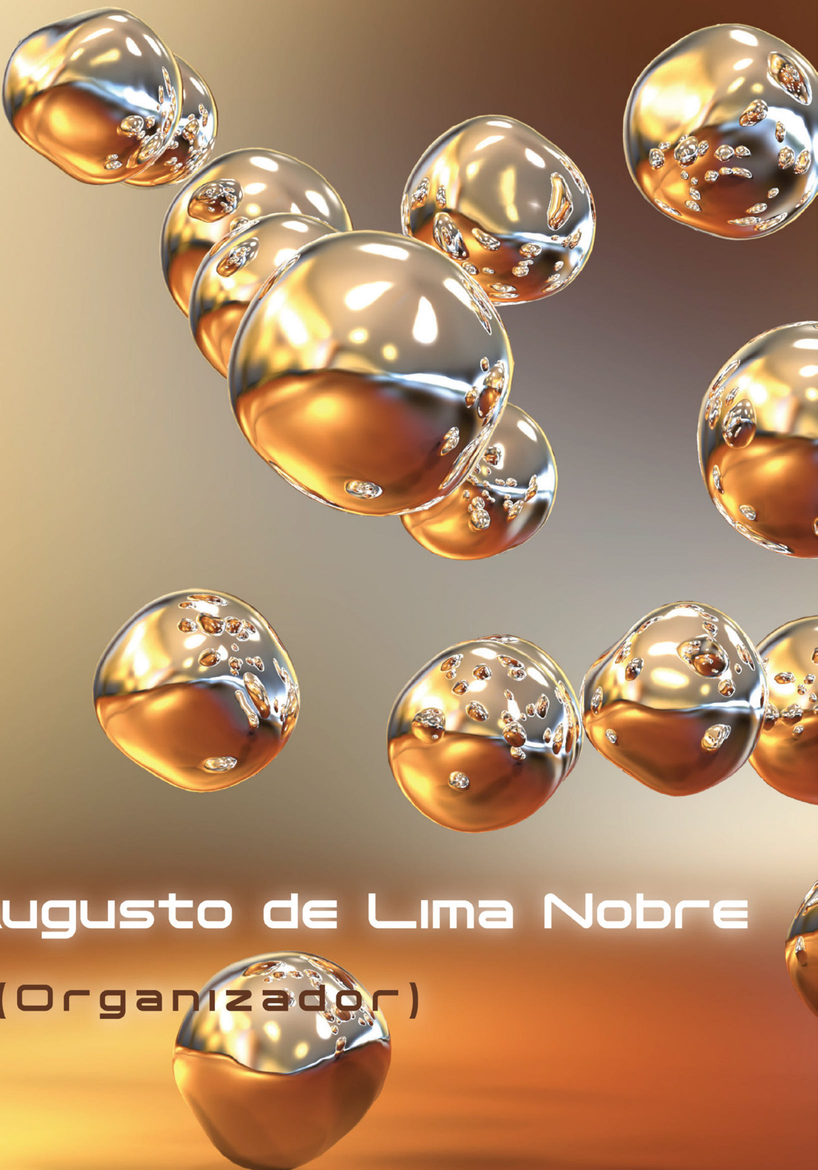
THE GREAT WORLD OF NANOTECHNOLOGY



Marcos Augusto de Lima Nobre

(Organizador)

VOL II

EDITORA ARTEMIS
2021

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PREFACE

The insertion of new and enhanced materials based on materials belonging to the Nano scale in the day-by-day has growth up in a silent way. In part, a number of works in the nanotechnology stemming of theoretical research using Density Functional Theory (DFT) and sophisticated simulation methods; another part is associated to the protected technologies associated to the military and patented nanomaterial and its process. In this sense, open access to recent aspects on the nanostructures application and properties can be reached in this book. Here, an interesting set of chapters gives opportunity of access texts that reach process and processing of nanostructures, applications of nanotechnology, advanced techniques to theoretical development. A broad set of nanostructures are here covered such as, nanocrystal, superficial nanograins, inner microstructures with nanograins, nanoaggregates, nanoshells, nanotubes, nanoflowers, nanoroad, nanosheets, Also, reveals new investigations areas as grainboundary of nanograins in ceramics and metals. A great number of software has been used as a tool of development of Science and Technologies for nanotechnology COMSOL Multiphysics 5.2. Phenomena and properties has been investigated by recent or classical techniques of materials characterization as Localized Surface Plasmon Resonance (LSPR), X-ray photoelectron spectroscopy (XPS), Field Emission Gun Scanning Electron Microscopy (FEG-SEM) with Energy Dispersive Spectroscopy (EDS), Raman Scattering Spectroscopy (RSS), X ray diffraction (XRD), ^{57}Fe Mössbauer spectroscopy, UV-vis spectroscopy, dynamic light scattering (DLS), Atomic Force Microscopy (AFM), and Field Emission Gun Scanning Electron Microscopy (FEG-SEM). In this sense, collections of spectra from Mössbauer spectroscopy, UV-vis spectroscopy and Infrared spectroscopy can be found. As a matter of fact, some chapter’s item can be seemed as specific protocols for synthesis, preparations and measurements in the nanotechnology.

I hope you enjoy your reading.

Prof. Dr. Marcos Augusto Lima Nobre

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CHAPTER 2

EFFECTS OF DIFFERENT ASPECT RATIOS AND JUNCTION LENGTHS ON THE COUPLED PLASMON GOLD NANOROD DIMERS

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ABSTRACT: We have explored the optical behaviour in dimmer of gold nanorod (AuNR) bridge by thin silica cylinder to sub-nanometre regime. To probe this model, Computational simulations were carried out to investigate the nanorod surface which was divided into small tetrahedral mesh with finer size. Furthermore, perfectly matched layer (PML) around the nanorod surface was applied to avoid any reflection artifacts on the simulation. The amplitude of the background oscillating field was one (1) Vm^{-1}. Our results reveal that an increase in aspect ratio causes a red shift in dimer connected mode, leading to significantly higher sensitivity 717 nm/RIU and figure of merit 16.9 compared to a single dimer having 300 nm/RIU sensitivity with similar dimensions. These findings suggest that using end to end

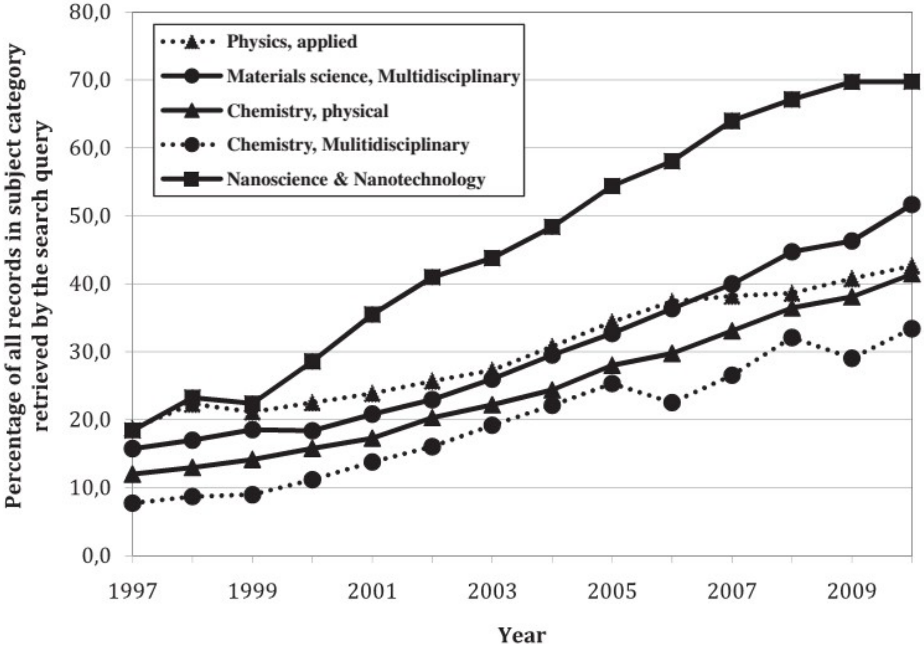
linked nanoscale structures could significantly play an important role in tuning far field spectral responses of plasmonic metal nanostructures for applications in LSPR sensing.

KEYWORDS: AuNR dimer. Figure of merit. Bulk Sensitivity. Perfectly matched layer.

1 INTRODUCTION

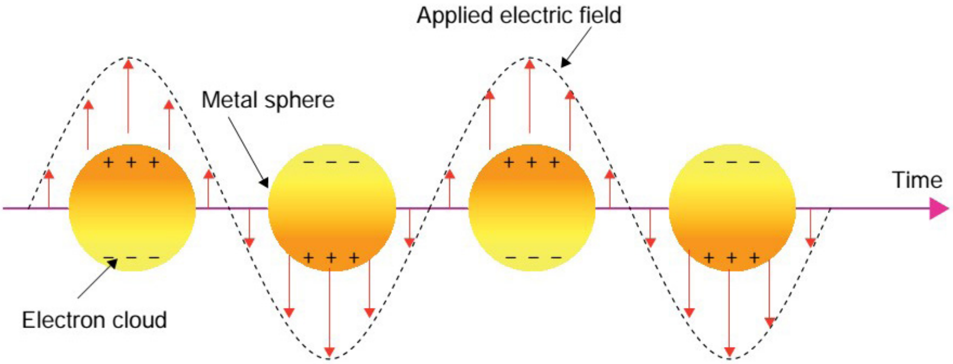
Modern civilization growth relies upon three pillars: materials, energy sources and information technology. Out of these three resources, materials are the basis for advancement in energy and information technology (Zhang et al., 2018). In past, each era was named after the material most dominant at that time e.g., Stone age, Bronze age, Iron age, polymer age etc. Thus, present era can be attributed as the Nanomaterial age. Nanotechnology is the study of the behavior of objects which fall between 10^{-9} to 10^{-6} meters regime (roughly 1 nm to 100 nm) (Grieneisen et al., 2011). When matter is reduced from its bulk to nanoscale, high surface-to-volume ratio, a key parameter of nanostructure plays a significant role to explore the novel and intriguing properties of the nanoparticles begin to emerge. Arguably "beginning" with the discovery of fullerenes, the last three decades have seen an expeditious investigation in nanoscience (Kroto et al., 1985). Due to the technology advancement in synthesis, control, and characterization of materials, the field of nanotechnology has seen tremendous growth. A brief description of rapidly growing field of nanotechnology in last decade is illustrated in Figure 1.

Figure. 1 - Graph displaying the proliferation of journals in the field of "nanoscience and nanotechnology" over the last decade. (Source: Adapted from (Grieneisen & Zhang, 2011).



As the name implies, nanoplasmonics is the study of plasmon resonance that occurs within nanostructures. In brief, the free electrons in a metal can be excited by the presence of an external electromagnetic (EM) field. This EM field displaces the electrons from their neutral orientation with respect to the fixed positive nuclei, and the resulting coulombic restorative force causes the electron cloud to oscillate at the system's natural frequency as a result of collective oscillations of the conduction electrons (Non-Propagating) prompted by electromagnetic radiation having a pertinent wavelength which is referred as Localized Surface Plasmon Resonance (LSPR) as depicted in Figure 2.

Figure. 2 - Schametic representation of the interacion of EM radiation and matellic nanostructure. (Source: Adapted from Zalevsky, Z. & Abdulhalim 2010).



Plasmonic nanostructures strongly interact with light resulting in size-dependent scattering, absorption and large enhancement in near electric field. These optical mechanisms of nanoscale particles have led to remarkable potential applications. A plethora of studies reveal that plasmonic properties of the metallic nanostructures have been demonstrated by controlling the geometry (size, shape), composition and the refractive index of their surrounding medium (Farooq and Araujo, 2018, Kelly *et al.,* 2003).

The spectrum of LSPR excitations have been the subject of intensive research efforts and encourage researchers to synthesize the growth of complex shapes nanostructures such as nanoshells, nanorice, nanocages, nanostars, nanorods and nanopyramids (Lee et al*.,* 2009), which shows plasmon peaks in various spectral regions.

Moreover, gold nanostructures are increasingly receiving attention as an important starting point for label-free sensing. LSPR sensors can be explored as fast, reliable, cheap and fairly facile tool for medical diagnosis. Various examples of LSPR biosensors were attributed to the diagnosis of relevant medical disease, as Alzheimer (Haes et al., 2005), preeclampsia (Hammond et al, 2005), influenza (Takemura et al., 2017) Dengue virus (Camara et al., 2013) and Candida albicans (Farooq et al., 2018) as well as for intracellular protein sensing (Jain et al., 2006).

El-Sayed and coworkers have theoretically suggested the use of coupled gold nanostructures for sensing (Hong et al., 2014). Several structural aspects of a nanochain rules the plasmonic features of coupled gold nanorods. Moreover, Pramod et al have investigated the effects of molecular link orientation on the optical properties of gold nanorod (AuNR) dimers (Pramod et al., 2008).

The basis of plasmonic sensors is the resonant coupling between the oscillations of free electrons, called plasmons, and incident visible light waves. By confining these oscillations within a nanostructure, the coupling efficiency is enhanced by the creation of LSPR states.

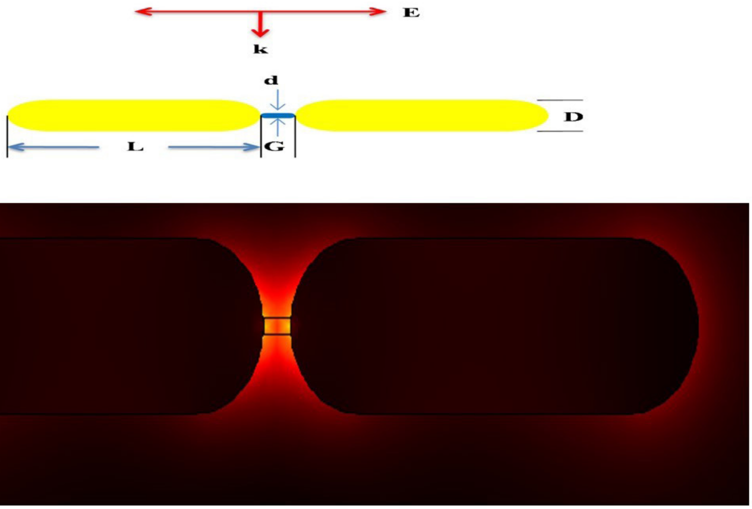
In this study, we evaluate the use of gold nanorod dimer as a sensing platform. Analyses of LSPR behavior of gold nanorod dimers, connected with silica nano-cylinder, with several aspect ratios and silica junction thickness, were investigated. In this work, crucial parameters that govern the LSPR molecular sensor performance, in particular figure of merit and bulk sensitivity was evaluated. Moreover, this work provides insights on the LSPR behavior due to embedding AuNR dimer in several surrounding media.

The performance of gold nanorod (AuNR) dimer linked end-to-end by thin dielectric junction, as a sensor platform has been investigated. Three-dimensional finite element simulations (COMSOL Multiphysics) in frequency domain were carried out to study the influence of local environment on the optical features of AuNR dimer, with different junction lengths and aspect ratios. This computational approach focused on understanding the LSPR spectral peak position and spatial distribution of electromagnetic field enhancement near the surface of individual gold nanorod dimer, in order to reveal the behavior of crucial parameters such as figure of merit and bulk sensitivity, which predicts the LSPR sensor performance. We find the plasmon peak position of end-to-end connected Au nanorod dimer exhibited red shift by at least 60 nm from single Au nanorod. The simulations reveal that silica linked dimer of gold nanorod sensing platform shows higher sensitivity (717 nm/RIU) as compared to individual gold nanorod. We observed that silica bridge dimer also exhibits a high figure of merit value, up to 16.9. Our proposed model put forth a new paradigm in LSPR based sensing applications.

2 SIMULATED MODEL ANALYSES

Finite Element Method (FEM) calculations were used to predict the plasmonic properties of the gold nanorod (AuNR) dimers which are linked with a thin silica cylinder. In the 3D simulations, the AuNR dimer surface was divided into small tetrahedral mesh elements with size‘extremely fine’. The dimers were modeled as shown in Figure. 3. The plasmonic dimers consist of two hemispherically-capped cylinders forming the gold nanorod (AuNRs) dimer with length = L, diameter = D and connected by a silica cylinder (length =G, diameter = d).

Figure. 3. 3D simulations model region composed of model nanostructure in embedding medium and PML layers.



The nanostructures geometry consisting of hemispherical caped cylinders of AuNR and linked through a silica cylinder. The plasmonic structure was probed by linearly polarized light along the long axis of dimer. Furthermore, perfectly matched layer (PML) around the nanoparticle was used to avoid any kind of reflection artifacts on the simulations. We have performed a plane wave electromagnetic field for the numerical model analysis using COMSOL Multiphysics software, Electromagnetic Waves and Frequency Domain interface, where the Electric field within the domain explores Maxwell's equations. The radius and thickness of the PML spheres were chosen, depending on the NPs diameter, such that further NPs size variations would not influence the simulation results as well as minimizing the reflection effects. To simulate the probe model, a background electric field $1\ Vm^{-1}$ was applied. The data of the metal dielectric functions (real and imaginary) for Au were obtained from Johnson and Christy (Johnson et al., 1972). To investigate which metal nanostructures is a good candidate for bio or chemical sensing applications as well as their efficiency can be characterized by measuring their RI based sensitivity. Bulk sensitivity (η_b), A sensing parameter which qualitatively analyse the sensing efficiency and correlates the change in LSPR wavelength as function of varying refractive index of the surrounding medium has been evaluated i.e: $\eta_b = \Delta\lambda LSPR / \Delta n$.Figure of Merit (FoM) is second analytical parameter which elucidate well sensor reliability by, FoM = $\eta_b / FWHM$, where (FWHM) is full width at half maximum or line width of the LSPR peak (Mahmood et al., 2019).

2.1 BULK SENSITIVITY

Sensitivity is one of the important parameters to characterize a sensor. For LSPR based sensors, bulk sensitivity is termed as the variation of LSPR peak position with respect to the change in RI unit (RIU) of the medium, and its unit is eV/RIU or nm/RIU (Farooq, and Araujo 2018). The most commonly employed equation for refractive index (RI) based sensitivity or bulk sensitivity can be written as:

$$\eta_B = \frac{\Delta\lambda}{\Delta n} \qquad (1)$$

where η_B represents bulk sensitivity, while $\Delta\lambda$ and Δn are respectively, Shift in LSPR peak wavelength and the refractive index change of a medium.

2.2 FIGURE OF MERIT

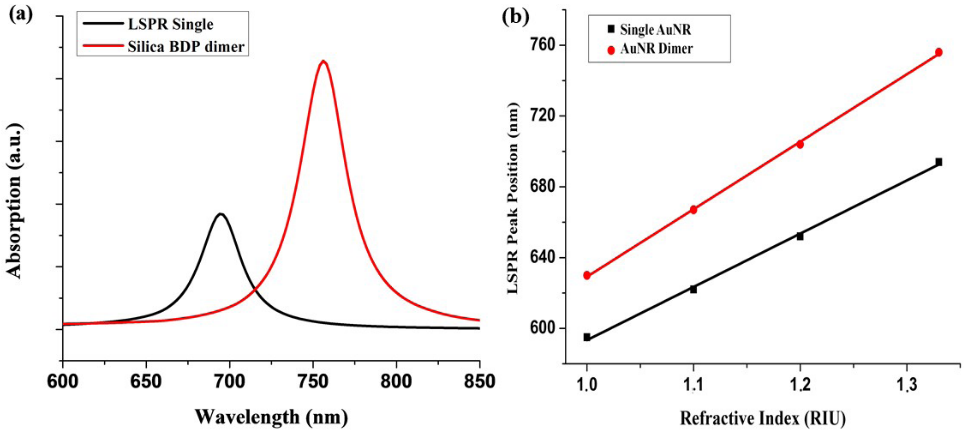
Sensing performance can also be evaluated by exploring the Figure of Merit (*FoM*) factor. The *FoM* is defined as the ratio of bulk sensitivity to the full width at half maximum (FWHM) (Farooq, and Araujo 2018), and is expressed as:

$$FoM = \eta_B / FWHM \qquad (2)$$

3 RESULTS AND DISCUSSIONS

The LSPR peak shift of single AuNR and silica connected AuNR dimer in various surrounding mediums with different RI values are presented in Figure. 4. LSPR peak position is linearly dependent on the variations of the surrounding medium RI,as shown in Figure.4 for Au single rod and AuNR dimer. For gold dimer bridged by silica cylinder having length G = 2 nm and thickness d= 1 nm, LSPR peak position can shift from 630 to 756 nm with RI increasing from 1.0 to 1.33, as depicted in Figure 4.

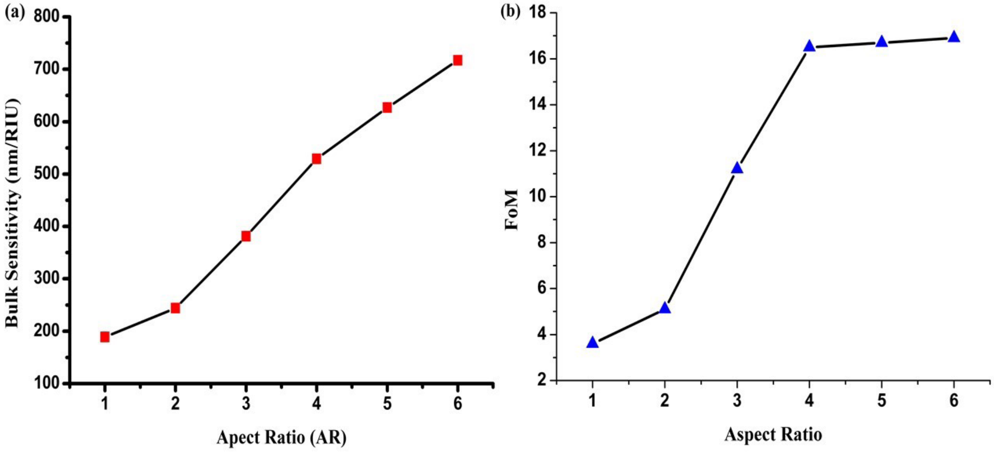
Figure. 4. LSPR peak shift of single AuNR and AuNR dimer connected with silica cylineder on changing the the refractive index of the surrounding Medium.



Numerical values for the bulk sensitivity of AuNR dimer were identified as 381 nm/RIU, which is higher than single nanorod value (300 nm/RIU). The AuNR dimer also presents a higher figure of merit (11.7) after linked by silica cylinder with appropriate aspect ratio (AR = 3).

As depicted in Figure. 5a, the aspect ratio of silica linked AuNR dimer increase, the bulk sensitivity of gold nanostructures enhances accordingly. The higher value of bulk sensitivity obtained at aspect ratio 6 (L = 30 nm, D = 5 nm), and the lower value at aspect ratio 1.

Fiure. 5. The bulk sensitivity (a) and FoM (b) of AuNR dimer with various aspect ratios, keeping constant silica connection length (G = 1 nm) and thickness (d = 1 nm).



Therefore, FoM of AuNR dimer also varies as a function of aspect ratio as shown in Figure 5b. The maximum value of FoM calculated in this work is 16.9, for aspect ratio equals to 6. This calculated value of FoM (16.9) of gold rod dimer is higher than the reported values of several nanostructures with different shapes, such as Au nanaorod (1.3) (Mayer et al, 2008), Au nanosphere (1.5) (Underwood and Mulvaney, 1994), Au nano-cresent (2.4) (Bukasov, and Shumaker-Parry, 2007), Au nanoshells (0.9) [14], Au bipyramide (4.5) (Burgin and Guyot-Sionnest, 2008) and Ag Nanoplate (2.5). Table 1 indicates the figure of merit and bulk sensitivity of different nanostructures (ensemble).

Table 1. The survey of bulk sensitivity and figure of merit of plasmonic nanostructures of various shapes

Nanostructures	Types	η_B (nm/RIU)	FoM	References
Au NR-dimer	---	717	16.9	Calculated
Au Nanoshells	Ensemble	314	0.9	Pramod et al, 2008

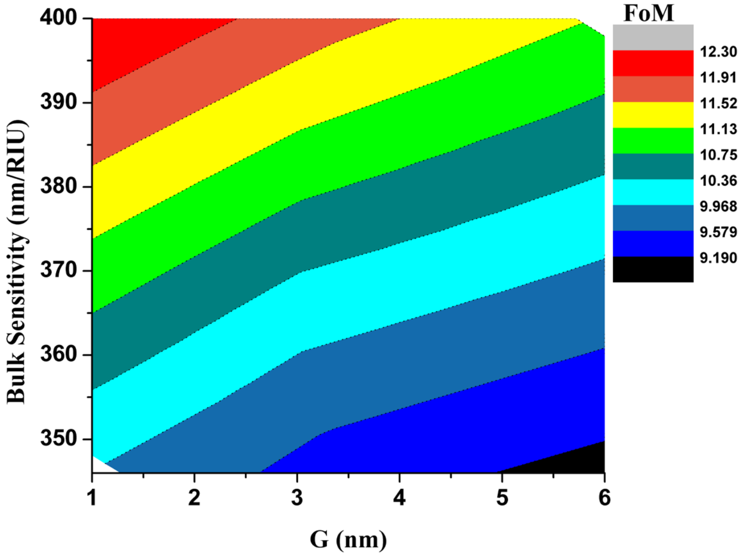
Nanostructures	Types	η_B (nm/RIU)	FoM	References
Au Nanospheres	Ensemble	90	1.5	Mulvaney et al, 1994
Au Nanorods	Ensemble	170	1.3	Mayer et al., 2008
Au Nano-Cresent	Ensemble	596	2.4	Bukasov et al, 2007
Au bipyramid	Ensemble	352	4.5	Burgin et al, 2008
Ag Nanoplate	Ensemble	406	2.5	Farooq et al., 2018

The FWHM of gold dimer spectrum is not so affected by increasing the aspect ratios, as compared to other ensemble shapes like spheres, shells etc. However, varying the AuNR aspect ratios of gold dimer can also affect the FoM due to change in radiation damping. Therefore, the FoM response of AuNR dimer is mainly dependent on the variations in bulk sensitivity and FWHM.

The impact of silica nano-cylinder junction length (G), connecting end-to-end gold nanorods, on the bulk sensitivity and FoM can be observed in fig 4. AuNR dimers with silica junction lengths from 1 to 5 nm were analyzed.

As silica linked cylinder length increases, the sensitivity and FoM of the nanostructured platform reduces. As FWHM of gold dimer spectrum is not so affected by the junction length FoM and bulk sensitivity presents similar behavior, as shown in Figure 6.

Figure.6. The bulk sensitivity and FoM of 30nmx10nm AuNR dimer as a function of silica nano-cylinder with different lengths (G); L= 30nm; D=10nm and d = 1 nm.



The higher FoM and sensitivity values were obtained for 1 nm junction length, Which was 12.25 and 397 nm/RIU respectively.

4 CONCLUSION

Localized Surface Plasmon Resonance phenomenon can drive the development of low-cost and accurate sensing. The establishment of high performance AuNR dimer LSPR sensor requires the description of sensing parameters (sensitivity and FoM) as a function of the AuNR aspect ratios and silica connection length.

The obtained computational results present a potential of the bulk sensitivity and FoM as function of the AuNR dimer connected end-to-end by silica nano-cylinder. By tuning the dimer aspect ratio from 1 to 6, substantial bulk sensitivity (717 nm/RIU) was obtained by embedding the nanostructure into several media. Moreover, higher FoM (16.9) was achieved by keeping the dimer aspect ratio 6.

Besides, the approach used in this work provides insight on the dimer LSPR behavior due to tuning the NR aspect ratio and silica junction length, establishing a new paradigm for engineering LSPR based sensor. The proposed approached can be extended to engineer an efficient and precise nanoscale sensor in molecular biosensing.

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