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RESEARCH ARTICLE

ANALYTICAL DESCRIPTION OF ENHANCEMENT FACTOR IN INDUCED OPTICAL BISTABILITY FOR ELLIPSOIDAL METAL/DIELECTRIC COMPOSITE CORE

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ABSTRACT

In this paper the enhancement factor of local field for pure ellipsoid metal/dielectric composite in linear host matrices is studied. The enhancement factor of local field which extremely enhanced is shown by analytical and numerical results. It is shown that the local field in metal ellipsoidal particles with dielectric core in an external varying electric field has two maxima at two different frequencies. The second maximum becomes more important with increment in the metal fraction.

INTRODUCTION

Nanoscience is a new emerging area of science that involves studying and working with matter at nanoscale, on the order of $10^{-9}m$. Structures in nanoscale, called nanostructures, are considered at the borderline of the smallest of human made-devices and the largest molecules of living systems. Nanostructures include all shapes wires, rods, dots-formed from all of the industrially important semiconductor materials [Bennink, 1999]. Nonlinear optics is the study of phenomena that occur as a consequence of the modification of the optical properties of a material system by the presence of light. Typically, only laser light is sufficiently intense to modify the optical properties of a material system. The beginning of the field of nonlinear optics is often taken to be the discovery of second-harmonic generation [Franken, 1961]. Shortly after the demonstration of the first working laser [Maiman, 1960]. Nonlinear optical phenomena are "nonlinear" in the sense that they occur when the response of a material system to an applied optical field depends in a nonlinear manner on the strength of the optical field. For example, second-harmonic generation occurs as a result of the part of the atomic response that scales quadratic ally with the strength of the applied optical field. Consequently, the intensity of the light generated at the second-harmonic frequency tends to increase as the square of the intensity of the applied laser light [InekeMalsh, 2002].

Certain nonlinear optical systems can possess more than one output state for a given input state. The term optical bistability refers to the situation in which two different output intensities are possible for a given input intensity, and the more general term optical multistability is used to describe the circumstance in which two or more stable output states are possible. Interest in optical bistability stems from its potential usefulness, as a switch for use in optical communication and in optical computing. Optical bistability was first described theoretically and observed experimentally using an absorptive nonlinearity as cited in [Piccione, 2014]. Optical bistability was observed experimentally for the case of a refractive nonlinearity real $\chi(3)$ [Bennink, 1999; InekeMalsh, 2002; Gibbs, 1976; Bohren, 1983]. The first studies reported about optical bistability in laser diode come from the sixties. Main works were done during eighties, most relevant are recompiled on mainly in passive optical bistability; following some of the previous works on optical semiconductor oscillators and amplifiers. It has been an intensive research topic due to the huge potential applications of these devices in different fields of technology, such as optical computing and optical communications and for the practical advantages of laser amplifiers: the presence of gain, fast response, low optical power requirements to achieve bistability etc. As a matter of fact, in optical computing, the nonlinear behavior exhibited by the laser amplifier leads to the possibility of using this kind of devices as basic components in the developing of logic gates.

In the other hand, in optical communications these devices could be employed in optical switching applications, optical signal regeneration and optical head packet processing, in addition the usual use in long range links [Yanik, 2003]. Optical bistability has been predicted by theory or demonstrated by experimental studies to exist in waveguiding resonators [Gibbs, 1985], Photonic crystal cavities [Wurtz, 2006; Min, 2008; Shen, 2008], sub wavelength metallic gratings [Daniel, 2012], metal gap waveguide nanocavities [Haes, 2004], and nanoantenna with amorphous silicon filled in the gap [El-Sayed, 2007]. It is important to achieve a deeper understanding of the basic physics of optical bistability at the nanoscale in order to design and realize high-performance nanophotonic switching devices. The interaction of light with metal surface results in the collective oscillation of the surface free electrons. This phenomenon is called surface Plasmon resonance. A strong resonance occurs roughly at the electromagnetic frequency, where, $\epsilon r = -2\epsilon m$ thus determining the surface plasmon resonance (SPR) frequency. For gold (Au), silver (Ag), and copper (Cu), the resonance condition is fulfilled at visible frequencies, making them the plasmonic metals of choice for optical applications. Different from the spectrum of bulk metals, the spectrum of noble nanoparticles have a very strong UV/visible absorption band. This absorption band results when the incident photon frequency is resonant with the collective excitation of the conduction electrons and is known as localized surface Plasmon resonance [Li, 2010].

The enhancement of local field in the small ellipsoidal metal/ dielectric particles: In a dilute gas of atoms the electric field E that produces the induced dipole moment on an atom is simply the applied electric field. In a solid, however, all of the dipole moments produced on other atoms in the solid make a contribution to the field acting on a given atom. The value of this microscopic field at the position of the atom is called the local field. The local field $ELF(r)$ is different from the applied electric field E_0 and from the macroscopic electric field E (which is the average of the microscopic field $ELF(r)$ over a region that is large compared to a unit cell). Clearly, the contributions to the microscopic field from the induced dipoles on neighboring atoms vary considerably over the unit cell [Mal'nev, 2012]. From the size dependence of the Surface Plasmon (SP), it is quite obvious that metal nanoparticles with non-spherical shape will show several SP resonances in their spectra. For instance, ellipsoidal particles with axes $a = b = c$ own three SP modes corresponding to polarizabilities along the principal axes. Moreover, an increase in the axis length leads to the minimization of the depolarization factor. For a spherical particle $L_a = L_b = L_c = 1/3$.

Thus, if the propagation direction and polarization of the electromagnetic wave do not coincide with the axes of the ellipsoid, the extinction spectra can demonstrate three separate SP bands corresponding to the oscillations of the free electrons along these axes. For spheroids one has: $a = b = c$ and the spectra exhibit two SP resonances. However, if the incident light is polarized parallel to one of the axes, only one single SP band corresponding to the appropriate axis. The band lying at higher wavelengths is referred to as the long axis, while the small axis demonstrates resonance at shorter wavelengths compared to the single resonance of a nanosphere of the same volume. The spectral separation of the two surface Plasmon bands of the ellipsoidal nanoparticle strongly depends on its aspect ratio which is defined as the ratio of the long to the

short axes. At the same time, it is clearly seen that for prolate and oblate spheroids having the same aspect ratio, the positions of SP resonances are different. Namely, the spectral separation between SP bands is higher for the nanoparticles having a zeppelin-like shape [Bohren, 1983].

Depolarization factor: The most general smooth particle one without edges or corners of regular shape is an ellipsoid with semi-axes $a > b > c$. To check these results we note that the sphere is a special ellipsoid for $a = b = c$. Only when the particle is in free space ($\epsilon_m = \epsilon_0$) are its depolarization factors independent of composition. In nature we note that there is no perfect sphere. Therefore, as we said a special class of sphere is ellipsoid when its depolarization is given by,

$$L_1 = L_2 = L_3 = \frac{a^3}{2} \int_0^\infty \left(\frac{dq}{a^2 + q} \right)^{\frac{5}{2}} = \frac{1}{3}$$

A special class of ellipsoids is the spheroids, which have two axes of equal length; therefore, only two of the geometrical factors of L_1, L_2, L_3 is independent because of the relation

$$L_1 + L_2 + L_3 = -abc \int_0^\infty \frac{dq}{f(q)} = 1$$

The prolate (cigar-shaped) spheroids, for which $b = c$ and $L_2 = L_3$, are generated by rotating an ellipse about its major axis; the oblate (pancake-shaped) spheroids, for which $b = a$ and $L_1 = L_2$, are generated by rotating an ellipse about its minor axis.

MATERIALS AND METHODS

Methodology: We have employed numerical and computational simulation methods using MATLAB program by developing suitable computer codes to study how depolarization factor L affect the enhancement factor in the metal/dielectric/semiconductors. These research works have been carried out analytically and numerically.

Materials: We used MATLAB Software for the analytical and numerical simulation to develop program code for our model equation and simulating the dielectric function of the composite materials. To make our result effective we have compared with physics thesis published nationally and internationally. To manage long analytical and numerical expression for scientific work and to simplify bulged equations into figural expressions Mathematic a software was used.

RESULTS AND DISCUSSION

Enhancement Factor of local field for metal/dielectric composite: As input intensity is increased, the field inside the cavity also increases, lowering the absorption that the field experiences and thus increasing thus increasing the field intensity still further. If the intensity of the incident field is subsequently lowered, the field inside the cavity tends to remain large because the absorption of the material system has already been reduced. Note that over some range of input intensities; more than one output intensity is possible. This is called induced optical bistability which means that some nonlinear optical systems can produce two different output intensities for a given input intensities or, in particular, the given value of an external electric field may produce several

values for the local field and the polarization. In this section, we consider the local field in metal ellipsoidal particles while accounting for the nonlinear part of $\epsilon(\omega, E)$ and it is used for the presence of small field $\chi|E|^2$. For the ellipsoid shaped particle as we kept dielectric function, (DF) in the core of metal/semiconductor particle as shown as (Figure 1), and then this DF covered by metallic/ semiconductor particle, finally the whole covered by host. From this (Figure 1) we see the dielectric function ϵ_d is at the center of metallic dielectric ϵ_m function. The dielectric and metallic dielectric function is covered by host ϵ_h as (Figure 1) using this we have derive the enhancement factor A. However, to derive we start using Laplace's equation in spherical coordinate. For our case we want to derive enhancement factor A for ellipsoid particle by using this spherical coordinates as reference. Now, we have to use the geometrical factor to shift into ellipsoid shape particle [Bohren, 1983]. To simplify our derivation we have the following two basic cases: The potential is the same for $r = r_1$ and $r = r_2$ and it is continuous at boundary.

Displacement vector is continuous and the same at the boundary for $r = r_1$ and $r = r_2$. From Laplace's equation ellipsoidal in coordinates (Bohren and Huffman 1983; Mal'nev Shewamare, 2012). Now, after certain steps of manipulations, we got the following three basic equations for my numerical manipulation for certain range of radius difference. However, the distribution of the electric potential in the system is described by the following expressions for they are the solutions of the Laplace equations of the dielectric core, metal and the host matrix, respectively.

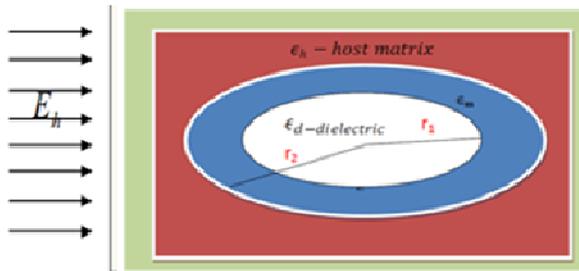


Figure 1. The construction of ellipsoidal by the combination of dielectric ϵ_d in core, metallic dielectric ϵ_m outside coverage of dielectric and finally host matrix ϵ_h external coverage of dielectric and metallic

$$\Phi_1 = -E_h \text{Arcos}\theta, r \leq r_1 \quad (1)$$

$$\Phi_2 = -E_h \left(Br - \frac{C}{r^2} \right) \text{cos}\theta, r_1 \leq r \leq r_2 \quad (2)$$

$$\Phi_3 = -E_h \left(r - \frac{D}{r^2} \right) \text{cos}\theta, r > r_2 \quad (3)$$

Where, Φ is potential, A and B is constants, r is radius. They are the solutions of the Laplace equations of the metal inclusion and the host matrix, respectively. Here Φ is potential, E_h is the applied field, r and θ are the coordinates of the observation point (the beginning of the coordinate in the center of the inclusion and the z axis is along E_h). We obtain a system of linear algebraic equations for unknown coefficients A and B from the continuity conditions of the potential and the displacement vector at the boundaries of metal-host matrix. To solve the above equations by using the following two cases:

Case I: At the boundary potential is the same for $r = r_1$ and $r = r_2$ and it is continuous

Case II: Displacement vector is continuous and the same at the boundary for $r = r_1$ and $r = r_2$

$$A = \frac{\epsilon_m}{\epsilon_d} \left(B + \frac{2C}{r_1^3} \right) \quad (4)$$

And setting the values of unknown constant values A and B to find enhancement

$$B = \frac{\epsilon_h(\epsilon_m + L(\epsilon_d - \epsilon_m))}{b + a\epsilon_h(1-L)} \quad (5)$$

Now, we have to use depolarization factor L, considering the particle as perfect sphere ($L = 1/3$) by considering equation (4)

$$A = \frac{\epsilon_h \epsilon_m}{\epsilon_m^2(LP(1-L)) + \epsilon_m[\epsilon_h(1-L) - \epsilon_hLP(1-L) + L\epsilon_d(1-P) + L^2P\epsilon_d] + \epsilon_h\epsilon_dLP(1-L)} \quad (6)$$

To simplify equation (6) we use the following denotations:

$$a_1 = LP(1-L)$$

$$a_2 = \epsilon_h(1-L) - \epsilon_hLP(1-L) + L\epsilon_d(1-P) + L^2P\epsilon_d$$

$$a_3 = \epsilon_h\epsilon_dLP(1-L)$$

Therefore, equation (6) becomes

$$A = \frac{\epsilon_h \epsilon_m}{a_1 \epsilon_m^2 + a_2 \epsilon_m + a_3} \quad (7)$$

By splitting in to its real and imaginary part of this above equation and by putting the value of the metallic dielectric below equation into above we get;

$$\epsilon_m = \epsilon'_m + i\epsilon''_m$$

$$\epsilon_m^2 = \epsilon'^2_m - \epsilon''^2_m + 2i\epsilon'_m\epsilon''_m$$

By taking the module of above equation

$$|A|^2 = \frac{|\epsilon_h|^2 |\epsilon_m|^2}{(a_1 \epsilon_m^2 + a_2 \epsilon_m + a_3)^2}$$

$$|A|^2 = \frac{|\epsilon_h|^2 (\epsilon'_m + i\epsilon''_m)^2 (\epsilon'_m - i\epsilon''_m)^2}{(a_1 (\epsilon'_m + i\epsilon''_m)^2 + a_2 (\epsilon'_m + i\epsilon''_m) + a_3)^2}$$

$$|A|^2 = \frac{|\epsilon_h|^2 (\epsilon'^2_m + \epsilon''^2_m)}{(a_1 (\epsilon'^2_m - \epsilon''^2_m) + a_2 \epsilon'_m + a_3)^2 + (2a_1 \epsilon'_m \epsilon''_m + a_2 \epsilon''_m)^2} \quad (8)$$

This equation (8) is called enhancement factor. Electrons in metals at the top of the energy distribution (near Fermi level) can be excited in to other energy and momentum states by photons with very small energies, thus they are essentially 'free' electrons. The optical response of a collection of free electrons can be obtained from the Lorentz harmonic oscillator model by simply 'climbing the springs' that is by setting the spring constant k is equal to zero. Therefore, for $\omega_o = 0$, that dielectric function for free electron is given by;

$$\epsilon = \epsilon_\infty - \frac{\omega_p^2}{\omega^2 + i\nu\omega} \quad (9)$$

Let an electromagnetic wave impinge on a metal particle in the form of a rotational ellipsoid embedded in, a dielectric host matrix. The dielectric function of the particle is assumed to

depend on the frequency ω and the local electric field (inside the particle) and can be presented in the form,

$$\epsilon(\omega, E) = \epsilon(\omega) + \chi(\omega) |E|^2 \tag{10}$$

Where, $\chi(\omega)$ is the complex kerr coefficient, and the linear parts of dielectric function is;

$$\epsilon(\omega) = \epsilon'(\omega) + i\epsilon''(\omega) \tag{12}$$

Thus, using equation (9) in the Drude form, we can derive as follows by equating (9) and (11) by rationalizing its conjugate and it becomes,

$$\epsilon'(\omega) + i\epsilon''(\omega) = \epsilon'_\infty + i\epsilon''_\infty - \left(\frac{\omega_p^2}{\omega^2 + i\nu\omega} \times \frac{\omega^2 - i\nu\omega}{\omega^2 - i\nu\omega} \right) \tag{13}$$

This equation (13) has real and imaginary, hence, we have to identify in to their real and imaginary

$$\epsilon'(\omega) + i\epsilon''(\omega) = \epsilon'_\infty + i\epsilon''_\infty - \frac{\omega_p^2\omega^2}{(\omega^4 + (\nu\omega)^2)} + \frac{i\omega_p^2\nu\omega}{(\omega^4 + (\nu\omega)^2)} \tag{14}$$

And let us splitting equation (9) into real and imaginary

$$\epsilon'(\omega) = \epsilon'_\infty - \frac{\omega_p^2\omega^2}{(\omega^4 + (\nu\omega)^2)}$$

$$i\epsilon''(\omega) = i\epsilon''_\infty + \frac{i\omega_p^2\nu\omega}{(\omega^4 + (\nu\omega)^2)}$$

Simplifying this finally we get

$$\epsilon'(\omega) = \epsilon'_\infty - \frac{\omega_p^2\omega^2}{(\omega^4 + (\nu\omega)^2)}$$

$$\epsilon''(\omega) = \epsilon''_\infty + \frac{\omega_p^2\nu\omega}{(\omega^4 + (\nu\omega)^2)} \tag{15}$$

Table 1. Numerical values of physical quantities

Used physical quantity	Value assigned for each physical quantity
ϵ_h	2.25
ϵ_d	0.5
P	0.99
ϵ_∞	4.6
γ	0.0115
a_1	$L.P(1-L)$
a_2	$\epsilon_h(1-L) - \epsilon_hLP(1-L) + L\epsilon_d(1-P) + L^2P\epsilon_d$
a_3	$\epsilon_h\epsilon_dLP(1-P)$
ϵ'_m	$\epsilon_\infty - \frac{1}{(Z^2 + \gamma^2)}$
ϵ''_m	$\frac{\gamma}{Z(Z^2 + \gamma^2)}$
Z	0.38, 0.54
L	0.34, 0.38

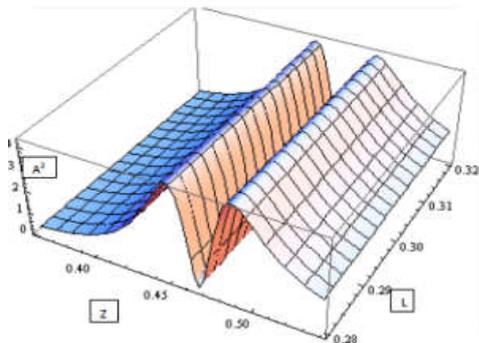


Figure 2. Enhancement factor $|A|^2$ for 3D of a silver nanoparticle versus z and L; $\epsilon'_h = 2.25, P = 0.99, \epsilon'' = 0, \epsilon'_\infty =$

4.6, $\epsilon''_\infty = 0, \gamma = 0.0115, \omega_p = 1.46 \times 10^{16} \text{ rad/sec}, \nu = 1.68 \times 10^{14} \text{ rad/sec}$.

where,

ω_p^2 –is plasma frequency of electrons in the metal

ν –is their collision frequency

ϵ_∞ –is a constant that can be a function of frequency and depend on the type of metal. Now, we have to assign value for enhancement factor A of equation (5) and set their value in table form as follows. Using above listed numerical value we have use to draw enhancement factor by varying depolarization factor L versus dimensionless frequency z of the following (Figure 2).

Where, ω_p is plasma frequency, in which it given by: $\omega_p = \sqrt{\frac{Ne^2}{m_e\epsilon_0}}$, which is called Drude plasma frequency, m_e mass of electron, N is used for number of electron, e is an electron, P is fraction volume. From figure 1 we have to understood that for dielectric function ϵ_d kept at center of small ellipsoidal particle. The depolarization factor L and dimensionless frequency z play a key role for enhancement by fixing depolarization. For example at point $Z_1 = 0.38, Z_2 = 0.54$ and $L_1 = 0.34, L_2 = 0.38$. Therefore, as we see from (Figure2) the dielectric function have an effect to enhance by presence local field in the region, the enhancement factor is increased.

Enhancement Factor of Local Field for ellipsoidal metal/Dielectric Composite in 2D for depolarization factor L for sphere:

Now here, we have looking enhancement factor drawn by two dimension (2D), while (Figure 2) is drawn by three dimensions (3D). The physical quantities used in (Figure2) the same to (figure 3). But they have difference in plotting 2D and 3D in using depolarization factor. From, (Figure 3) It is shown that with the change of L from lower value to high value, namely, with the transition of from dielectric property to metallic property, the level values of the enhancement factor of the local field increase. Compared with the case of no dielectric layer, the metal-like dielectric layer makes the threshold values increase; while the dielectric like layer makes the level values decrease. Therefore, from (Figure 3) enhancement factor for metallic dielectric function increased, while dielectric function make enhancement factor to decrease.

Enhancement Factor of Local Field for ellipsoidal Metal/Dielectric Composite for oblate and prolate:

Where the oblate shaped objective have the equatorial diameter greater than the polar diameter, whereas, prolate having the polar diameter greater than the equatorial diameter. Using geometrical factor L for oblate $L_1 = 0.3$ and prolate $L_2 = 0.44$, as we have to see from figure 4 no change effective change seen, except when the number value of L is increased and the enhancement increase from the transition of dielectric to metallic.

Enhancement Factor of Local Field for ellipsoidal Metal/Dielectric Composite for sphere, oblate and prolate shape:

And let us see what it seems while we combine for depolarization factor perfect sphere, oblate and prolate shaped and it look like the following, In (Figure 5), we present $|A|^2$ of composites of small ellipsoidal metal/dielectric separated by dielectric layer verses the resonant frequency Z for three different depolarization factor values; $L_1 = 0.3, L_2 = 0.37$ and $L_3 = 0.44$. We find that the depolarization factor plays an important role in enhancement factor behavior. It is shown that

with the change of L for oblate, prolate and sphere, namely, with the transition of dielectric property to metallic property,

have two maximum peaks for depolarization factor L and dimensionless frequency z . Nonlinear optics is the study of phenomena that occur as a consequence of the modification of

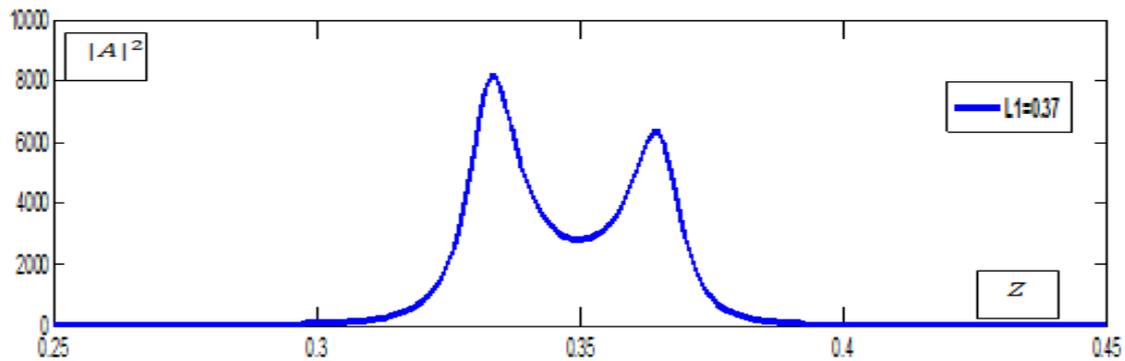


Figure3. Enhancement factor $|A|^2$ for 3D of a silver nanoparticle versus z and L ; $\epsilon'_h = 2.25$, $P = 0.99$, $\epsilon'' = 0$, $h = 0$, $\epsilon'_\infty = 4.6$, $\epsilon''_\infty = 0$, $\gamma = 0.0115$, $\omega_p = 1.46 \times 10^{16} \text{ rad/sec}$, $\nu = 1.68 \times 10^{14} \text{ rad/sec}$.

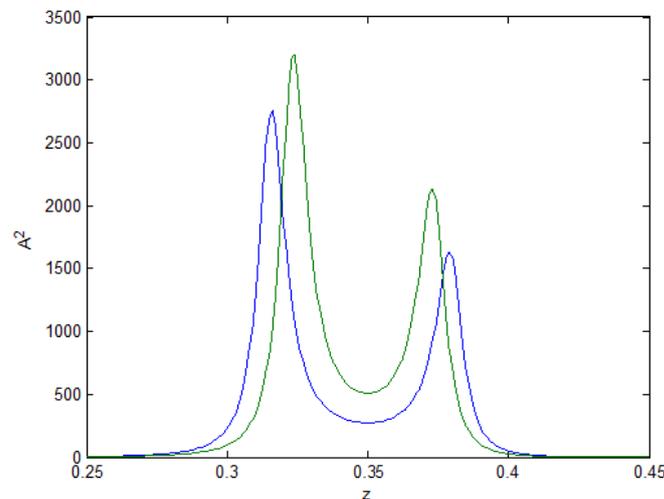


Figure 4. Enhancement factor for the oblate and prolate shape, when $L_1 = 0.3$ and $L_2 = 0.44$ and other quantities are the same to (Figure 3).

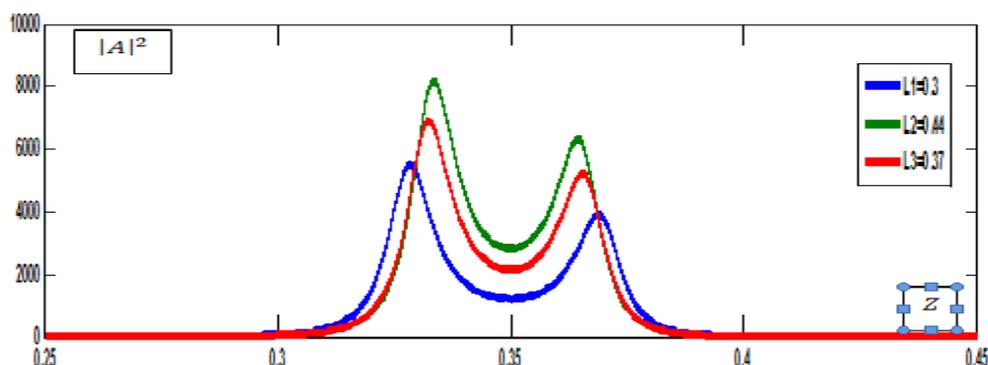


Figure 5. Enhancement factor for the oblate, pure Sphere and prolate shape respectively, when $L_1 = 0.3$, $L_2 = 0.37$ and $L_3 = 0.44$ and other quantities are the same to (Figure 3)

the point values of the enhancement factor of the local field stay the same in three of shapes.

Conclusion and Recommendation

We now discussed the main theoretical conclusions that follow from this study. From first section we have to studied for incident intensity the dielectric function in ellipsoidal nanoparticle have a great effect on enhancement factor and it

the optical properties of a material system by the presence of light. The degree of optical nonlinearity in a material depends upon the strength of the optical field, and varies in different materials. However, even if they give us the same result for both geometrical shapes, using spherical is recommended than ellipsoidal in seek of calculation and determining and explaining and researcher doing their paper in ellipsoidal shape than spherical shape. It is shown that the enhancement factor of the local electric field in metal spherical or ellipsoidal

nanoparticles with dielectric cores imbedded in a dielectric matrix have two maxima on two resonant frequencies. The second maximum for the inclusions with large dielectric cores covered by a thin metal shell is comparatively small. With increasing in a metal fraction in the inclusion, both enhancement factors grow. Due to very small nonlinearities in naturally occurring materials, large optical fields are necessary to realize measurable nonlinear phenomena. The necessities of high intensity sources to observe the effects of optical nonlinearity severely limit its use in practical applications, especially in low-powered devices. To realize such devices, the enhancement of nonlinear material properties is required. Therefore we recommend you anybody who interested to do his/her research related to linear, nonlinear optics and nanoparticles it is better to do a research using experiment is more reliable than it theoretical explanation because it done by checking every activity when local electric field maximized and minimized. The future work will aim at studying the change that will be observed by varying the parameters considered like depolarization L, dielectrics, and the metal fraction in the inclusion p .

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