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RESEARCH ARTICLE

LOCAL FIELD ENHANCEMENT OF CYLINDRICAL CORE-SHELL NANOPARTICLE COMPOSITES IN PASSIVE AND ACTIVE DIELECTRIC CORE

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ABSTRACT

In this paper, we investigated how local field enhancement (LFE) and induced optical bistability (IOB) of cylindrical core-shell nanoparticle composites (NPCs) with passive and active dielectric cores were affected by the metal fraction (p), and dielectric constant of host matrix. We have determined the expressions of the electric potentials for cylindrical core-shell NPCs by solving Laplace's equations in the quasi-static limit. The equation of IOB was derived from the equation of local field enhancement factor (LFEF) by incorporating Drude-Sommerfeld model into the expressions. The host dielectric and the dielectric of the core are interfaced with the metal shell. The LFEF significantly rises at two resonant frequencies with increasing p and dielectric constant in both passive and active dielectric core. The findings reveal that S-like peaks of IOB are created in both passive and active dielectric cores of cylindrical NPCs, no matter how p, and dielectric constant change or remain constant. In NPCs, both in passive and active dielectric cores, an increase in any of these parameters results in switching-up and switching-down threshold points where optical bistability (OB) resonances prevail. Within passive and active dielectric cores, increasing p shows the incident field required at each switching-up threshold point also increases and the bistable region produced gets wider. Additionally, it was found that the bistable area of the IOB in active dielectric cores of cylindrical core-shell NPCs is reduced when the host dielectric constant increases.

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INTRODUCTION

Enhancing the local electric field within the metal-dieletric (shell-core) composite is one of the key components in the development of the nonlinear optical effect. The differences in the dielectric characteristics between the host matrix and the composite, as well as the nanoscale sizes and shapes of the metal-dielectric composite, are factors that contribute to the enhancement of the local electric field within the metal-dielectric composite. Additionally, the surface plasmon resonance that results from localized surface plasmonic involves the other components for strengthening the local electric field inside the metal-dielectric composite (Stroud, 1989; Law, 1998; Sarychev, 2000). Due to various potential applications, including surface enhanced Raman spectroscopy (Prokes, 2007), metal enhanced florescence (Liu *et al*., 2010), quantum electrodynamics (Quan *et al*., 2009; Katz, 2012), nonlinear optical effect (Gorodetsky, 1996), quantum optomechanics (Van Thourhout, 2010), optical sensors (Anker, 2008) and nano-optical tweezers (Juan, 2011), the increased magnitude of the local electric field of the incident electromagnetic radiation in composites of metal coated nanoparticles with dielectric core is of significant importance. It is well known that if an incident radiation frequency is close to the surface plasmon frequency, the local electric field in the inclusions can be significantly increased. (Neeves, 1989). This issue was investigated in relation to optically induced bistability (Kalyaniwalla, 1990; Haraguchi, 2008) and it is acknowledged that such an enhancement only occurs on one resonant frequency. It is obvious that the nonlinear portion of the dielectric function (DF) only matters if the electric fields are comparable to the inner atomic fields. Currently, laser radiation is capable of creating such fields. An anomalous amplification of the local field occurs when the incident electromagnetic wave frequency approaches the metal's surface plasmon frequency. This is an amazing characteristic of pure metals and dielectric tiny particles covered in metal (Buryi *et al*., 2011). Despite being theoretically and experimentally realized, optical induced bistability (OIB) continues to be of great interest due to the wide range of potential applications (Fischer *et al*., 1995; Szoke, 1969; Gibbs, 1976) because of its numerous possible applications. The most interesting systems for studying IOB are composites made of metal-covered dielectric particles with nonlinear dielectric functions enclosed in a linear host matrix. The key idea here is that IOB is based on the inclusions' nonlinear dielectric function. Inclusions (local fields) with frequencies near to the surface plasmon frequency of the metal have an elevated electric field amplitude due to incident intense radiation. The core's nonlinear dielectric function (DF) is now important because to this enhancement (Kalyaniwalla, 1990; Gehr, 1997). The local field enhance at the focal point of spherical nanoinclusions in a linear dielectric host matrix was investigated by Sisay and Mal'nev (Mal, 2013).

When the frequency of the incident electromagnetic wave approaches the surface plasmon frequency of the metal component of the inclusions, the results of these research outperform those of anomalous enhancement of the local field.

The aim of this study is a thorough theoretical and numerical analysis the effect of metal fraction and host matrix dielectric constant on enhancement of local field and optical bistability in cylindrical core-shell nanoparticle composites in the electrostatic approximation of core-shell composite that implanted in linear host matrix.

Local Field Enhancement of Cylindrical Core-shell Nanocomposites: In classical electrodynamics, the Laplace equation (i.e., $\boldsymbol{\nabla^2 \phi = 0}$) in a cylindrical coordinate system has a general form given by equation

$$\frac{\partial^2\phi}{\partial r^2}+\frac{1}{r}\frac{\partial\phi}{\partial r}+\frac{1}{r^2}\frac{\partial\phi}{\partial\theta^2}+\frac{\partial\phi}{\partial z^2}=0$$

In a cylindrical coordinate system, the potential is two-dimensional and choosing it is not a function of z-axis. In this case, Eq. (1) can be reduced to the form

$$\frac{\partial^2\phi}{\partial r^2}+\frac{1}{\partial r}\frac{\partial\phi}{\partial r}+\frac{1}{r^2}\frac{\partial\phi}{\partial\theta^2}=0$$

The solution of Eq. (2) can yield the potential distribution at different regions of a composite of metal coated dielectric core cylindrical nano inclusions embedded in a linear dielectric host matrix as:

$$\phi_d = -E_h A r cos\theta, \qquad r \le r_1$$

$$\phi_m = -E_h(\left(Br-\frac{C}{r}\right)cos\theta, \qquad r_1 \le r \le r_2$$

$$\phi_h = -E_h(\left(r-\frac{D}{r}\right)cos\theta, \qquad r \ge r_2$$

Where ϕ_d, $\phi_m$and $\phi_h$are potentials in the dielectric core, metallic shell and the dielectric host matrix, respectively, ϵ_h the applied field (for the cylindrical inclusion it is perpendicular to its axis r_1 and r_2 are the radii of the dielectric core and the metal shell, respectively, and A, B, C and D are unknown coefficients). We can calculate the enhancement factor A using this. The unknown coefficients can be obtained from the electrostatics boundary conditions. Under the long-wave approximation, the case in which the wavelength of the incident electromagnetic wave is greater than the size of the particle, we can use the following electrostatics boundary conditions in order to get the value of the coefficients (Chylek, 1990). 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 E is different from the applied electric field $E_h$and from the macroscopic electric field E (which is the average of the microscopic field E over a region that is large compared to a unit cell). Clearly, the contributions to the microscopic field from the induced dipoles on neighbouring atoms vary considerably over the unit cell (Buryi, 2011). From the continuity conditions of the electric potential and the displacement vector on the interface dielectric core metal and metal host matrix, we obtain the system of linear algebraic equations for the unknown coefficients and from the continuity condition of the displacement vector,

$$A=\frac{4\epsilon_h\epsilon_2}{p\nabla}$$

Where, $p = 1 - (r_1^2/r_2^2)$ - is the metal volume fraction in the inclusion. Eq. (3) indicates the local field enhancement factor (LFEF) of cylindrical metal. Recall that dielectric function of the dielectric inclusion is given by:

$$\epsilon_m = \epsilon_\infty - \frac{1}{z(z+iz)}$$
$$\epsilon'_m = \epsilon'_\infty - \frac{1}{z(z+iz)}$$
$$\epsilon''_m = \epsilon''_\infty + \frac{1}{z(z+iz)}$$

Where ϵ'_m and ϵ''_m are real and imaginary parts of ϵ_m, respectively, $z=\omega/\omega_p$is dimensionless frequency, $\omega$is the frequency of the incident radiation, $\omega_p$is the plasma frequency of the inclusion metal part, $\upsilon$is the electron collision frequency and $\gamma=\upsilon/\omega_p$. By squaring LFEF, we have

$$|A|^2=\frac{16\epsilon_h^2}{p^2}\left|\frac{\epsilon_m}{\nabla}\right|^2$$

Where

$$\nabla = \epsilon_m^2 + q\epsilon_m + \varepsilon_d\epsilon_h,$$
$$\nabla = \left(\frac{2}{p}-1\right)\epsilon_d + \left(\frac{2}{p}-1\right)\epsilon_h$$

Therefore, the local field enhancement factor becomes

$$|A|^2 = \frac{16\epsilon_h^2(|\epsilon'_m|^2 + |\epsilon''_m|^2)}{p^2(|\nabla'|^2 + |\nabla''|^2)}$$

Induced Optical Bistability (IOB) of Cylindrical Core-shell Nanocomposites: Metallic nanoparticles have the ability to sustain coherent electron oscillations known as surface plasmon (SP) leading to electromagnetic fields confined to their surface. The formation of SP are due to the electric field of an incoming radiation that induces the formation of a dipole or a polarization of charges on the nanoparticle surface. The local electric field E can be presented in the form

$$E = AE_h$$

Where, A - Enhancement factor, E-local field, E_h-applied field.

We consider a cylindrical dielectric particle (the core) of a radius $r_1$covered by a metal shell of radius r_2. Let the core be a nonlinear dielectric of the Kerr type with nonlinear dielectric function

$$\tilde{\epsilon}_d = \epsilon'_d + i\epsilon''_d + \chi|E|^2$$

Where,ϵ'_d - the linear part and ϵ''_d imaginary part of dielectric function of the core, χ- the nonlinear kerr coefficient. Substituting Eq. (6) in to Eq. (4), we get

$$|A|^2 = \frac{16}{p^2}\left|\frac{\epsilon_h\epsilon_m}{\sigma}\right|^2 \frac{1}{\left|\frac{\nabla}{\sigma}\right|^2 + 2Re\left(\frac{\nabla}{\sigma}\right)\chi|E|^2 + |\chi|E|^2|^2}$$

By squaring Eq. (5) and multiply by χwe have

$$\chi|E|^2 = |A|^2\chi|E_h|^2$$

Substituting Eq. (7) in to Eq. (8)

$$\chi|E|^2 = \frac{16}{p^2}\left|\frac{\epsilon_h\epsilon_m}{\sigma}\right|^2 \frac{\chi|E_h|^2}{\left|\frac{\nabla}{\sigma}\right|^2 + 2Re\left(\frac{\nabla}{\sigma}\right)\chi|E|^2 + |\chi|E|^2|^2}$$

Recall that the modulus of the dielectric function of metal-dielectric inclusion is given by

$$\nabla' = \epsilon'^2_m - \epsilon''^2_m + q\epsilon'_m + \epsilon'_d\epsilon_h$$

$$\nabla'' = 2\epsilon'_m\epsilon''_m + q\epsilon''_m + \epsilon''_d\epsilon_h$$

$$\sigma' = \left(\frac{2}{p} - 1\right)\epsilon'_m + \epsilon_h$$

$$\sigma'' = \left(\frac{2}{p} - 1\right)\epsilon''_m$$

And getting $X = \chi|E|^2$and $Y = \chi|E_h|^2$, then, the above equation becomes

$$\eta Y = X^3 + aX^2 + bX$$

Where $\eta = \frac{16}{p^2}\left|\frac{\epsilon_h\epsilon_m}{\sigma}\right|^2$, $b = \left|\frac{\nabla}{\sigma}\right|^2$and $a = 2\left(\frac{\nabla'}{\sigma'}\right)$. Eq. (9) is called induced optical bistability (IOB)

RESULTS AND DISCUSSION

We investigated the effects of varying p and $\epsilon_h$on the LFE and IOB of cylindrical core-shell NPCs in passive and active dielectric cores. The model considered in the study, specifically consists a passive and active dielectric core, a silver (Ag) shell, and a host matrix.

Table 1. The parameters used for numerical evaluations are:

Used Parameters	Value assigned
ϵ'_d	6.0
ω_p	1.4×10^{16}
υ	1.68×10^{14}
γ	1.15×10^{-2}
ϵ'_m	$\varepsilon'_\infty - \frac{1}{z^2+\gamma^2}$
ϵ''_m	$\varepsilon''_\infty + \frac{\gamma}{z(z^2+\gamma^2)}$

Effect of metal fraction and host dielectric constant on Local Field Enhancement (LFE): We have seen the effect of metal fraction and host dielectric on the LFE of cylindrical core-shell NPCs in passive and active dielectric cores. Fixing the values of ϵ_h and changing the metal fraction by the same amount produces LFE of different peaks in passive and active dielectric cores Fig.1 and 2.

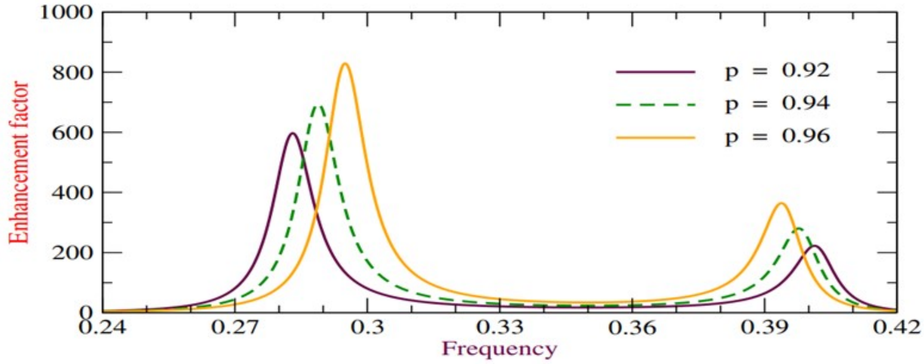

Fig. 1. LFE of cylindrical core-shell silver nanocomposites in passive dielectric core (ϵ_d''= 0.0) with parameters ϵ_∞= 4.5, ϵ_h= 2.25 and different values of p.

When the metal fraction increases, the amplitude of local field enhancement factor also increases in both passive and active dielectric cores Fig.1 and 2. Further, comparison of the results from Fig. 2 that shows the value of LFE occurs for each value of the increase in p is larger in active dielectric core. Fig.1 and 2 shows that, when the radius of the core increases, i.e., when the p value decreases, the enhancement factor of cylindrical core-shell nanocomposites decreases leading to smaller amplitude. On the other hand, when the metal fraction increases, the enhancement factor increases. Hence, it could be said that the LFE in the passive and active dielectric core can be controlled by adjusting the metal fraction or size of the core-shell nanocomposites. The embedding host matrix permittivity is one of the parameters that affects the LFE of nanoparticle composites (NPCs). The result shows that when the value of ϵ_h increases, the local field enhancement increases in both types of cores. When the value of host dielectric constant ϵ_h= 2.15, the values of enhancement factors are nearly 700 and 1350 in passive and active dielectric cores Fig. 3 and 4, respectively.

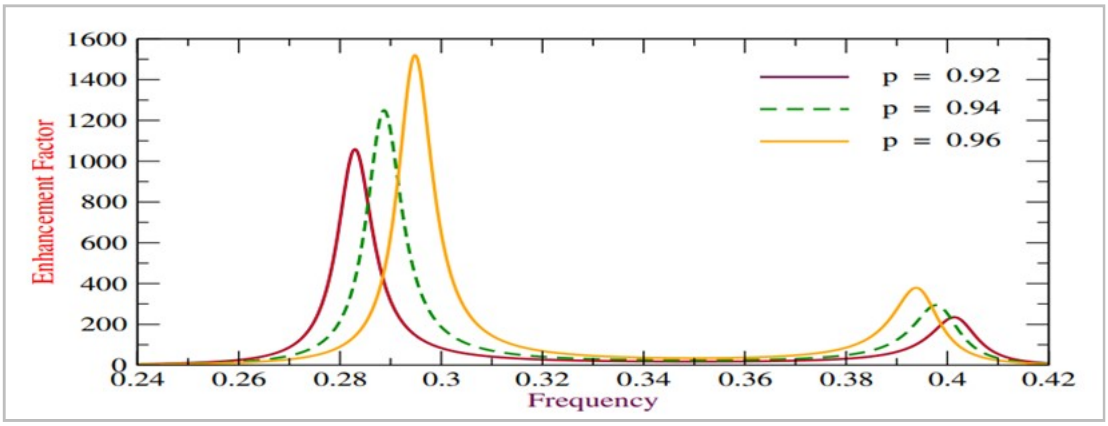

Fig. 2. LFE of cylindrical core-shell silver nanocomposites in active dielectric core ($\epsilon_d'' = -0.112$) with parameters ϵ_∞= 4.5, ϵ_h= 2.25 and different values of p

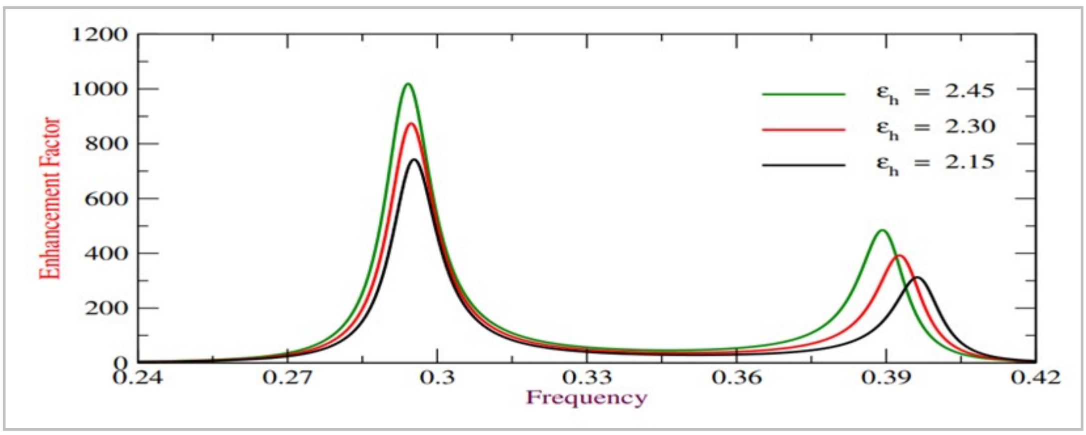

Fig. 3 LFE of cylindrical core-shell silver nanocomposites in passive dielectric core ($\epsilon_d'' = 0.0$) with parameters ϵ_∞= 4.5, p = 0.96 and different values of ϵ_h

Moreover, it could be observed that increasing the dielectric constant of the embedding medium increases of the LFE factor in both passive and active dielectric cores of cylindrical core-shell nanocomposites. Generally, the LFE of cylindrical core-shell nanocomposites in passive and active dielectric core is sensitive to the changes in p and ϵ_h. From figure 5, we obtained that there are different maximum value of the local field enhancement factor for different values of active dielectric core ($\epsilon''_d < 0$). The negative sign implies that additional dielectric function is given to the imaginary part of active dielectric core. When affecting the natural property of the dielectric function of the host matrix by applying additional dielectric function on it, the amplitude of the graph increases. Therefore, for the active dielectric core ($\epsilon''_h < 0$), the LFEF can be maximized by varying the original property of imaginary part of the dielectric function of the dielectric core, this resembles like that of increasing the density of cylindrical core-shell silver NPCs.

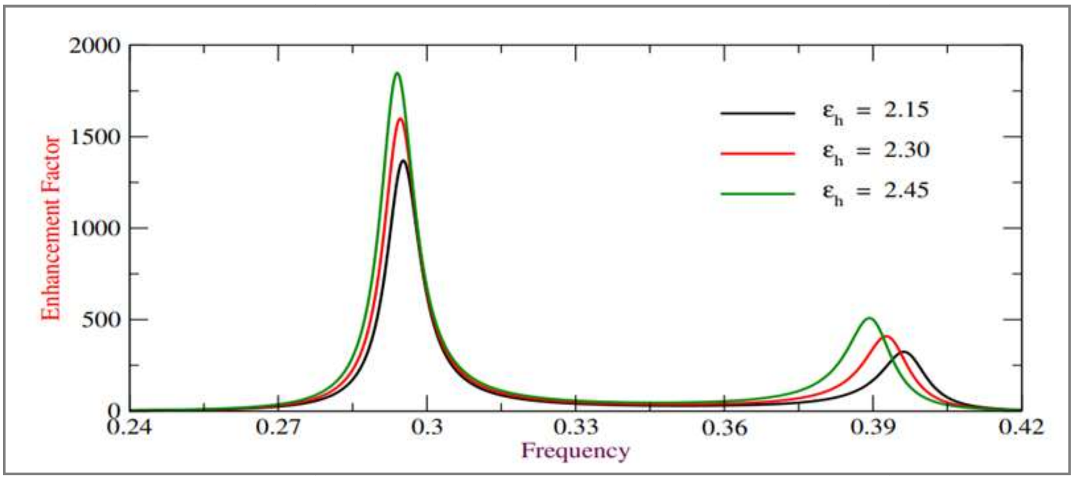

Fig. 4 LFE of cylindrical core-shell silver nanocomposites in active dielectric core ($\epsilon''_d = -0.112$) with parameters ϵ_∞= 4.5, p = 0.96 and different values of ϵ_h

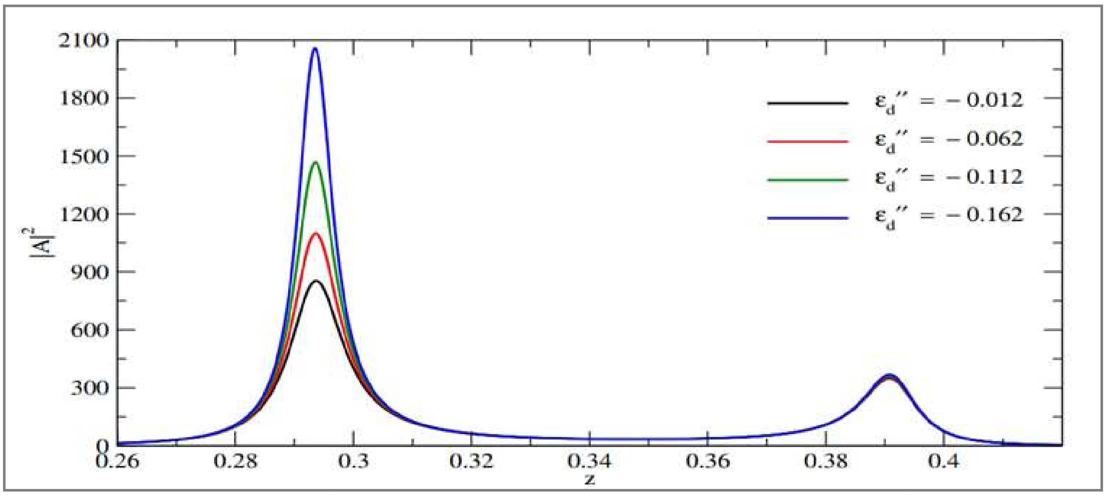

Fig. 5. LFE of cylindrical core-shell silver nanocomposites in active dielectric core with parameters p=0.96, ϵ_∞= 4.5, ϵ_h= 2.25 and different values of ϵ''_d.

Effects of metal fraction and host dielectric constant on Optical Bistability (OB): We have also seen the effect of metal fraction and host dielectric constant on the optical bistability (OB) of cylindrical core-shell nanocomposites in active dielectric cores. Fixing the values of $\epsilon_h$and changing the metal fraction by the same amount produces OB of different peaks and bistability regions in active dielectric cores (Fig. 6). When the metal fraction increases, the incident field required at each switching-up threshold points also increases in active dielectric cores (Fig. 6). However, the switching-down points for various values of p occur at nearly the same incident electromagnetic field.

Further, comparison of the results from Fig. 6 that shows the value of applied field at which switching-up of optical bistability (OB) occurs for each value of the increase in p is larger in active dielectric core. When the radius of the core increases, i.e., when the p value decreases, the bistable threshold of cylindrical core-shell NPCs decreases leading to smaller bistable outputs as shown in Fig. 6. On the other hand, when the metal fraction increases, the switching-up threshold field increases and the bistable region produced gets wider. Hence, it could be said that the OB in active dielectric core can be controlled by adjusting the metal fraction of the core-shell NPCs. The embedding host matrix permittivity is one of the parameters that affects the induced optical bistability (IOB) of nanoparticles. However, the effect was not extensively studied in active dielectric cores of cylindrical core-shell nanoparticle composites. To address this, we have used the varying values of host dielectric constant $\epsilon_h$at constant p and investigated the result for cylindrical core-shell NPCs in active dielectric cores. The result shows that when the value of $\epsilon_h$increases, the switching-up threshold field decreases in both types of cores (Fig. 7). Hence, it could be said that by using larger value of host dielectric constant ϵ_h, the switching-up threshold of IOB of cylindrical core-shell NPCs can be obtained at smaller value of incident field.

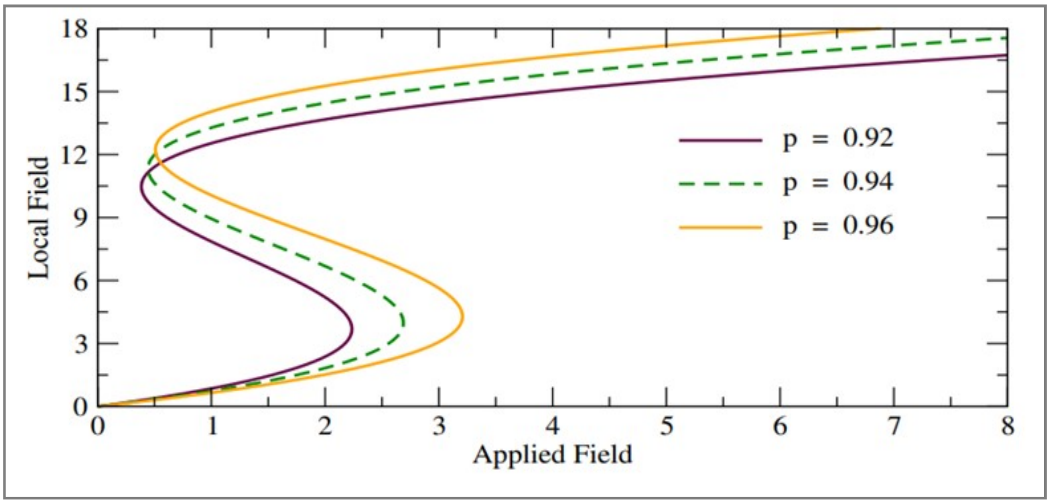

Fig. 6 IOB of cylindrical core-shell silver nanocomposites in active dielectric core ($\epsilon_d'' = -0.112$) with parameters ϵ_∞= 4.5, ϵ_h= 2.25 and different values of p

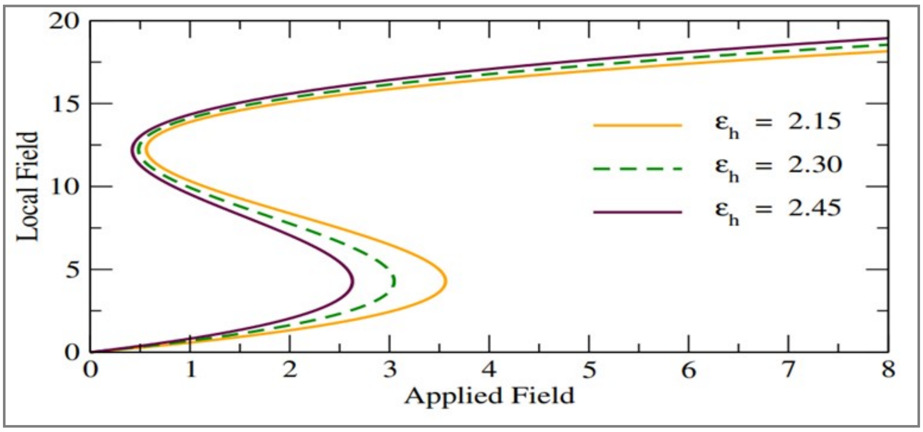

Fig. 7 IOB of cylindrical core-shell silver nanocomposites in active dielectric core ($\epsilon_d'' = -0.112$) with parameters ϵ_∞= 4.5, p = 0.96 and different values of ϵ_h.

Additionally, one can observe that increasing the surrounding dielectric constant produces no change in the switching-down threshold field, especially in the active dielectric core. The IOB of cylindrical core-shell NPCs in active dielectric core is sensitive to the changes in p andϵ_h. Changing those parameters under different conditions can lead to the possibility of tuning the bistable thresholds and the bistable regions which enables one to design various types of nanodevices for practical applications in nonlinear optics.

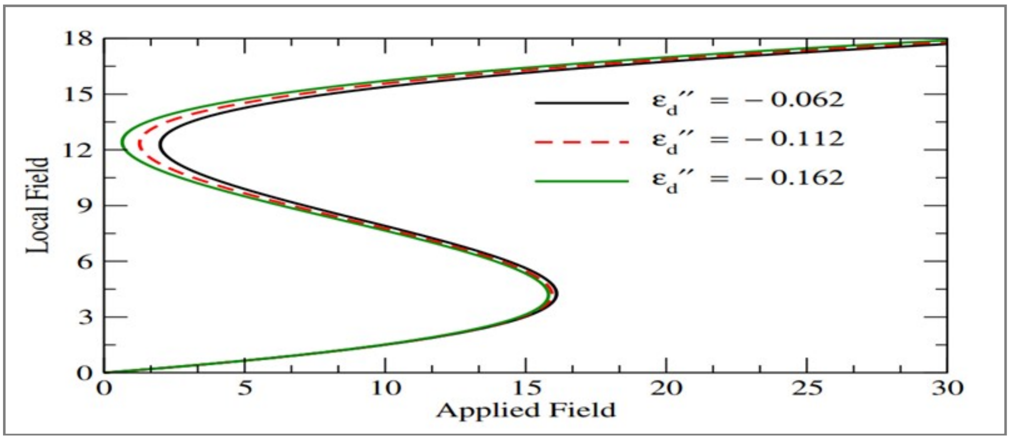

Fig. 8 IOB of cylindrical core-shell silver nanocomposites in active dielectric core with parameters p=0.96, ϵ_h= 2.25 and different values of ϵ_d''

From fig. 8, optical bistability is illustrated in the *Y-X* plane and we observed *S-like* curves. Increasing of incident field from zero to and gives increasing of local field monotonically. However, after a certain decreasing the value of incident field gives increasing of the local field. Using linear stability analysis this branch of solution is unstable. That means, if the system is initially in this state, it will rapidly switch to one of the stable solutions through the growth of small perturbations. So, with increasing of incident field from zero to and when it passes the turning point in the lower branch then immediately it switching up to the upper branch. On the other hand, if the input intensity is slowly decreased, the system will remain on the upper branch and the output intensity will continue and at the turning point switching down to the lower branch. Fig. 8 shows that as the imaginary part of the dielectric function of the active dielectric core increases, the width range of optical bistability or the threshold width rises. This wider threshold width enables the system to oscillate highly, or increases the activation of the system.

SUMMARY AND CONCLUSION

We proposed the effect of both passive and active dielectric cores on local field enhancement (LFE) and induced optical bistability (IOB) of cylindrical core-shell NPCs by adjusting p, and $\epsilon_h$as well as doing a root analysis of the IOB. The findings show that, when the metal fraction and dielectric of host matrix increases, the amplitude of local field enhancement factor also increases in both passive and active dielectric cores. It indicates that, when the radius of the core increases, i.e., when the p value decreases, the enhancement factor of cylindrical core-shell nanocomposites decreases leading to smaller amplitude.
Also, we studied that the IOB of the cylindrical coreshell NPCs is attained at a lower applied field in the passive dielectric core than the active one, regardless of how p, or $\epsilon_h$vary or are maintained constant. Furthermore, it could be observed that bistability formed by varying the intensity of the incident electric field, regardless of whether the dielectric core is passive or active. Moreover, there is an effect on LFE and the IOB of cylindrical core-shell NPCs in passive and active dielectric cores when p is considered. Likewise, fixing the values of $\epsilon_h$and varying the p, however, produces S-like bistability regions in active dielectric cores. Yet, as p increases, the incident field required at each switching-up threshold point also increases, in active dielectric cores. However, the results show that the intensities at which switching-up of IOB occurs for each value of the increase in p are larger in the active dielectric core. Moreover, when $\epsilon_h$increases, the corresponding switching-up threshold fields decrease. For a larger value ofϵ_h, the switching-up threshold of the IOB of cylindrical core-shell NPCs can be obtained at a smaller value of the incident field. Also, for cylindrical core-shell NPCs, it could be observed that increasing the dielectric constant of the embedding medium decreases the bistable region of IOB in both passive and active dielectric cores of spheroidal core-shell NPCs. We observed that by varying the metal fraction, and dielectric function of the NPCs host medium, it is possible to control the values of LFE and IOB in cylindrical core-shell NPCs.

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Conflict of interest: The authors have no conflicts to declare.

Author contributions: SG and SS: conception and design of the model, performed the analytic calculations, analysing and interpreting the results. SH drafted manuscript preparation. All authors are reviews the results and approved the final version of the manuscript.

Data availability: This manuscript has no associated data or the data will not be deposited.

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Ethics conduct: Not applicable.

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