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Tailoring Plasmonic Properties of Silica-Coated Gold and Silver Nanostructures

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ABSTRACT

The performance of plasmonic sensors is primarily determined by two critical factors: the bulk refractive index sensitivity (RIS) and the linewidth (or full-width at half maximum, FWHM) of the localized surface plasmon resonance (LSPR) peak. To achieve optimal sensor functionality, it is essential to maximize RIS while maintaining a narrow resonance spectrum. These parameters are often collectively assessed using the product RIS and FoM, where FoM (figure of merit) is defined as RIS/FWHM. While complex plasmonic nanostructures are widely recognized for their high sensitivity, they frequently suffer from broad LSPR peaks, which can compromise detection limits. In this research, we utilized full-wave electromagnetic analysis, grounded in Mie theory, to model dielectric-shell/metal-core nanoshells—specifically Au coated SiO_2 and Ag coated SiO—as effective LSPR sensors. By optimizing the nanoshells' geometry, we calculated the highest RIS × FoM values, obtaining ~479 nm/RIU² for Ag coated SiO and ~364 nm/RIU² for Au coated SiO_2. Our findings indicate that this multilayer core-shell design can be extended to other material systems, enabling the development of plasmonic sensors with improved accuracy, stability, and sensitivity across a wide spectral range.

Keywords- Localized Surface Plasmon Resonance, Bulk Sensitivity (RIS), Figure Of Merit (FoM)

Introduction

Over the past two decades, researchers have extensively investigated how nanoparticle geometry and composition influence their optical behavior. When light strikes noble-metal nanostructures, it can excite localized surface plasmon resonances (LSPR)—these are collective oscillations of conduction electrons driven

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by electromagnetic waves at particular wavelengths. (Farooq et al., 2023b) The wavelength of LSPR is closely associated with nanoparticle characteristics such as shape, size, and metal type, which in turn govern optical phenomena like absorption, scattering, and extinction, and make them useful for biosensing applications. (Saylan et al., 2019)

Plasmonic nanostructures remain integral to chemical and biological sensing platforms due to their unique optical properties. In LSPR-based sensing, these metallic nanostructures enhance localized electromagnetic fields, significantly boosting detection sensitivity. (Farooq et al., 2018) Two critical parameters for evaluating these sensors are the bulk refractive index sensitivity (RIS), measured as the shift in the plasmon peak per unit change in refractive index ($\Delta\lambda LSPR/\Delta n$), and the Figure of Merit (FOM), calculated as the ratio of RIS to the full width at half maximum (FWHM) of the plasmon peak. (Mahmood, 2019)

Since the resonant wavelengths of Localized Surface Plasmon Resonance (LSPR) shift in response to variations in the surrounding dielectric environment, it is crucial to optimize the geometry and composition of nanoparticles to fine-tune sensor performance. (Farooq et al., 2023b) For instance, nanostructures with sharper edges or specific shapes—such as rods, stars, or triangular prisms—tend to exhibit greater sensitivity and narrower resonance peaks, which enhance their Figure of Merit (FOM). Consequently, achieving high-performing LSPR sensors depends on balancing strong bulk sensitivity with sharp resonance characteristics. (Farooq et al., 2023a)

Moreover, theoretical studies have examined Au/Ag nanoshells—typically consisting of a gold–silver core coated with a silica shell whose thickness can be varied at the nanoscale—to explore how this architecture affects optical tunability via surface plasmon resonance (SPR). These simulations were conducted using the Finite Element Method (FEM) implemented in COMSOL Multiphysics, a commercial software platform that solves Maxwell's equations to accurately predict electromagnetic properties and local electric field distributions around core–shell nanostructures (Mahmood et al., 2019).

To determine the scattered field distribution and extinction cross section, the nanoaggregates surface was divided into extremely small mesh elements up to finer

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size. The amplitude was fixed 1 Vm^{-1} for background field oscillations. A hindrance was created in shape of perfectly matched layer around the nanostructure to limit the simulation from any reflection.

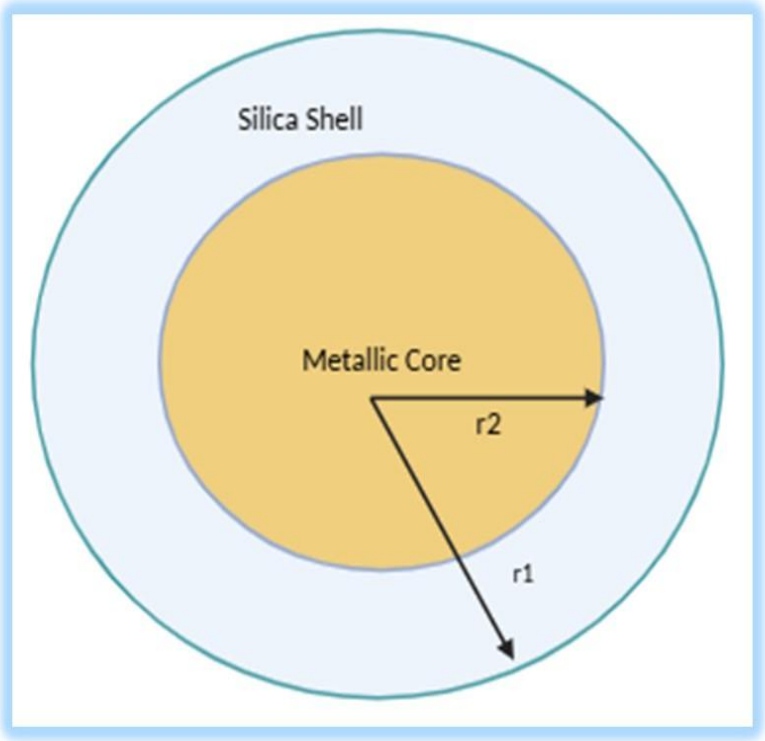


Figure. 1: Schematic Diagram

Figure 1 depicts the schematic geometry of the Au/Ag silica-coated nanoshell investigated in this study. The innermost region is identified as the core, characterized by a radius (r1) and a dielectric function epsilon. The surrounding layer represents the shell, with a radius (r2) and a dielectric function (epsilon_d), where the shell thickness is defined as (t = r2 – r1).

Mathematical Modelling

The interaction between the core-shell metallic nanostructures and electromagnetic radiation in this work is described using Mie theory, which provides a comprehensive solution to Maxwell's equations under appropriate boundary conditions. (Kiran et al., 2022a)

The basic model for the electronic properties of a metal is the Drude model, based on the classical description which makes the approximation of a free electron gas/plasma that moves within a crystalline lattice of fixed positive nuclei of a metal.

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The dielectric function for a free electron is:

$$\varepsilon = 1 - \frac{\omega_p^2}{\omega^2 + i\gamma\omega} \quad (1)$$

With real and imaginary parts:

$$\varepsilon_{real} = 1 - \frac{\omega_p^2}{\omega^2 + \gamma^2} \quad (2)$$

$$\varepsilon_{img} = 1 - \frac{\omega_p^2 \gamma}{\omega(\omega^2 + \gamma^2)} \quad (3)$$

The Drude model, as described by Bohren & Huffman (1983), explains the optical behavior of free electrons in metals. When a metal is subjected to an external electromagnetic field, the resulting non-uniform charge distribution generates an internal electric field. This field induces oscillations, exerting a force on the electron plasma and causing it to shift away from its original uniform equilibrium position. The electric field set up due to the displacement of electron plasma can be expressed by means of Gauss's Law in eq. (4):

$$E = \frac{-\rho x e}{\varepsilon_0} \quad (4)$$

Where 'ρ' is the free electron density, 'x' is the displacement from mean equilibrium position, 'e' charge on an electron and 'ε_0' is the permittivity of free space. As aforementioned, the 'E' exerts a force on free electron gas/plasma yields E.e. By comparing this relation 'E.e' with Newton's 2nd law can be written as:

$$E.e = m_e \cdot \frac{\partial^2 x}{\partial t^2} \quad (5)$$

Here m_e is the effective mass of an electron. By putting the eq. (4) in eq. (5) implies that:

$$\frac{-\rho x e^2}{\varepsilon_0} = m_e \cdot \frac{\partial^2 x}{\partial t^2} \quad (6)$$

$$\frac{\partial^2 x}{\partial t^2} + \frac{\rho x e^2}{\varepsilon_0 m_e} = 0 \quad (7)$$

$$\frac{\partial^2 x}{\partial t^2} + \omega^2 x = 0 \quad (8)$$

After substitution Eq. (8) takes the form of simple harmonic oscillator. It is clear from the comparison of eq. (7) and eq. (8), the natural frequency at which the free electrons in a metal will naturally oscillate, called the plasma frequency 'ω_p', can be

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determined as particularly expressed in eq. (9):

$$\omega_p = \sqrt{\frac{\rho e^2}{\varepsilon_0 m_e}} \quad (9)$$

When light strikes a metal, the electron plasma within the material exhibits long-range correlations, leading to collective oscillations driven by Coulomb forces. This phenomenon is known as plasma oscillation (Bohren & Huffman, 1983). The frequency of these oscillations is specific to plasmons present in the bulk material. For metals, this frequency typically lies within the visible and ultraviolet regions of the electromagnetic spectrum, ranging approximately from 3 eV to 20 eV (Bohren & Huffman, 1983).

Results and Discussion

In this studied model, our primary objective is to optimize the figure of merit by adjusting the refractive index (RI) of the surrounding medium. Despite their relatively simple core-shell structure, these metallic nanostructures demonstrate significant refractive index tunability, driven by their localized surface plasmon resonance (LSPR) effect. (Mahmood et al., 2021) Figures 2 & 3 illustrate the behavior of the LSPR wavelength (λ_{LSPR}) and the extinction spectra of metallic core/dielectric shell nanoparticles in response to changes in the refractive index of the adjacent medium. For both nanostructures, variations in the RI lead to notable shifts in the extinction spectra within the visible range, accompanied by pronounced red shifts. These shifts are clearly associated with an increase in the intensity of the extinction peaks.(Yasmeen et al., 2024)

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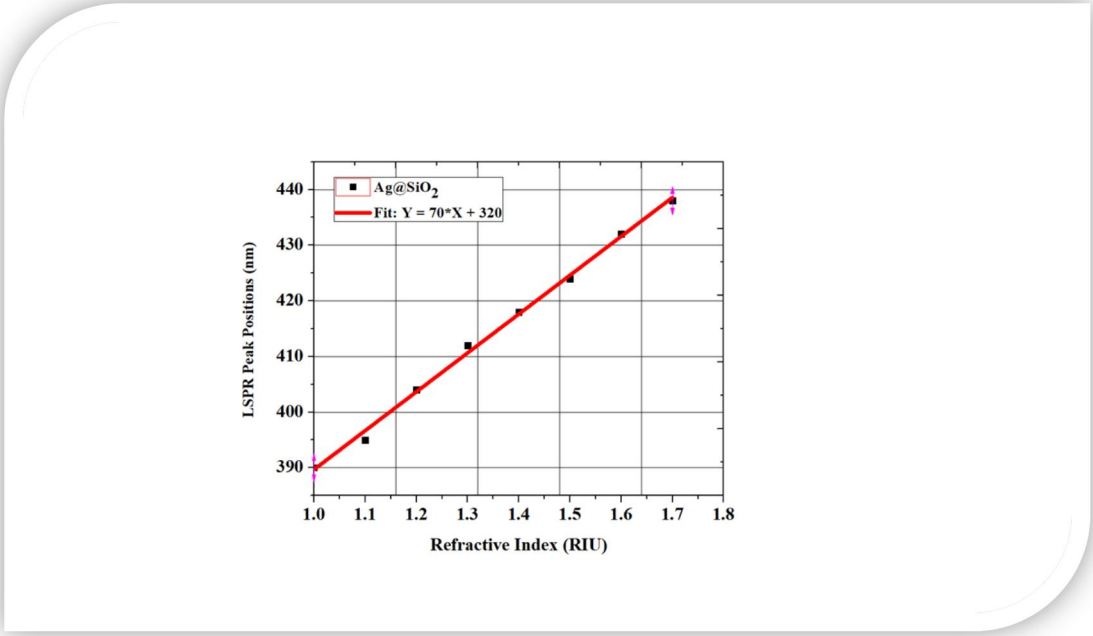


Figure. 2: The LSPR extinction of Ag

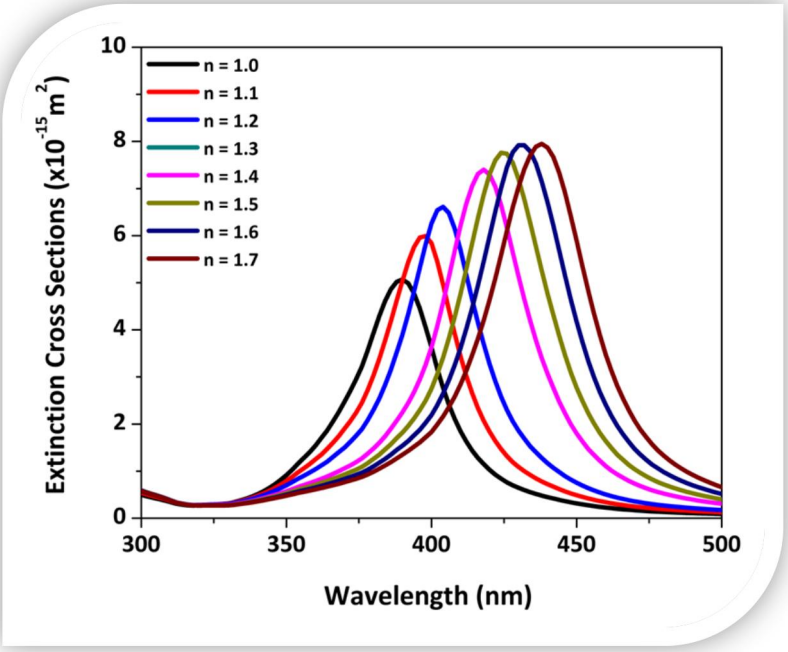


Figure. 3: The LSPR Extinction of Ag

For Au coated SiO_2 nanoshells, the extinction spectrum gradually moves toward longer wavelengths within the visible range, with the resonance peak reaching

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around 540 nm. On the other hand, Ag coated SiO_2 nanoshells first exhibit a blue shift into the near-UV region before stabilizing at approximately 430 nm in the visible spectrum.(Shad et al., 2024) Figure 4 depict the electric field distributions linked to the dipole modes of the nanoshells. These field profiles were generated at the localized surface plasmon resonance (LSPR) wavelength specific to metal nanostructure. When exposed to linearly polarized light, the dipole resonance shows a field pattern with two distinct lobes, emphasizing the plasmonic dipole nature.(Shad et al., 2022)

The LSPR resonance wavelength is determined not just by the real part of the metal's dielectric function but also by the refractive index of the surrounding medium. In refractive-index-based LSPR sensing, bulk sensitivity refers to the degree of resonance peak shift in reaction to variations in the local refractive index. (Salman et al., 2025)

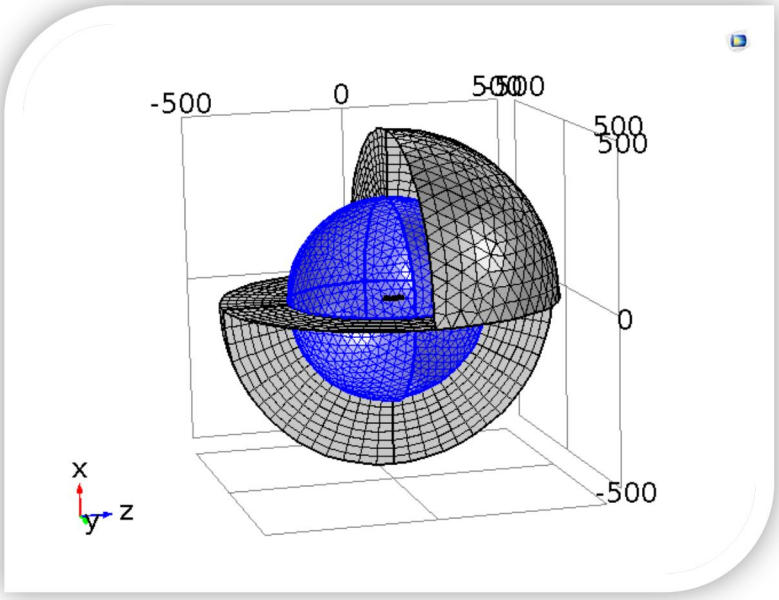


Figure. 4: Electric field profile for nanostructure in dielectric media

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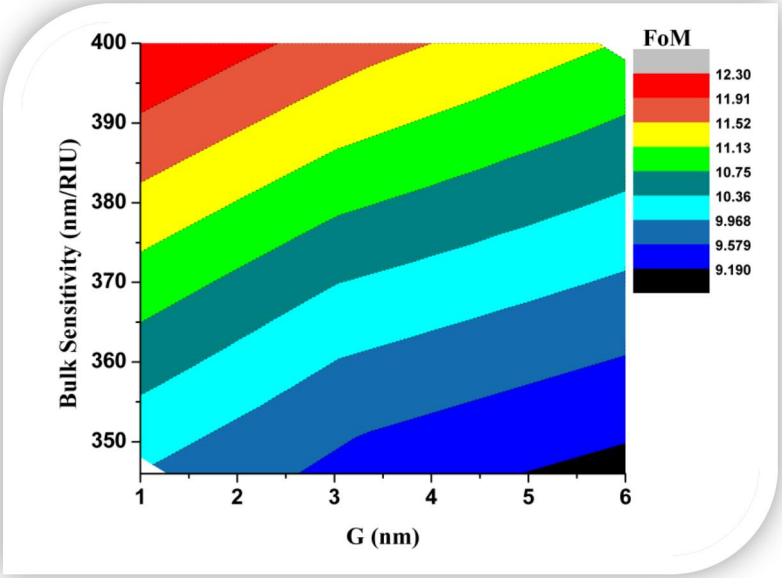


Figure. 5: The sensitivity of gold and silver nanoshells as a function of their respective silica shell thickness

Figure 5 illustrates the sensitivity response of the plasmonic sensor when the thickness of the Ag and Au cores is set at 30 nm, while the SiO2 shell radius is varied.(Kiran et al., 2022b) As anticipated, increasing the shell thickness leads to a reduction in sensitivity for both metallic cores, with the Ag nanoshell exhibiting a linear decrease. Based on the observed behavior of this structure, the Ag coated SiO_2 nanostructure appears to be more effective for high molecular sensing, particularly at smaller shell thicknesses (e.g., 5 nm), compared to the Au coated SiO_2 shell, making it a promising candidate for molecular biosensing applications. (Farooq et al., 2023c)

Conclusion

The sensing capabilities of a nanostructure featuring a metallic core (Au/Ag) coated with a SiO2 shell were examined, focusing on the RIS×FoM relationship, which quantifies sensing performance through the product of high bulk sensitivity and a sharp localized surface plasmon resonance (LSPR) spectrum. By utilizing the RIS×FoM parameter, the optimized performance of the LSPR sensor was determined, yielding values of 479 nm/RIU^2 for the silver (Ag) core and 364 nm/RIU^2 for the gold (Au) core, respectively.

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References

Farooq, S., Del-Valle, M., Dos Santos, M.O., Dos Santos, S.N., Bernardes, E.S., Zezell, D.M., 2023a. Rapid identification of breast cancer subtypes using micro-FTIR and machine learning methods. Appl. Opt. 62, C80–C87.

Farooq, S., Mahmood, H.Z., Rativa, D., Bouchonneau, N., Lins, E., Fontana, J., de Araujo, R.E., 2018. Optimizing gold nanorods dimer structure for sensing platform, in: 2018 SBFoton International Optics and Photonics Conference (SBFoton IOPC). IEEE, pp. 1–4.

Farooq, S., Rativa, D., De Araujo, R.E., 2023b. Quantitative Analysis of High Performance Plasmonic Metamolecules for Targeted Deep Tissues Applications. Plasmonics 18, 2475–2482. https://doi.org/10.1007/s11468-023-01960-4

Farooq, S., Rativa, D., Said, Z., Araujo, R.E.D., 2023c. High performance blended nanofluid based on gold nanorods chain for harvesting solar radiation. Appl. Therm. Eng. 218, 119212. https://doi.org/10.1016/j.applthermaleng.2022.119212

Kiran, I., Shad, N.A., Munir Sajid, M., Zeeshan Mahmood, H., Javed, Y., Hanif, M., Ali, R., Sarwar, M., Nosrati, H., Danafar, H., Sharma, Surender K., 2022a. Emerging Nanomaterials as Radio-Sensitizer in Radiotherapy, in: Sharma, Surender Kumar, Nosrati, H., Kavetskyy, T. (Eds.), Harnessing Materials for X-Ray Based Cancer Therapy and Imaging, Nanomedicine and Nanotoxicology. Springer International Publishing, Cham, pp. 59–75. https://doi.org/10.1007/978-3-031-04071-9_3

Kiran, I., Shad, N.A., Sajid, M.M., Mahmood, H.Z., Javed, Y., Sarwar, M., Nosrati, H., Danafar, H., Sharma, Surender K., 2022b. X-ray Triggered Photodynamic Therapy, in: Sharma, Surender Kumar, Nosrati, H., Kavetskyy, T. (Eds.), Harnessing Materials for X-Ray Based Cancer Therapy and Imaging, Nanomedicine and Nanotoxicology. Springer International Publishing, Cham, pp. 201–216. https://doi.org/10.1007/978-3-031-04071-9_7

MAHMOOD, H.Z., 2019. A study of metallic and polymeric nanostructure-solution based platforms for optical and chemical arbovirus biosensing.

Mahmood, H.Z., Farooq, S., Lins, E.C., 2019. Optimizing the Plasmonic Sensing of

Online ISSN 3007-3197
Print ISSN 3007-3189
http://amresearchreview.com/index.php/Journal/about

Silica Coated Au/Ag Nanoshells. Int J Sci Eng InvestigIJSEI 8, 140–145.

Mahmood, H.Z., Jilani, A., Farooq, S., Javed, Y., Jamil, Y., Iqbal, J., Ullah, S., Wageh, S., 2021. Plasmon-based label-free biosensor using gold nanosphere for dengue detection. Crystals 11, 1340.

Salman, M., Mahmood, Z., Akhtar, K., Muhammad, A.D., Tahir, W.S., Iqbal, M., Javeed, Y., 2025. Investigating the Effects of Cerium Doping on the Chemical and Optical Properties of Lanthanum Phosphate Nanoparticles. Kashf J. Multidiscip. Res. 2, 31–39.

Saylan, Y., Akgönüllü, S., Yavuz, H., Ünal, S., Denizli, A., 2019. Molecularly imprinted polymer based sensors for medical applications. Sensors 19, 1279.

Shad, N.A., Jameel, A., Sajid, M.M., Afzal, A.M., Javed, Y., Ullah, A., Asghar, A., Mehmood, Z., Kiran, I., Munawar, A., Qayyum, M.A., Sarwar, M., 2022. Fabrication of Spike-Like Spherical Iron Manganite Nanoparticles for the Augmented Photocatalytic Degradation of Methylene Blue Dye. J. Electron. Mater. 51, 900–909. https://doi.org/10.1007/s11664-021-09371-z

Shad, N.A., Rakha, A., Qayyum, M.A., Siddiqi, M.H., Mahmood, Z., Nazir, S., Khan, M.F., Sajid, M.M., Rehman, R.A., Riaz, A., 2024. Zn3 (VO4) 2/Bi2WO6 composite based versatile platform for cotinine sensing and latent fingerprints development by using multiple modalities. Mater. Sci. Eng. B 301, 117203.

Yasmeen, T., Ali, M., Hashmi, M.U., Hashmi, M.A., Mehmood, Z., 2024. A Comparative Study of Advanced Machine Learning Ensemble Techniques for Classification of Breast Cancer. J. Comput. Biomed. Inform. 8.