrons at the surface of a metal at a certain frequency is known as Plasmones. In the case of a nanoparticle the size of the particle is too small as compared to the wavelength range. We are concern to find the enhance electric field and specific wavelength and frequency. Here we have studied the optical properties, near-field and far-field in COMSOL Multiphysics using finite element method.

COMSOL Multiphysics is a software environment for the modeling and simulation of any physics based system. COMSOL Multiphysics is a finite element analysis, solver and Simulation software / FEA Software package for various physics and engineering applications, especially coupled phenomena, or Multiphysics. For the calculations of near field and far field we use COMSOL Multiphysics 4.2. COMSOL Multiphysics also offers an extensive interface to MATLAB and its toolboxes for a large variety of programming, preprocessing and post processing possibilities. In post processing the data is analyze in MATLAB 2012.

The finite element method is a numerical method seeking an approximated solution of the distribution of field variable in the problem domain that is difficult to obtain numerically. The problem is divided into several elements; each has a very simple geometry. Finite element method mainly consist of four steps: Modeling of geometry, meshing, specification of material property, and specification of boundary, initial and loading condition. The finite element method (FEM) is the dominant discretization technique in structural mechanics. The basic concept in the physical interpretation of the FEM is the subdivision of the mathematical model into disjoint (non-overlapping) components of simple geometry called finite elements or elements for short. The response of each element is expressed in terms of a finite number of degrees of freedom characterized as the value of an unknown function, or functions, at a set of nodal points.

In this study, we have used the finite element method (FEM) to examine the transition from silver Nano shells. Both the near- and far-field effects of core offset and total particle size are considered, with an emphasis on spectral evolution and focused field enhancements. We conclude that, for a given pair of inner and outer shell radii, phase retardation and core offsets can be used together to design nanoparticles with a desired scattering and absorption ratio at the dipolar resonance.

II. Results and Discussions

The near- and far-field optical properties of Nano shells are solved numerically in the frequency domain using the scattered field formulation. Problem definition, solution and analysis were all conducted using Matlab (R2012a) in conjunction with the scripting functions of a commercially available FEM package (COMSOL Multiphysics 4.2 with the RF module).

The 3D simulation space was composed of four spherical volumes: a core, a shell, an embedding medium and a perfectly matched layer (PML). A plane wave, used for excitation, was inserted on the inside of PMLs surrounding the embedding medium. Large field enhancements, resulting from Plasmon resonances, required the application of mesh constraints to ensure convergence of the simulation in the visible and near-infrared (NIR) (400-900 nm). The Nano shells surface was restricted to a maximum triangle mesh side length of 25nm with maximum element growth rate of 1.5. Specifying that elements adjoining the nanoparticle surface could be no more than 1.4 times the size of surface elements. Far-field extinction spectra were obtained by summing the far-field absorption (*Q*abs) and scattering (*Q*scat) efficiencies. Near-field enhancements at a point is defined as the total electric-field amplitude (*E*tot) at the nanoparticle surface normalized to the incident field magnitude (*E*tot/*E*inc) where, on resonance, the total electric field near the particle surface is dominated by scattering (*E*tot _ *E*scat).

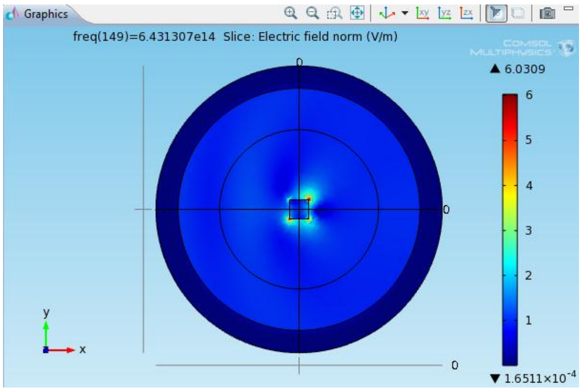

Figure 1 Simulated enhanced electric field at wavelength= 466.4681 nm, f=6.4313e14 hz, with minimum electric field value 1.6511e-4 and maximum 6.0609.

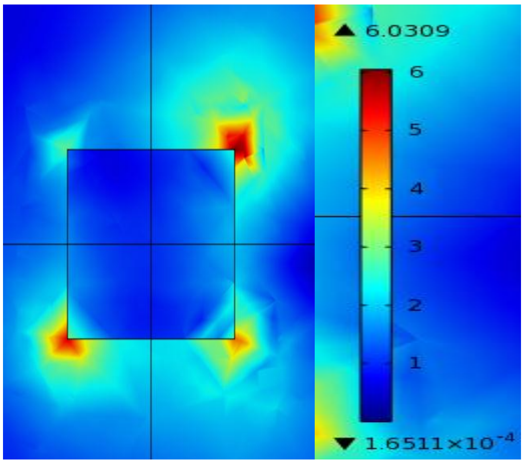

Figure 2. Hotspot of electric field Polarization in y-axis and propagation in x-axis with minimum electric field 1.6511e-4 and maximum 6.0309**.**

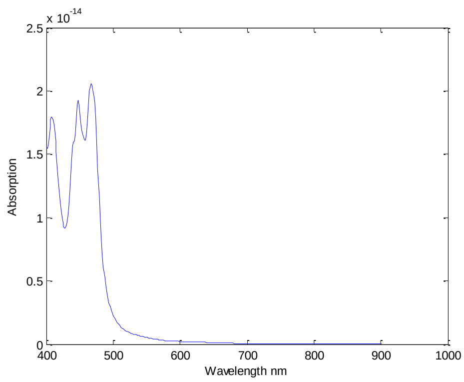

Figure 3. Absorption spectra at the surface of block shape nanoparticle, peak value at wavelength= 466.4628nm.

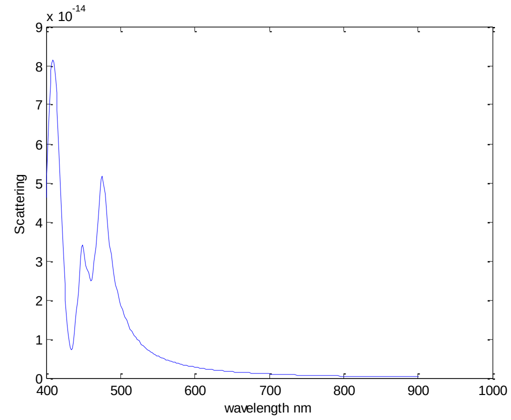

Figure 4. Scattering spectra of electric field at the surface of shell of radius =250nm of the dielectric air. Peak value of scattering at wave length 409.145nm.

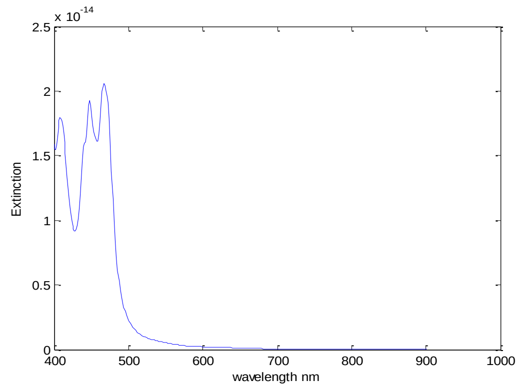

Figure 5. Extinction spectra Extinction= absorption + scattering, peak value is at wavelength= 466.4681nm.

After simulation in COMSOL Multiphysics we analyze the data in Matlab. We take the volume integration at the surface of nanoparticle and export data to matlab to get the electric field absorption spectra as in figure 3. And analyze the surface integration data to get scattering spectra as in figure 4. The extinction spectra is the summation of absorption and scattering data and the peak value of the extinction is at wavelength 466.4681nm. Then we analyze the simulation for the peak valve of extinction. Extinction peak is at the frequency (149)= 4.31307e14 to get enhanced electric field as shown in figure 1. The electric field polarization is in y-axis and propagation is in x-axis. The zoomed hotspot in figure 2, shows the enhanced electric field due to the enhanced oscillation of Plasmons. The minimum and maximum electric field is calculated 1.6511e-4 and 6.0309 respectively.

III. Conclusion

In this study we have observed the specific wavelength from the range 400-900nm at which the electric field is maximum. We have shown that the broad wave length can be tune to the nanoparticle by finite element method. This type of tuning is possible by finding the specific wavelength and frequency of the extinction peak value at which the Plasmones are more excited. In the future we will analyze behavior of the nanoparticle to the mid infrared and far infrared. The nanotechnology makes the products Lighter, Stronger, Faster, Smaller and more Durable.

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