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Research Article

STUDY OF ELECTRO-OPTIC INTERACTIONS FOR SILVER NANOPARTICLES

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ABSTRACT
Semiconductor nano-materials are more commonly studied than metallic ones. However, recent applications of metallic nanoparticles in biomedicine have sparked intense interest in this area. The controlled particle size combined with the stealth ligand on their surface allows them to hide from the immune system, enabling them to circulate in the blood for longer periods of time. It is vital to study electro-optic interactions for the creation of successful biomedical sensors using silver nanoparticles. In the present study, we examined variations in the extinction spectra and electric field intensity along with variations in light polarization, semiconductor medium, and particle size of silver nanoparticles using Nanosphere Optics Lab Field Simulator. The peak extinction wavelength shows a significant increase with size, along with the bandwidth. There were significant differences in the results due to changes in embedding medium. Hence, we may conclude that the silver nanoparticles may find applications in a variety of fields, including medical, health care, industrial catalyst and consumer products, due to their unique tunable electro-optical properties.

Keywords: Metallic Ag nanoparticles, Electric field variations, Extinction coefficient, Solid medium dependences.

1. INTRODUCTION
The application of nanoparticles in the real world is proving to be very versatile and beneficial for the next evolution of civilization. One of the most studied of these is semiconductor nanoparticles used mostly in optoelectronics applications. However, the advent of technology and knowledge made it possible to create metallic nanoparticles as well [1]. In comparison with their semiconductor counterpart, metallic nanoparticles are less explored. Metallic nanoparticles have recently attracted the attention of a large number of researchers. The use of metallic nanoparticles in biomedical sciences and engineering has fascinated scientists for decades. Most nanoparticles used in biotechnology fall within the range of 10 to 500 nanometers, rarely exceeding 700 nanometers. These nanoparticles allow various types of communication with biomolecules on and within cells in a way that can be decoded and related to a variety of biochemical and physiological properties [2]. Furthermore, its potential application in drug delivery system and noninvasive imaging offered a number of advantages over conventional pharmaceuticals [3]. The nanoparticles must be stable, biocompatible, and selectively directed to specific sites after systematic administration in order to be utilized fully. Cancer cells, for example, can be targeted with more precise technique for recognizing them. This is possible by conjugating the nanoparticle with an appropriate ligand, with specific binding activity towards the target cells. Also, nanoparticles can be used as platforms to attach multiple therapeutic substances to them, which enables the concentration of these substances to be increased at the pathological site. Nanoparticles (>3-5 nm) with different sizes can change the concentration and dynamics of the active molecule. By controlling particle size in combination with a surface coating with a stealth ligand, they can hide from the body's immune system, allowing them to circulate in the blood for a longer period of time [4]. The use of nanoparticles, such as magnetic nanoparticles (iron oxide), gold and silver nanoparticles, nanoshells, and nanocages, as therapeutic agents has increased over the past decade. The study of metallic nanoparticles is a very exciting and interesting field of research because of its immense applications in biomedicine. The use of metallic nanoparticles can be useful to develop products that have antimicrobial properties and have the potential to improve shelf life of food products [5]. There are many important uses of gold (Au) and silver (Ag) nanoparticles, including nano biotechnology, biosensor technology, cell structure

visualization, targeted drug delivery, and water purification [6]. Electro-optic interactions have a key role to play in making successful biomedical sensors using Ag and Au nanoparticles, which is why their study is important. In this work we utilized Nanosphere Optics Lab Field Simulator [7] to simulate and predicts the behavior of metallic silver nanoparticles when they interact with light. This study investigates variations in extinction spectra and electric field intensity of silver nanoparticles with variations in light polarization, semiconductor medium, and particle size.

2. THEORETICAL BACKGROUND

Metallic nanoparticles have optical properties similar to semiconductor quantum dots, but their underlying physics is completely different. In an electric field, the conduction band electron cloud in small spherical metallic nanoparticle irradiated by light oscillates coherently because of the oscillating electric field, as shown in schematic diagram in Fig. 1.

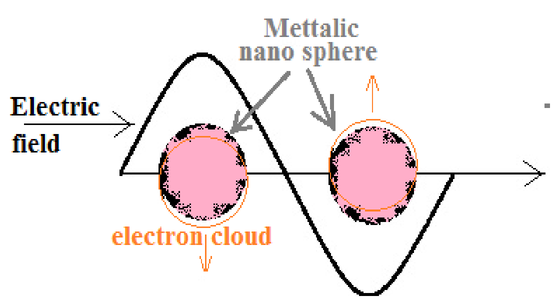


Fig. 1: Plasmon oscillations in metallic nano sphere in the presence of electric field

A restoring force arises from Coulomb's attraction between electrons and nuclei when the electron cloud is displace relative to the nuclei, causing an oscillation in the electron cloud. The oscillation frequency, depends on four factors: density of electrons, effective electron mass, shape, and size of the charge distribution. It is called the dipole plasmon resonance of the particle because it consists of a collective oscillation of electrons. The plasmon frequency of a metal like silver is influenced by other electrons such as those in d-orbitals, which makes calculating the plasmon frequency difficult using electronic structure calculations. However, the plasmon frequency can easily be related to metal dielectric constant (or refractive index), which are measurable as a function of wavelength for bulk metal. In order to correlate a metal nanoparticle's dipole plasmon frequency with its dielectric constant, we consider the interaction of light with a spherical particle that is much smaller than its wavelength. Under these conditions, the electric field of light could be regarded as constant, and the interaction would follow electrostatics rather than electrodynamics.

Localized Surface Plasmon Resonances (LSPR) are well known to occur when visible light excites collective oscillations of electrons inside the metals. In other words, LSPR is a coupled oscillation of electron density and electromagnetic waves. These are unlike the surface plasmons, which are actually electromagnetic waves propagating along the metal-dielectric interface. Because the nano particle's surface is curved, it exerts an effective restoring force on the driven electrons, so a resonance can be formed and field amplification occurs inside and outside the particle. As a consequence, metal nanoparticles scatter light at the LSPR frequency effectively.

The excitation of LSPR in metal nanoparticles is the most efficient process by which light interacts with matter and defines the optical properties of nanoparticles. The LSPR frequency can be successfully tuned within a broad spectrum, by varying the refractive index of the surrounding medium or using nanoparticles of different shapes and sizes [8]. In gold and silver nanoparticles, the resonance occurs in the visible region of the electromagnetic spectrum. This fact is evident by the bright colors displayed by particles immersed into transparent matrix (such as glass or aqueous suspension) in both transmitted and reflected light. The phase matching is not necessary for LSPR to get excited by incident light directly, as it is for surface plasmon-polaritons.

3. COMPUTATIONAL/SIMULATION DETAILS

In contrast to semiconductor nanoparticles, where the blue shift is caused by electron/hole energy quantization and produces major changes in their optical properties, the changes of metallic nanoparticles can be explained by using a classical dielectric picture. Specifically, we solve the Laplace and Maxwell's equations to see how an electric field interacts with a spherical nanoparticle depending on following two boundary conditions,

1. Surface of the sphere has a continuous electric potential.
2. Electric field displacement has a continuous normal component.

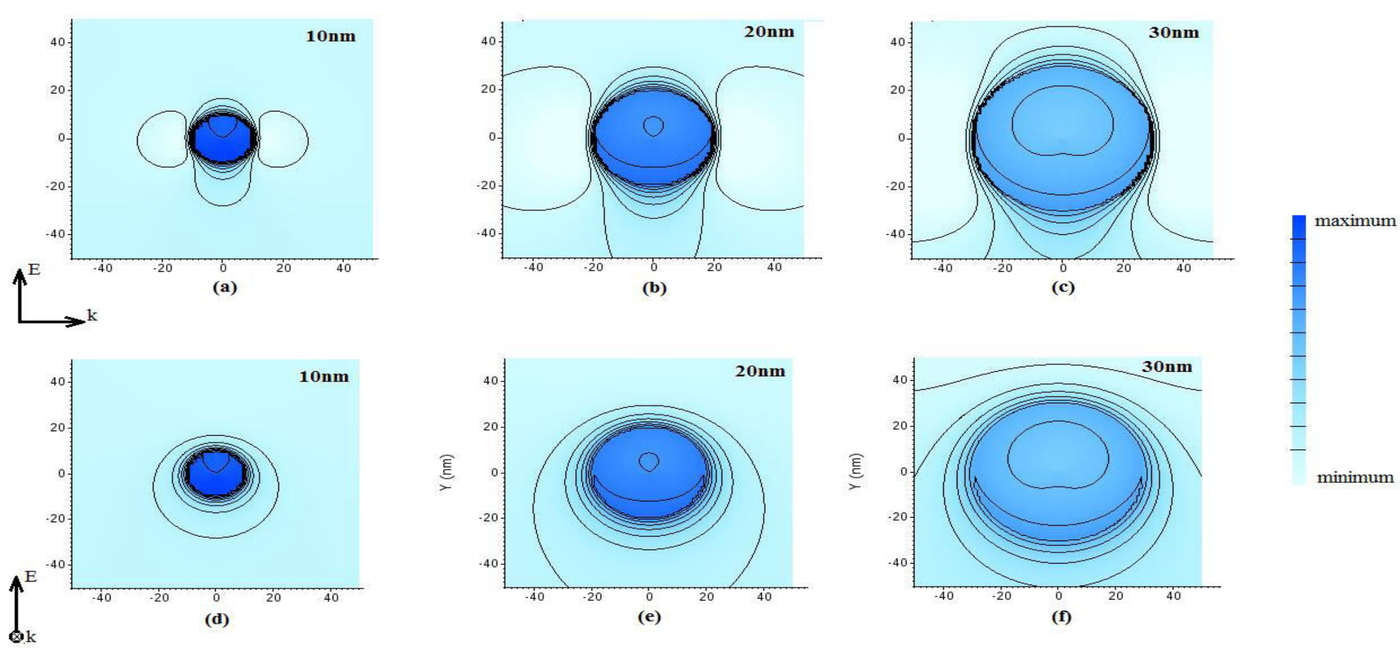
The radiation incident on the sphere is absorbed in part, scattered in part, and may be transmitted in part. These equations are then solved to obtain the peaks for absorption, scattering, and extinction spectra. The extinction coefficient, which is equal to the sum of the absorption and scattering coefficients, presents the total amount of radiation that the nanoparticle intercepts.

In order to obtain the present results, we used Nanosphere Optics Lab Field Simulator [7], which simulates the behavior of metallic nanoparticles in contact with light. This simulator uses Mie's theory to calculate the aborption, scattering, and extinction spectra of metallic spherical nanoparticle. The electric field induced by electromagnetic radiation, as well as the absorption, scattering, and extinction of spheres of Ag is computed with this tool. The refractive index of the surrounding medium, the radius of the nanoparticle to be studied, the Bessel function order, polarization of the light and the wavelength of the incoming radiation can be varied in order to derive results and predict the nature of nanoparticles. In the first step, we compute the wavelength at which the maximum of the extinction spectrum occurs for a nanoparticle of a given size, with the electric field kept at zero. The maximum electric field occurs at the wavelength of the extinction peak, so the wavelength of the incident light is assigned that value, and the tab 'Calculate Electric Field' is clicked. We then, compute the various extinction spectra and electric field distributions for Ag nanoparticles by incident radiations at wavelength 329nm.

4. RESUTLS & DISCUSSION

The electric field enhancements $|\boldsymbol{E}|^2$ with all multipoles, at 10, 20, and 30 nm sliver nonospheres in vacuum, are shown in Fig. 1, when light with the wavelength equal to peak extinction wavelength is incident on it. Two planes are chosen for the plots: one is formed by the polarization and **k** vectors (Fig. a, b, c), and the other is perpendicular to the polarization vector (Fig. d, e, f). We observe that for 10nm particles, the electric field is less distributed in the area, but its intensity is higher. However, particle intensity for 30nm particles is distributed, but its intensity is not as high as that for 10nm particles. So, as the size of the nanoparticle increases, the electric field becomes more distributed, but its intensity decreases. Moreover, such dipole fields exhibit d-orbital (distorted) shaped electric fields around the nanospheres. As shown in the graphic, the d-orbital lobes are asymmetrical. This may be attributed to small electric quadupole components arisen due to alternating positive and negative charges.

Fig. 2 shows the absorption, scattering, and extinction (absorption + scattering) spectrums for silver nano-particles of sizes 10, 20, and, 30nm when light of wavelength 329nm get incident on these. This illustrate the fact that absorption and scattering efficiencies peaks differ both in magnitude and wavelengths. The scattering of light is minimum for 10nm and maximum for 30nm nanoparticles indicating strong size dependence.



(Fig. a,b,c) for cross-section containing the propagation vector and polarization axes and (Fig. d, e, f) for cross-section perpendicular to propagation.

Fig. 1: E-field contours for radius 10, 20, and 30 nm Ag-Nano spheres

In the plot shown in Fig. 2 (c), we can see that as the nanoparticle size increases, the wavelength at which the extinction coefficient peak occurs also increases. In addition to peak extinction wavelength, bandwidth also increases with size, while peak extinction wavelength rises significantly, as illustrated in table 1.

We examine the nature of even bigger Ag nanospheres with lengths of 25, 50, and 75nm. Fig. 3 illustrates the electric field variations for these nanoparticles. These results show that if the size of the nanoparticle is increased further, the electric field will become even more diffuse with a lesser intensity. The electric field contours around the nanosphere become more asymmetrical. In these cases, electric field variations confirm the hybridization of plasmon modes near-field enhancement of metallic nano-particles as suggested by Huang *et. al* [9]. Even so, plasmonic resonances in metallic nanoparticles are still undergoing intense research with the aim of helping develop practical nanoscale optical sensors [10].

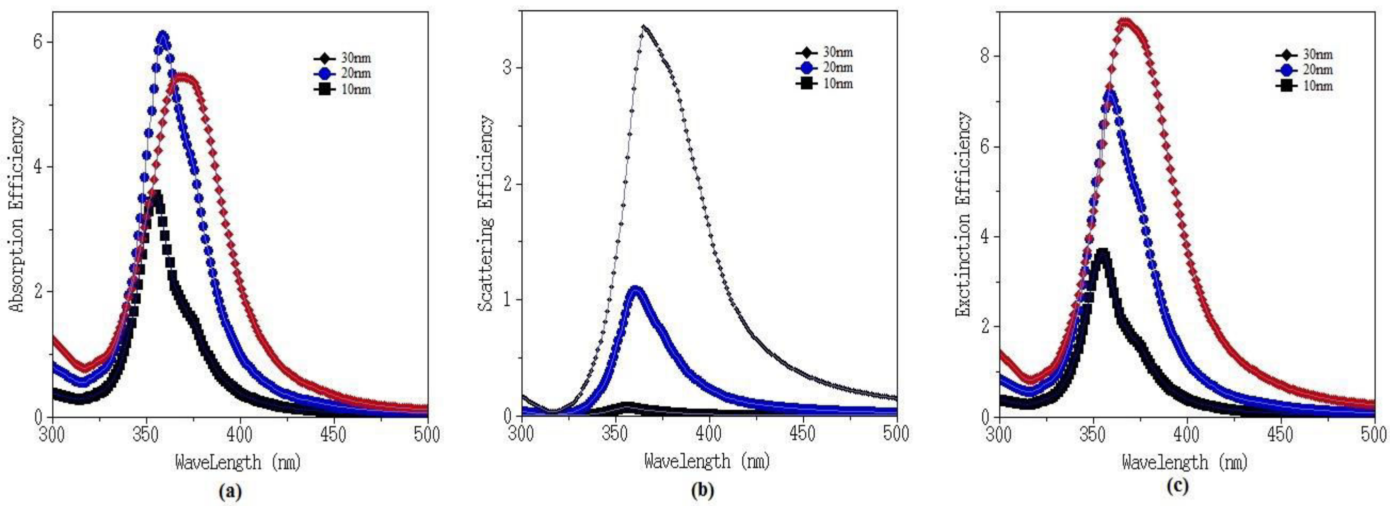
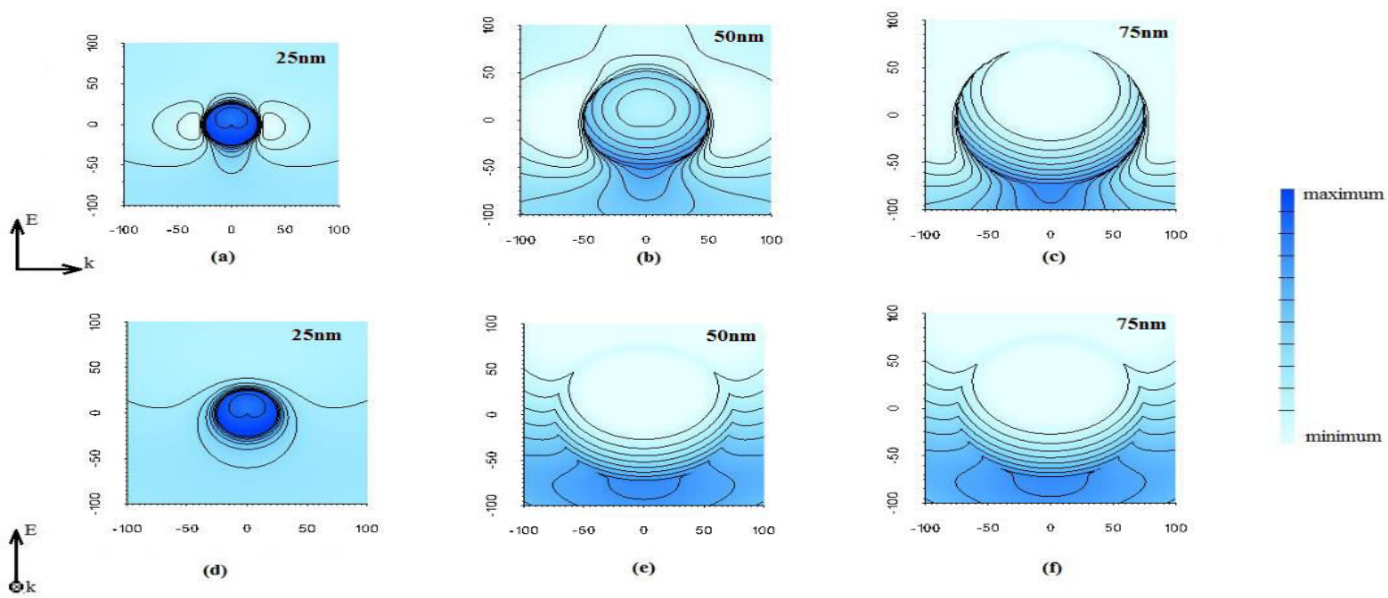


Fig. 2: (a) Absorption, (b) scattering, and (c) extinction efficiencies for Ag-Nano spheres of size 10, 20, and 30nm



(Fig. a, b, c) for cross-section containing the propagation vector and polarization axes and (Fig. d, e, f) for cross-section perpendicular to propagation

Fig. 3: E-field contours for radius 25, 50, and 75 nm Ag-Nano spheres

Table 1: Peak extinction coefficients parameters for small size Ag-Nano spheres of size 10, 20, and 30nm

Size of Ag-Nano particle (nm)	Wavelength for Extinction coefficient peak (nm)	Peak strength for Extinction coefficient peak	Full wave half maximum-Bandwidth (nm)
10	355	3.20	30
20	358	7.34	40
30	367	8.88	50

The extinction spectra of big Ag nanoparticles can be seen in Fig. 4. We can observe that as the size of Ag-nanoparticles increased more the peak extinction wavelengths also increase, hence it shows a redshift. Although the increasing size of the nanosphere causes the peak extinction amplitude to decrease and, the bandwidth increases pronouncedly. The comparison of Fig. 2 (c) and Fig. 4 shows that the peaks of larger metallic nanoparticles are clustered together and are wider than those of smaller nanoparticles. As a result, Ag-nanoparticles exhibit different properties depending on their size ranges. On the general, we may call nanoparticles larger than 25nm as big whereas those with smaller radii may be called small.

The effect of water media on Ag-nanoparticle of size 25nm on extinction efficiency is shown in Fig. 5. Both the magnitude and the position of the peak for extinction efficiency shows a strong dependence on media type. As a result of this dependence, water-immersed Ag-nanoparticles are finding new thrust in the area of LASER [11] and third-order non-linearity [12] generation.

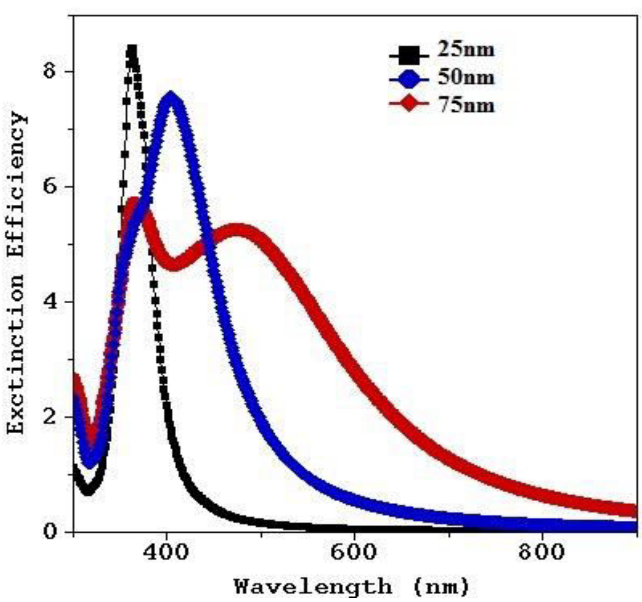


Fig. 4: Extinction efficiencies for Ag-Nano spheres of size 25, 50, and 75nm

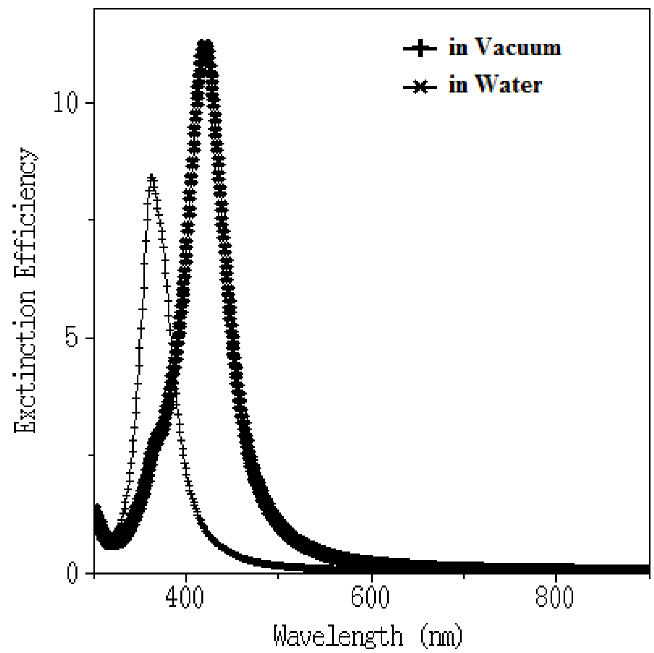


Fig. 5: Extinction efficiencies for Ag-Nano spheres of size 25nm in vacuum and water media

Fig. 6 shows the variation of the extinction spectrum of 25nm silver nanoparticle when placed in different solid mediums such as Flint glass, Si, GaAs, and Ge, while vacuum indicates the absence of any solid medium. As the nanoparticle is placed inside a medium with increasing refractive index, the wavelength at which peak extinction occurs also increases. We found that the peak wavelength of extinction is highest under Ge medium. In table 2, we summarized these observations, however, the peak extinction efficiency does not vary much.

Fig. 7 illustrates the variation of electric field intensity in the plane perpendicular to the electric field vector and propagation vector. It shows that the intensity of the electric field decreases as the refractive index of the medium increases and is found to be almost the same for GaAs and Ge media. In all solid medium the intensity is found to be very low in comparison to the case without a medium.

Table 2: Peak extinction coefficients parameters for 25nm Ag-Nano spheres embedded under different solid materials

Medium	Refractive index	Wavelength for Extinction coefficient peak (nm)	Peak strength for Extinction coefficient peak	Full wave half maximum-Bandwidth (nm)
Vacuum	1	364	8.4	35
Flint glass	1.60	471	13.0	60
Silicon	3.45	909	13.2	183
GaAs	3.93	1018	12.9	221
Ge	4.10	1060	12.8	225

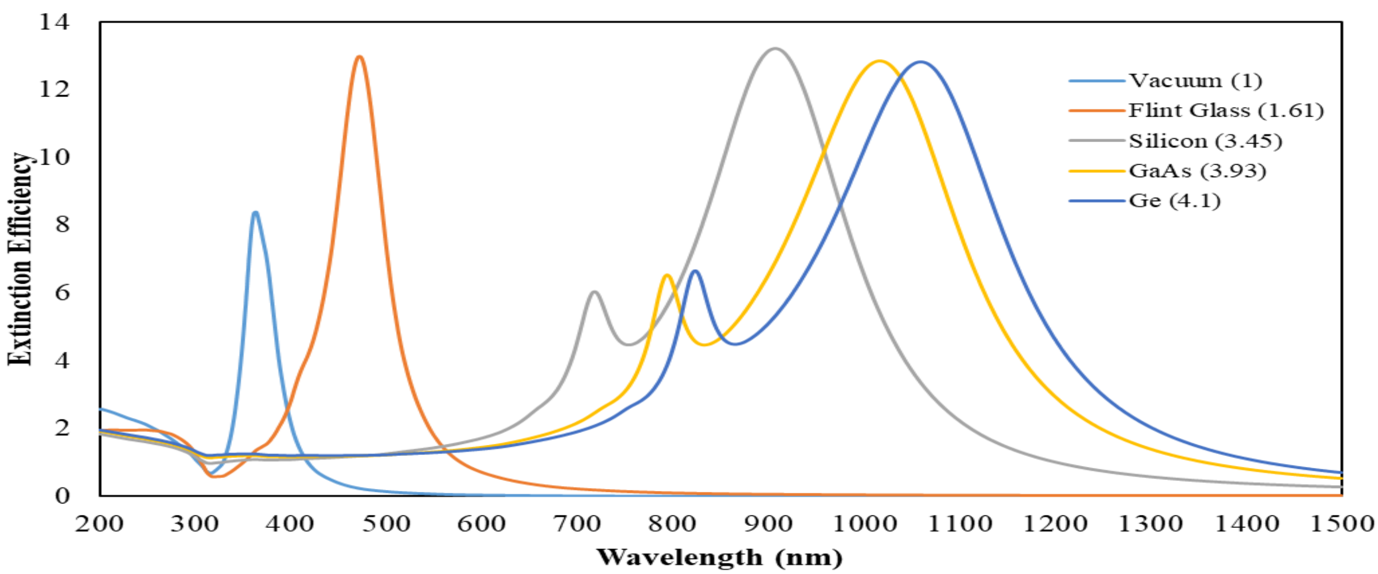


Fig. 6: Extinction spectra of 25nm silver nanoparticle when it is placed in different solid mediums with different refractive indexes

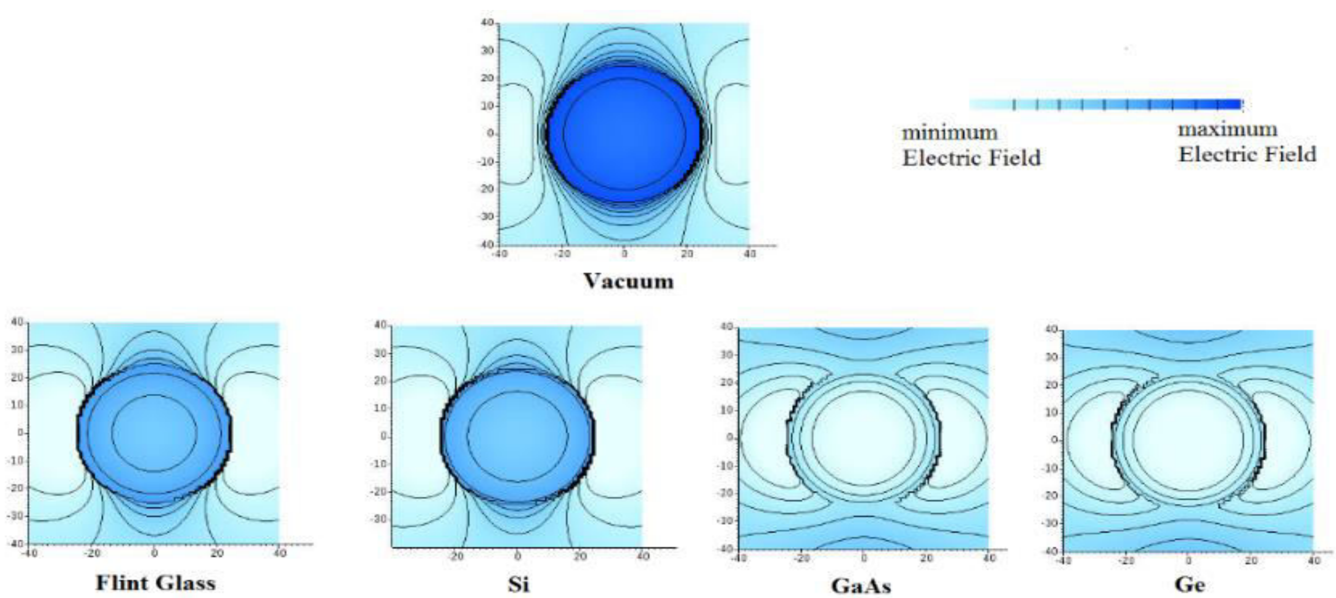


Fig. 7: E-field contours for radius 25nm for different solid medium, for cross-section perpendicular to electric field and propagation vector

5. CONCLUSION

An understanding of optical interaction with metallic nanoparticles is crucial in describing a variety of physical phenomena and helps in finding the real-time applications. In the present work, we investigated the variation of extinction spectra and electric field intensity of silver nanospheres according to Mie's theory by varying their size and surrounding medium. A radially-distributed electric field was determined to be governed by collective excitations of conduction electrons. These electrons oscillate coherently when metallic sphere get irradiated by visible and near-IR regions of electromagnetic spectrum. It has been found that the opto-electronic interactions are highly dependent upon size of metallic nanoparticle. The extinction amplitude for large particles decreases as the size grows, but the opposite occurs for small particles. An increase in bandwidth is observed as the size of the nanoparticle increases. Field intensity is found to get greatly reduced when nanoparticles are embedded in solid semiconductor medium, and the quantum of this decrease is found to increase with the refractive index of the solid. According to the analysis conducted in this work, silver nanoparticles are a good candidate for a variety of applications, including sensors for medical health care, industrial catalysts and consumer products.

6. REFERENCES

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