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Triangular Nanoparticle Based Plasmonic Biosensor

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Abstract: This paper presents the theoretical investigation of a novel metal-insulator-metal based plasmonic perfect absorber for biosensing applications. The electromagnetic simulations are performed using finite integration technique (FIT) based simulation softrware i.e. CST Microwave Studio. The electromagnetic analysis are useful in demonstrating the effect of field enhancement in the sensing region of a biosensor. It also depicts the spectral shift of field enhancementas a function of variations in the refractive indices of a sensing medium defined as a sensitivity of biosensor. If the spectral shift is high with a small variation in refractive index of a sensing medium, then sensor is said to be a highly sensitive. The sensitivity of a plasmonic sensors depend on the geometry of the structure. Here, a novel metal-insulator-metal based PPA structure is considered for analysis. The novel approach uses triangular gold nanoparticles at the vicinity of the sensing medium. Due to the sharp edges of the triangular nanoparticles, high field is enhanced towards the sensing medium as compared to the conventional metal-insulator-metal based PPA biosensors. The simulation results show effects of field enhancement, spectral shifts of the absorption in the sensitivity. Results are useful for the design of a novel PPA biosensor.

Keywords: Biosensing; SPR biosensor; LSPR biosensor; PPA; Triangular Nanoparticles; Spectral Sensitivity

1. INTRODUCTION

When the light energy is subjected to a metal through a suitable medium its particles interacts with the free electrons of metal. Proper light illumination produces the collective oscillations at the interface of metal and dielectric. Plasmonics is the study of this interaction and collective oscillations.

Plasmons are the free oscillating electrons of a metal. The antenna based on optical excitation of plasmons is called plasmonic antenna. When the incident light is subjected to excite the plasmon, the reflected light is detected by the detector simultaneously (Homola, 2003). By detecting changes in the light intensity the detector detects properties of the material (i.e. refractive index) at which the plasmons are existed. Plasmonic antennas are widely used for medical diagnosis, environmental monitoring, drug screening, and food safety. These antennas offer label-free biomarker detection, rapid test time and portability (Homola, 2003), (Piliarik and Homola 2009), (Zhao *et al.*, 2014).

Recently, it is proved that plasmonic biosensing family is the most developed and advanced optical label free technology. Plasmonic biosensing family falls into two categories i.e. surface plasmon resonance (SPR) and localized surface plasmon resonance (LSPR) sensors. SPR sensors are based on the excitation of propagating surface plasmons (PSPs) that are excited on metallic-layer and propagate along the interface or metal-dielectric layer. Whereas, When the light is subjected on noble metal nanoparticle a collective oscillation of electrons is produced that is called LSPR. The condition when oscillation of electrons on nanoparticle surface matches with the incident EM field is called "Resonance". The resonant oscillation produces large EM field at the surface of the nanoparticle which is helpful in the surface enhanced raman spectroscopic (SERS) sensing of analytes (such as chemical and biological molecules). LSPR biosensors offers many advantages including no labeling requirement, low cost, good reproducibility, easy instrumental setup and high sensitivity than conventional schemes (Zhao *et al.*, 2014). Another configuration of plasmonic biosensor has emerged recently known plasmonic perfect absorber (PPA) biosensor (Lu *et al.*, 2018). The PPA is a combination of SPR and LSPR configuration. It consists of a dielectric spacer sandwiched between metal nanoparticles and metal layer on glass substrate. It works on the principle of perfect absorption. There are two types of absoption in the PPA strucuture: one is due to plasmons (at the interface between metal and dielectric) and the other is due to waveguide (dielectric

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spacer). Due to the presensence on metal layer and metal nanoparticles, it combines the effects of both SPR and LSPR biosensors.

(Fig. 1) shows the setups of plasmonic biosensors with their response curves. The setups are comprised of prism/glass (light green), metal layer (yellow box), and a flow cell (blue box). The light is incident and reflected from a prism on the metal structures for coupling. The flow cell consists of analytes (red balls) and ligands (y shaped). Analytes are the biomolecules that are to be detected. Whereas, ligands are the bio-recognition elements. The principle of detection of biomolecules is based on the coupling on analyte to the ligand. When an analayte interacts with the ligand, the dielectric property of ligand or flow cell (also known as dielectric material) is changed. By this way, a biomolecule is recognized. Different biomolecules lead to different different dielectric material. **(Fig. 1 (a))** shows the Kretschmann configured SPR biosensor setup. In SPR setup, the light is incident/detected through a prism (light green triangle) on the metal layer (yellow box). Incident light is used to detect changes in the dielectric material with the interaction of analytes with the ligands. When a light is incident on the metal layer with a principle of total internal reflection (TIR) then absorption of light occurs.

This lead to the generation of PSPs (i.e. all the incident light is coupled) at the interface between metal and dielectric material. This effect can be observed with a response curve of SPR, by measuring reflectivity as a function of wavelength of light. The dip in the reflectivity at a specific wavelength shows the generation of a PSPs. The generation of PSPs is highly dependent on the dielectric material (Homola, 2003). The changes in the dielectric material are observed by the shifts of the reflectivity dip to different wavelengths. **(Fig. 1 (b))** shows the configuration of a LSPR biosensor setup. In LSPR setup, the light is incident/detected through dielectric material on the metal nanoparticles (yellow ball). Incident light is used to detect changes in the dielectric material with the interaction of analytes with the ligands. When a light is incident on the metal nanoparticles, then absorption of light occurs. This lead to the generation of LSPRs (i.e. all the incident light is coupled) at the interface between metal and dielectric material. This effect can be observed with a response curve of LSPR, by measuring absorption as a function of wavelength of light. The peak in the specific at a specific wavelength shows the generation of a LSPRs. Like PSPs, the generation of LSPRs is also highly dependent on the dielectric material (Homola, 2003). The changes in the dielectric material are observed by the shifts of the absorption peak dip to different wavelengths in LSPR curve. **(Fig. 1 (c))** shows the shows the setup of a PPA biosensor. In PPA setup, the light is incident/detected through dielectric material (i.e. flow cell) on the metal nanoparticles (yellow ball). Incident light is used to detect changes in the dielectric material with the interaction of analytes with the ligands. When a light is incident on the metal nanoparticles, then absorption of light occurs. This lead to the generation of LSPRs (i.e. all the incident light is coupled) at the interface between metal and dielectric material. The absorbed light from the metallic nanoparticles impinges into the metallic layer from dielectric spacer. That light is absorbed at the dielectric layer lead to the excitation of waveguide modes. The light is also absorbed at the metal layer and lead to the generation of PSPs. By this way, the PPA has the properties of LSPRs and SPRs. This effect can be observed with a response curve of PPA, by measuring absorption as a function of wavelength of light. The peak in the specific at a specific wavelength shows the generation of absorption plasmonic as well as waveguides waves. Like PSPs and LSPRs, the absorption peak of PPA is also highly dependent on the dielectric material (Homola, 2003). The changes in the dielectric material are observed by the shifts of the absorption peak dip to different wavelengths in PPA curve.

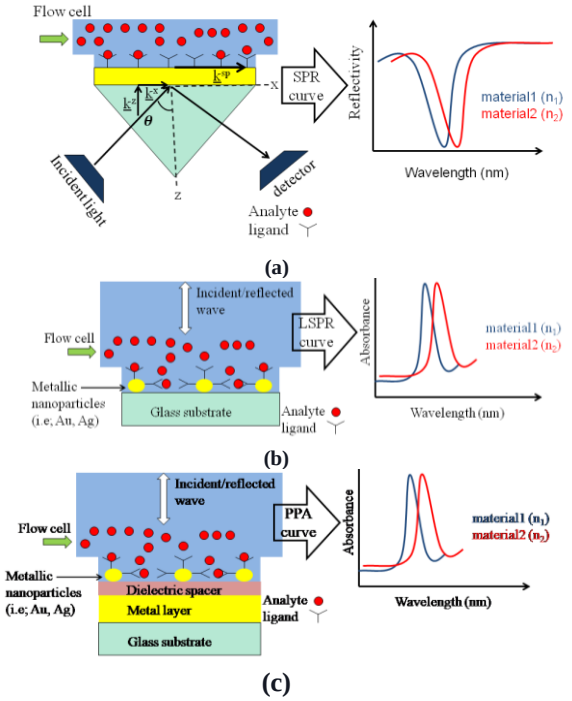


Fig. 1: Plasmonic biosensor setups: (a) SPR (Kretschman configuration), (b) LSPR, and (c) PPA

The sensitivity of plasmonic biosensors can be measured by (Piliarik and Homola 2009) as given in **eq. (1)** ,

$$S = \frac{\delta Y\ (wavelength)}{\delta n_{eff}} \frac{\delta n_{eff}}{\delta n} \qquad \textbf{eq (1)}$$

Where, δY(wavelength), δn_{eff}, and δn indicate the changes in output of the sensor (i.e. reflectivity or absorption as a function of wavelength), effective refractive index of dielectric material and refractive index of dielectric material, respectively. The refractive index in **eq(1)** is the square root of the permittivity (which is dielectric material property).

This paper is divided in to five sections. Section 1 describes the introduction of the and explaination of plasmonic biosensors (SPR, LSPR, and PPA). Section 2 reviews the literature of plasmonic biosensor. Section 3 illustrates the methodology of the work. Section 4 discusses results of the plasmonic biosensor. At the end, section 5 concludes the research work.

2. LITERATURE REVIEW

The Sensitivity and detection limit are main performance characteristics for plasmonic biosensor. Pang et al. investigated the sensitivity of nano hole array SPR biosensor for various modes (Pang 2007). Kretschmann configuration commercial SPR is developed with Sensitivity is 1110nm/RIU. Its sensitivity can still be improved. Gerardo made advances in plasmonic biosensors and analysed their performance (Alves *et al.*, 2016), From this work it is concluded that detection limit of LSPR (10ng/ml) is much higher than SPR (0.7μg/ml). (Lu *et al.* 2018) numerically investigated a PPA structure (Lu *et al.*, 2018). Spectral sensitivity of proposed PPA is 840nm/RIU. This sensitivity value is considered as benchmark value for current PPA biosensor. Jamali A. used disc shape nano particles to design PPA. He measured angular sensitivity of PPA biosensor 140°/RIU.Homola has reviewed the SPR biosensor technology including SPR fundamentals, advances and applications of SPR biosensors (Zhao *et al.*, 2014). In this review different SPR biosensing formats are discussed which are direct detection (used for medium size analyte detection), inhibition assay (used for small size analyte) and sandwich assay (used for large size analyte). Areas of applications of SPR biosensor are medical diagnosis, environmental monitoring, biotechnology, food safety, drug screening, and security (Zhao *et al.*, 2014), (Alves *et al.*, 2016), (Jamali and Witzigmann (2014), (Lu *et al.* 2018). Unified-theoretical model for the resolution of SPR sensor is reported in (Piliarik and Homola 2009). This theory indicates that SPR sensors are independent of SPRs excitation method or the modulation method and are dependent on properties of source and detector. A novel and reusable LSPR biosensor is proposed by Zhao *et al.* (2014) (Alves *et al.*, 2016), to detect the Squamous Cell Carcinoma Antigen (SCCA) in cervical cancer patients. This biosensor is comparatively advantageous in terms of free-labelling, good sensitivity; less cost and short assay time hence it is potential alternative of other clinical serological diagnosis strategies. (Breault-Turcot and Masson 2012),has developed the nano-structuring of thin gold film in order to enhance the sensitivity of SPR biosensor. The noise reduction algorithms are also proposed for improvement of signal to noise ratio which proportionally improves the detection limits of SPR in Pico molar range to nano-molar range. A Kretschmann configuration integrated SPR sensor is proposed by Soelberg *et al.* (2019). The proposed biosensor is rapid, portable, inexpensive and usable for coinciding analysis of multiple analytes. Six analyses are analysed to detect the environmental pollutants and small organics including spores, nerve agents, viruses, toxic proteins, and whole microbes. Liu et al. has proposed smart phone based fibre optic SPR that is miniaturized, inexpensive and portable alternative of conventional bulk SPR (Liu *et al.*, 2015). Through fibre optic the sensing element and optical components are connected on phone case. Due to the simple installation and removal of SPR its flexibility and simplicity is enhanced. LED light of phone is used as light source and camera works as detector. Information is extracted from the refractive index changes due to the changes in light intensity recorded continuously with 0.5second interval (Liu *et al.*, 2015). Lu et al. proposed a PPA structure (Dielectric patch array mounted on metal plane (DAM)) for biosensing applications (Lu *et al.*, 2018). Observed sensitivity and figure of merit (FOM) are 840nm/RIU and 84/RIU respectively (Lu, *et al.* 2018). (Gerardo *et al.* 2016) reviewed different techniques of SPR and LSPR to design a portable, miniature, sensitive plasmonic antenna for clinical and bio analytical applications (Lopez *et al.*, 2016), generated an array of triangular gold nano particles through lithography (Jamali *et al.* 2012), and concluded that optical properties of nano particle vary by tuning its morphology compared finite integration technique FIT to discrete dipole approximation DDA (Pang 2007). Sensitivity (to refractive index change) of rhombic hybrid gold-silver nanostructure is calculated using DDA and FIT as well. Both techniques show same accuracy. In addition DDA's advantage is shorter simulation time. Islam et al. has presented two port SPR biosensor model along with a graphene layer (Islam and Kouzani (2012),. Graphene layer strengthen the adsorption of the bio molecules hence sensitivity increases.

3. METHODOLOGY

The objective of this work is to design a biosensor which provides better sensitivity as compared to conventional SPR and LSPR sensors. Here, a PPA based configuration for biosensor is designed for the improvement in sensitivity. The flow chart of the research work is depicted in **(Fig. 2)**. The plasmonic biosensors such as SPR, LSPR, and PPA are modelled

and simulated, separately. The modelling and simulations are performed by using 3D electromagnetic simulation software package (i.e. CST Microwave Studio). Then, the electromagnetic analysis are executed on each plasmonic biosensor. After that, sensitivity are measured for each biosensor by using **(eq. 1)**. The PPA biosensor has the ability to improve the sensitivity by varying geometrical structure of the PPA (Jamali and Witzigmann (2014)). If the PPA has the less sensitivity as comared to SPR and LSPR sensor, then the geometrical paramteres of PPA are changed accordingly.

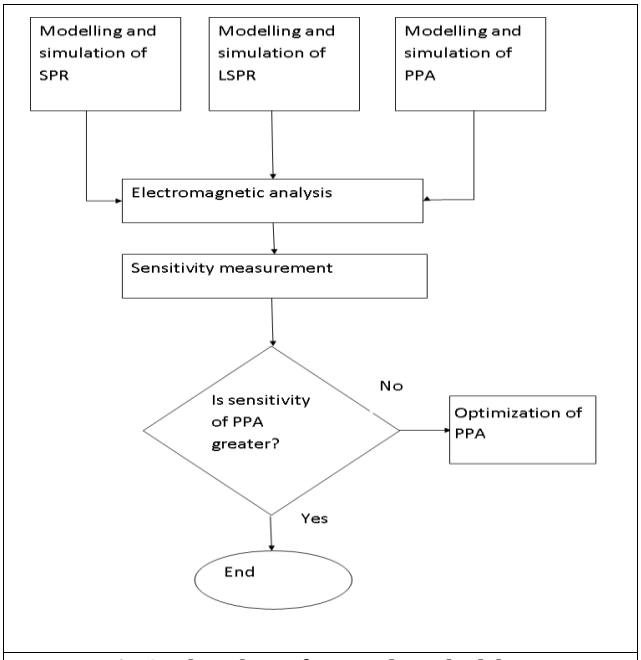


Fig. 2: Flow chart of research methodology

This paper explains the simulation model of a PPA biosensor only. The readers who are interested in details of the modeling of SPR and LSPR biosensors they can go through (Jamali, 2015). The sensitivity of triangular nanoparticles based PPA structure is designed and compared with conventional SPR and LSPR sensors.

The basic model of a triangular gold nanoparticles based PPA biosensor is shown in **(Fig. 3)**. The triangle is a three dimensional isosceles triangle with side lengths of 100 nm and thinckness of 30 nm. The PPA structure consists of three layers placed on the glass substrate. The thicknesses of three layers are t_1 , t_2 and t_3 are 30 nm, 40 nm, and 200 nm, respectively. The first layer comprises of a periodically arranged triangular gold nanoparticles that has periodicity "p" of 500 nm. Second and third layers are dielectric spacer and gold layer. The light waves are incident from top of the PPA structure and reflected lights are also observed on top of PPA structure.

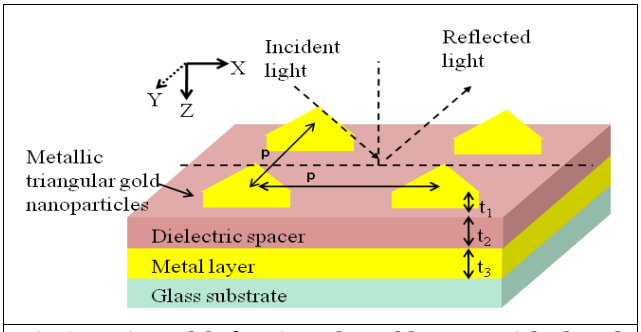


Fig. 3: Basic model of a triangular gold nanoparticles based PPA biosensor

The material specifications of a PPA structure are provided in **(Table 1)**.

Table 1: Material specifications of a PPA structure

Material	Specification
Dielectric material	Refractive index= 2.08
Drude metal	Collision frequency=2.89×10^{14} Cycles /sec Plasma frequency=1.04×10^{16} Hz
Glass	Refractive index= 1.5

The modeling of a PPA biosensor is depicted in **(Fig. 4)**. PPA consists of a periodically arranged triangular gold nanoparticles along lateral direction of a structure. Unit cell (consist of a single triangular nanoparticle) can be taken to save computational time and memory. Therefore, a unit cell boundary conditions are applied along the lateral direction i.e. the x and y direction of PPA. The unit cell simulates the infinitely arranged periodic structure. The light waves are incident from the top of the structure, therefore, perfectly matched layer boundary conditions are applied the vertical direction (z-direction) of the PPA structure. The electric field is polarized along the x-direction and y-direction for transvers magnetic (TM), and transverse electric (TE) polarization, respectively.

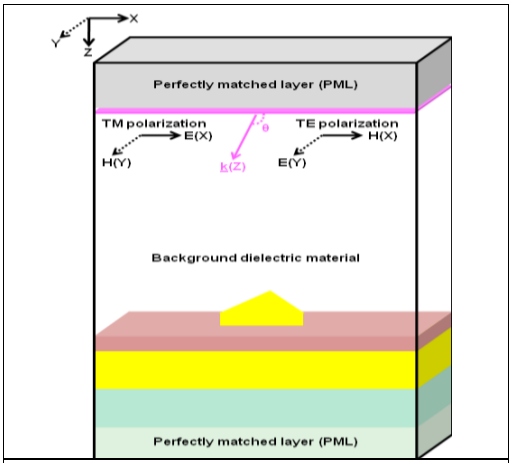
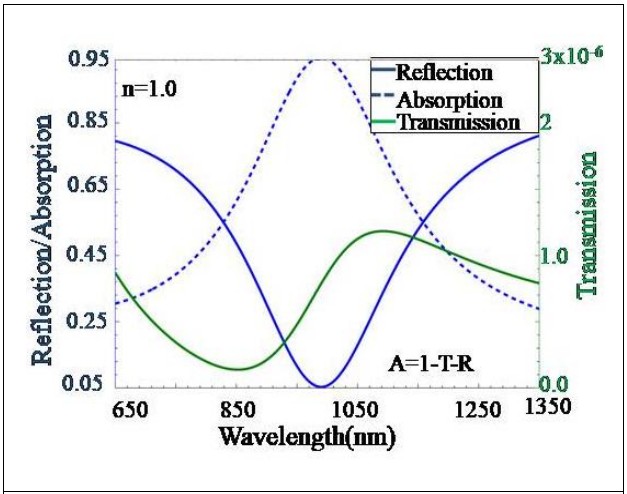


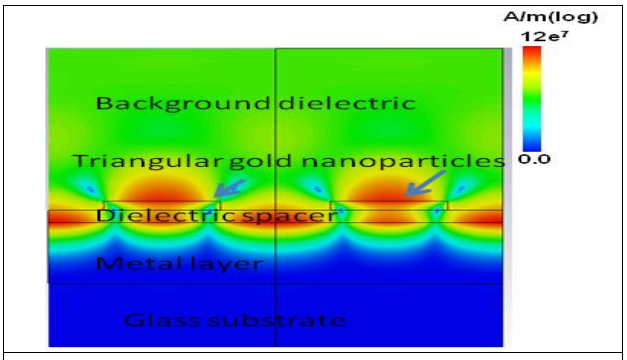
Fig. 4: Computational domain of a PPA biosensor

4. RESULTS

This paper focuses on the electromagnetic analysis of the triangular nanoparticles based PPA biosensor. The triangle based PPA structure is modelled as depicted in **(Fig. 4)**. The simulation results of a unit cell PPA structure with air (n=1.0) as a background dielectric material are obtained for wavelength ranges from 650-1350 nm **(Fig. 5)**. The triangle based PPA structure is excited with TE and TM polarizations. The light waves are traveling along vertical direction (i.e. z-direction) at normal incidence. The PPA response curves (transmission (T), reflection (R) and absorption(A)) are computed for both polarizations as a function of wavelengths. The A is calculated in postprcessing from R and T spectra with A=1-T-R. The similarity in the response curves are observed for TE and TM polarizations, as shown in **(Fig. 5(a))**. It is due to the symmetry of the structure along the x and y-directions with normal polarizations. The dip/peak in the reflection/absorption is obtained at 980 nm. The transmission is negligibly small for all wavelengths ranging from 650-1350 nm. The results show 95% absorption at a wavelength of 980 nm with the novel triangular gold nanoparticles based PPA structure. **(Fig. 5(b))** depicts the field distribution along the PPA structure at a wavelength of 880 nm. It can be observed that the field is highly enhanced at the interfaces between gold and dielectrics. This field is generated due to the excitation of surface plasmons, which occurs at the metal/dielectric interface. The plasmonic field decays exponentially along dielectric media. Another field is also observed at the dielectric spacer. This field is due to the excitation of a waveguide mode. The plasmonic waves can only be generated with TM polarizations, it can not be excited with TE polarizations. While the waveguide mode is excited by TE polarizations. At a wavelength of 880 nm, the plasmonic and waveguide modes are coupled together lead to 95% absorption.



(a)



(b)

Fig. 5: Simulation results of a triangular nanoparticles based PPA biosensor: (a) PPA curve for TE/TM polarizations with normal incidence, and (b) Field distribution along PPA structure at a wavelength of 980 nm

The simulation results of TE and TM polarizations with oblique angles of incidences at a specific wavelength of 980 nm are depicted in **(Fig. 6)**. More than 90% absorption is obtained with TM polarization for tilted angles from 0-60^0. For TE polarization, more than 85% absorption obtained for tilted angel ranging from 0-50^0. More than 50% absorption is obtained from 50-60^0. TE polarization has less absorption as compared to TM polarization. These results support previous observation obtained from the result of field distribution shown in **(Fig. 5(b))**. That, the TM polarization leads to the excitation of plasmonic modes, whereas, TE polarization excites waveguide modesin triangular gold nanoparticles based PPA structure. These observations are similar to the observations obtained in previous works of (Jamali and Witzigmann, 2014) and (Lu *et al*. 2018).

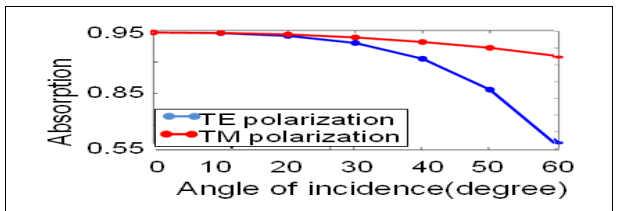


Fig. 6: The response of a PPA biosensor with TE and TM polarizations by impinging light wave at oblique angles from 0-60^0 at a wavelength of 980 nm.

After the electromagnetic analysis, the triangular gold nanoparticles based PPA structure is tested for biosensing. The background dielectric material of computational domain **(Fig. 4)** is replaced from air (n=1.0) to water (n=1.33). The simulation are performed with TM polarization to excite the plasmonic modes. The variation in the background dielectric material causes wavelength shift of absorption from 980 nm to 1160 nm in the PPA curve. A shift of 180 nm is observed. This is called red-shift, as the absorption curve shifts to the higher wavelength. After that a suitable angle of incidence (44.5^0) is obtained, which provides maximum absorption with water as a background dielectric medium.

(Fig. 7) shows the sensitive response of PPA based biosensor for a wavelength ranges from 900-1600 nm. The PPA response is obtained with TM polarization. The bulk refractive index of a dielectric medium is varied from 1.33 to 1.40 with a change of 0.01. Around 90% absorption is observed for all variations of refractive indices. It is also observed that the PPA response curve is smooth and depicts a shifts in the wavelength with variation of refractive indices. The sensitivity is computed by using **(eq. (1))**. The calculated sensitivity of a triangular gold nanoparticles based biosensor is 1020 nm/RIU. The sensitivity of simulated novel structure is higher than the SPR (Lopez G.A. *et al.* 2016), LSPR (Pang, L. *et al.* 2007), and PPA (Jamali and Witzigmann, 2014).

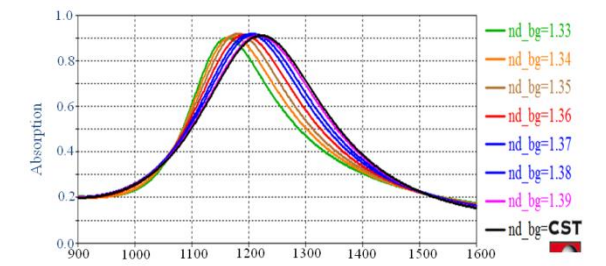


Fig. 7: Response of triangular gold nanoparticles based PPA biosensor with a refractive index variation from 1.33 -1.40.

5. CONCLUSION

This paper has presented the novel PPA structure based on triangular gold nanoparticles. The PPA structure is modelled, simulated by using CST Microwave studio. The electromagnetic analysis of novel PPA structure is performed. It has shown a 95% with normal incidence with TE and TM polarizations. Due to the symmetry of the structure at normal incidence, the PPA response curve has similarity with TE and TM polarization. The field distribution is also observed. The excitation of plasmonic and waveguides modes are observed with analysis of field distribution. The absorption spectra is also analyzed for oblique angles of incidences. It is depicted that the TM polarization provides more than 90%, whereas, TE polarization provides more than 55% absorption for tilted angles from $0\text{-}60^0$. The triangular based PPA structure is also tested for biosensing. Refractive index of back ground material is varied from 1.33-1.40. It has shown spectral shift of absorption peak with the variation of refractive indices. The sentivity is computed which is better than the SPR, LSPR and nano disk based PPA structures. Due to the sharper edges of the nanoparticle, the high field is enhanced at the sharp edges. This lead to the high sensitivity of a novel triangle based PPA. The demonstated results will help scientific for designing plasmonic sensor with high sensitivity.

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