Theoretical Study of Zirconium Nitride Based Surface Plasmon Resonance Sensor

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Abstract: This investigation presents a rigorous computational evaluation of a Surface Plasmon Resonance (SPR) sensor architecture employing the Kretschmann configuration. Optical performance was characterized using the Transfer Matrix Method (TMM) via angular interrogation at a 633 nm excitation wavelength. The optimized design achieved an angular sensitivity of 193.50°/RIU, a detection accuracy of 0.59 deg.$^{-1}$, a quality factor of 114.3 RIU^{-1}, and a figure of merit of 191.18 RIU^{-1} within a refractive index interval of 1.33 to 1.35. To quantify analytical efficacy and selectivity, critical performance metrics including detection accuracy, quality factor, and figure of merit (FOM), were systematically assessed. These findings highlight the sensor's substantial potential for advanced biomedical diagnostics and offer significant contributions to the fields of materials science and plasmonic instrumentation.

Keywords: *Plasmon, Angular Sensitivity, Kretschmann Configuration, Transfer Matrix Method.*

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I. INTRODUCTION

Surface Plasmon Resonance (SPR) has emerged as a premier label-free optical detection technology for analyzing biomolecular interactions, valued for its ability to provide real-time, quantitative data on the binding affinities and kinetics of membrane proteins interacting with ligands [1]. In a standard SPR assay, a target ligand is immobilized onto a sensor surface while a fluidic analyte is introduced across it [2]. The underlying optical mechanism relies on polarized light passing through a high-refractive-index prism; upon undergoing total internal reflection, it generates an evanescent wave that penetrates an adjacent thin metal film. When the momentum of this evanescent wave matches that of the free electrons in the metal, it induces a resonant excitation of surface plasmon waves (SPWs) [3]. A photodetector tracks the intensity of the reflected light as a function of the incidence angle, revealing a sharp drop in intensity known as the SPR dip at the specific resonance angle where energy absorption occurs. Because this resonance angle is highly sensitive to localized shifts in the refractive index directly adjacent to the metal surface, binding events can be accurately monitored without the need for fluorescent or radioactive labels [4].

The practical application of this phenomenon evolved through two foundational optical setups. In 1968, Otto introduced a configuration that resonantly excited SPWs via attenuated total reflection, utilizing an evanescent field that coupled to a silver substrate across a narrow air gap [5]. While historically significant, commercial viability was achieved through the Kretschmann configuration, which simplified the architecture by depositing the thin silver film directly onto the glass substrate [6]. In this design, the light undergoes total internal reflection at the backside of the metal film, efficiently exciting the plasmons on the outer sensing layer. Ultimately, the performance of these sensors is dictated by their sensitivity—their capacity to detect minute changes within the sensing boundary layer—which, in conventional Kretschmann systems, remains heavily governed by the specific material composition and precise thickness of the incorporated metal film [7-9].

Alam et al. reported a Kretschmann-configured SPR architecture incorporating two-dimensional materials, specifically MXene and MoS_2 thin films, for dental tissue characterization. Their study demonstrated that a bilayer MXene structure coupled with a monolayer MoS_2 film produced optimal sensitivities of 91.460°/RIU for dentin, 83.219°/RIU for enamel, and 104.744°/RIU for cementum

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[10]. Kumar et al. developed a highly sensitive and selective SPR biosensor employing MoS_2 quantum dots for label-free glucose detection, achieving a linear response over the 0.5-10 mM range with a detection limit of 0.31 mM [11]. Similarly, Z. Wang proposed an SPR sensor based on a $MoSe_2/Zr_2CO_2$ heterostructure, in which optimization of the multilayer stack and prism configuration substantially improved plasmonic absorption, resulting in a sensitivity of 92.48°/RIU and an approximately eightfold enhancement in the figure of merit relative to conventional gold-film SPR sensors [12]. In another study, D. Wang et al. introduced an optimized SPR platform incorporating WS2-graphene hybrid nanosheets, which enhanced plasmonic interaction, biomolecular adsorption, and structural tunability. The reported multilayer design exhibited a sensitivity of 224°/RIU, a quality factor of 96.97 RIU^{-1}, and dual-resonance behavior, highlighting its considerable promise for biochemical sensing applications [13].

In this study, an SPR-based sensor is proposed over a refractive index range of 1.33–1.35. The reflectance profile, resonance angle, and associated sensitivity are theoretically evaluated using the Fresnel equations and the transfer matrix method within the MATLAB computational environment.

II. THEORETICAL MODELLING AND SPR SENSOR CONFIGURATION

➢ *Design Consideration*

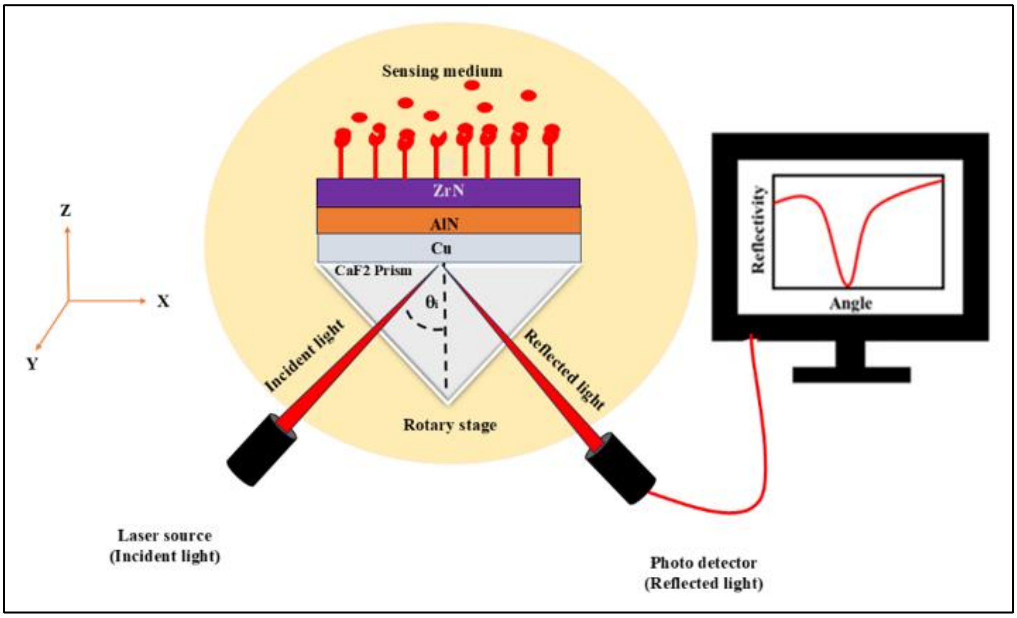

Fig 1 Proposed SPR Sensor.

The sensor utilizes the Kretschmann configuration shown in Figure 1 and is designed to maximize the Kerr response. Evaluation is performed at a wavelength of 633 nm, starting with a CaF_2 prism as the foundational layer, possessing a refractive index of 1.4329 [14] . The low-index prism promotes efficient optical coupling in line with Snell's law, thereby enhancing sensitivity. The subsequent coating is Cu with a complex refractive index of 0.5840 + 3.6466i, which supports the generation of surface plasmon polaritons. An AlN layer (n = 2.1496) is included to improve plasmonic mode confinement and further boost sensitivity [15-17]. Between the metal and the overlying two-dimensional (2D) material stack lies a zirconium nitride (ZrN) layer with a complex refractive index of 0.62 + 2.75293i [18-19].

➢ *Reflectivity:*

In the sensor's design and analysis, the transfer-matrix method (TMM) is employed as a highly accurate, model-independent technique to determine the device's reflectance magnitude. Surface plasmon wave (SPW) resonance occurs when the in-plane propagation constant of the SPW matches that of the incident p-polarized light. The p-polarized reflectance, Rp, of the structure is described by the standard transfer-matrix formulation [20].

$$Rp=\left|r_p\right|^2 \quad (1)$$

The variable r_p denotes the p-polarized reflection coefficient corresponding to the reflected wave within the N-layer stack, as defined by the following expression [21]:

$$r_p = \frac{(X_{11}+X_{12}Y_N)X_1-(X_{21}+X_{22}Y_N)}{(X_{11}+X_{12}Y_N)X_1+(X_{21}+X_{22}Y_N)} \quad (2)$$

➢ *Performance Parameter*

Evaluating surface plasmon resonance (SPR) sensor performance relies on key metrics such as sensitivity, the quality factor (Q), and measurement precision. Achieving optimal SPR sensor operation requires refining these performance indicators. Variations in the analyte's refractive index (RI) influence both the reflected signal intensity and the angular position of the SPR dip.

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$$\text{Sensitivity} = \frac{\Delta\theta_{res}}{\Delta n} \quad (3)$$

$$\text{DA} = \frac{1}{\text{FWHM}} \quad (4)$$

$$\text{QF} = \frac{\text{Sensitivity}}{\text{FWHM}} \quad (5)$$

$$\text{FoM} = \text{QF} \times (1 - R_{\min}) \quad (6)$$

III. RESULTS AND DISCUSSIONS

To get the sensor's high sensitivity, the RI of the coupling sensor should be low. CaF_2 is the best choice as a coupling prism. The prism with high RI provides a narrow resonance curve as compared to the lower RI prism, but other performance parameters, such as sensitivity, FWHM, resonance angle, and angular shift on the resonance curve are high for the lower RI prism. The flat end of the prism was coated with a 50-nm thick Cu film for a more significant quality factor and a deep SPR curve. The effect of having a variable number of AlN layers on top of the Cu film on the structure's sensitivity was investigated. A ZrN film of 0.53 nm was used to cover the AlN layer. The ZrN layer is selected due to a variety of reasons. It functions as a protective layer at room temperature, preventing Cu from oxidizing quickly and increasing the analyte's adsorption rates with the sensing medium.

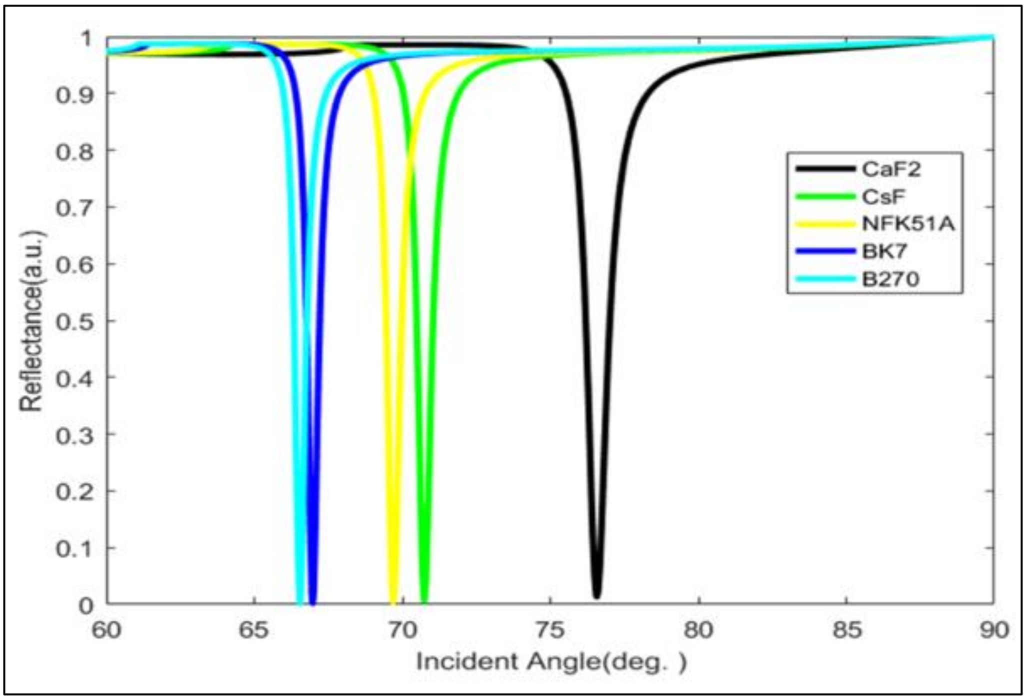

Fig 2 Reflectance vs. Incident Angle Curve for Different Prisms.

The simulation results presented in Figure 2 detail the reflectivity profile displacements across various glass prisms, specifically CaF_2, CsF, FK51A, BK7, and B270. Analysis indicates that the CaF_2 substrate facilitates the most significant displacement in the reflectivity profile while simultaneously achieving the minimum reflectance (R_{min}). To optimize biosensor resolution and responsiveness, it is imperative to minimize R_{min} toward zero, thereby ensuring the efficient transfer of p-polarized energy to surface plasmons and maximizing overall device efficacy. A primary objective of this study was the optimization of the copper (Cu) thin-film thickness through iterative computational modeling. Resonance is achieved when the incident wave vector matches the propagation constant at the interface, and refinement was conducted by targeting the absolute minimum reflectance at this state. It was observed that exceeding the optimal thickness results in an increased Rmin, indicating suboptimal surface plasmon activation. As demonstrated in Figure 3, Rmin reaches at a Cu thickness of 50 nm, beyond which reflectance begins to rise. Consequently, a 50 nm Cu film was identified as the ideal thickness, yielding an Rmin of 0.002 and a sensitivity of 193.50°/RIU. Comparative analysis of three distinct surface plasmon resonance (SPR) architectures was conducted, as illustrated in Figures 4a–c. Configuration-1, a conventional CaF_2/Cu structure, exhibited a resonance angle shift of 3.5° and an angular sensitivity of 152.50° RIU^{-1}, providing a baseline level of performance. To improve chemical stability and biomolecule affinity, Configuration-2 incorporated an Aluminum Nitride (AlN) passivation layer over the Cu film. This modification resulted in a resonance displacement of 3.75° and an improved sensitivity of 187.50° RIU^{-1}. Further enhancement was realized in Configuration-3 through the addition of a Zirconium Nitride (ZrN) layer. This composite architecture (CaF_2/Cu/AlN/ZrN) achieved a superior resonance angle displacement of 3.87° and a peak angular sensitivity of 193.50° RIU^{-1}. Based on these performance metrics, Configuration-3 is designated as the optimal design for high-sensitivity SPR sensing applications.

Table1. Performance Parameter of Various SPR Sensors.

Sr. No.	Device Structure	Sensitivity (°RIU^{-1})	DA ($deg.^{-1}$)	QF (RIU^{-1})	FoM(RIU^{-1})
1.	Prism+ Cu+ SM	152.50	0.99	150.99	50.83
2.	Prism+ Cu +AlN +SM	187.50	0.60	113.63	113.40
3.	Prism+ Cu +AlN +ZrN +SM	193.50	0.59	114.49	114.26

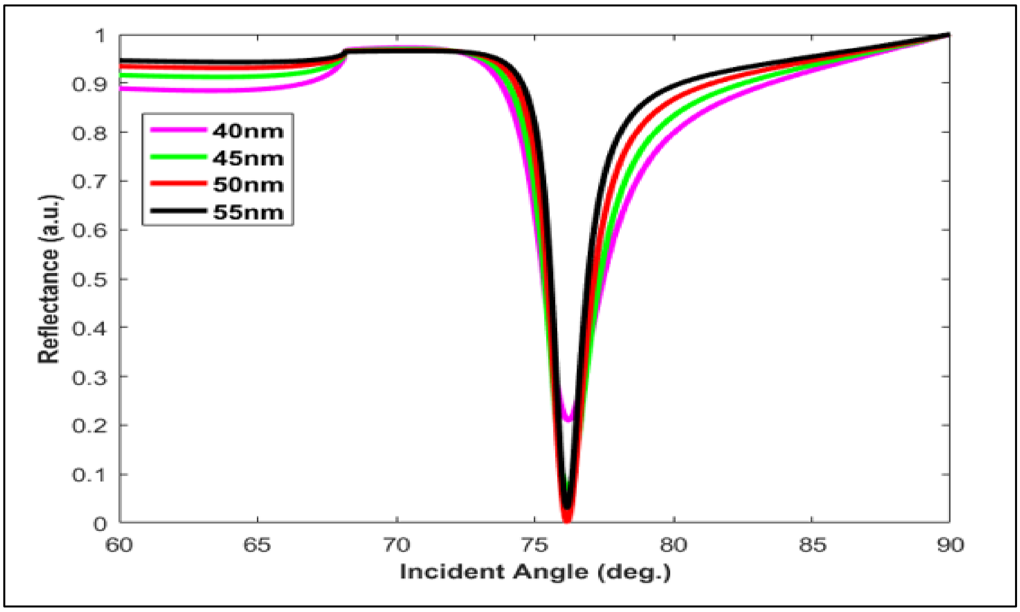

Fig 3 Metal Layer Thickness Optimization.

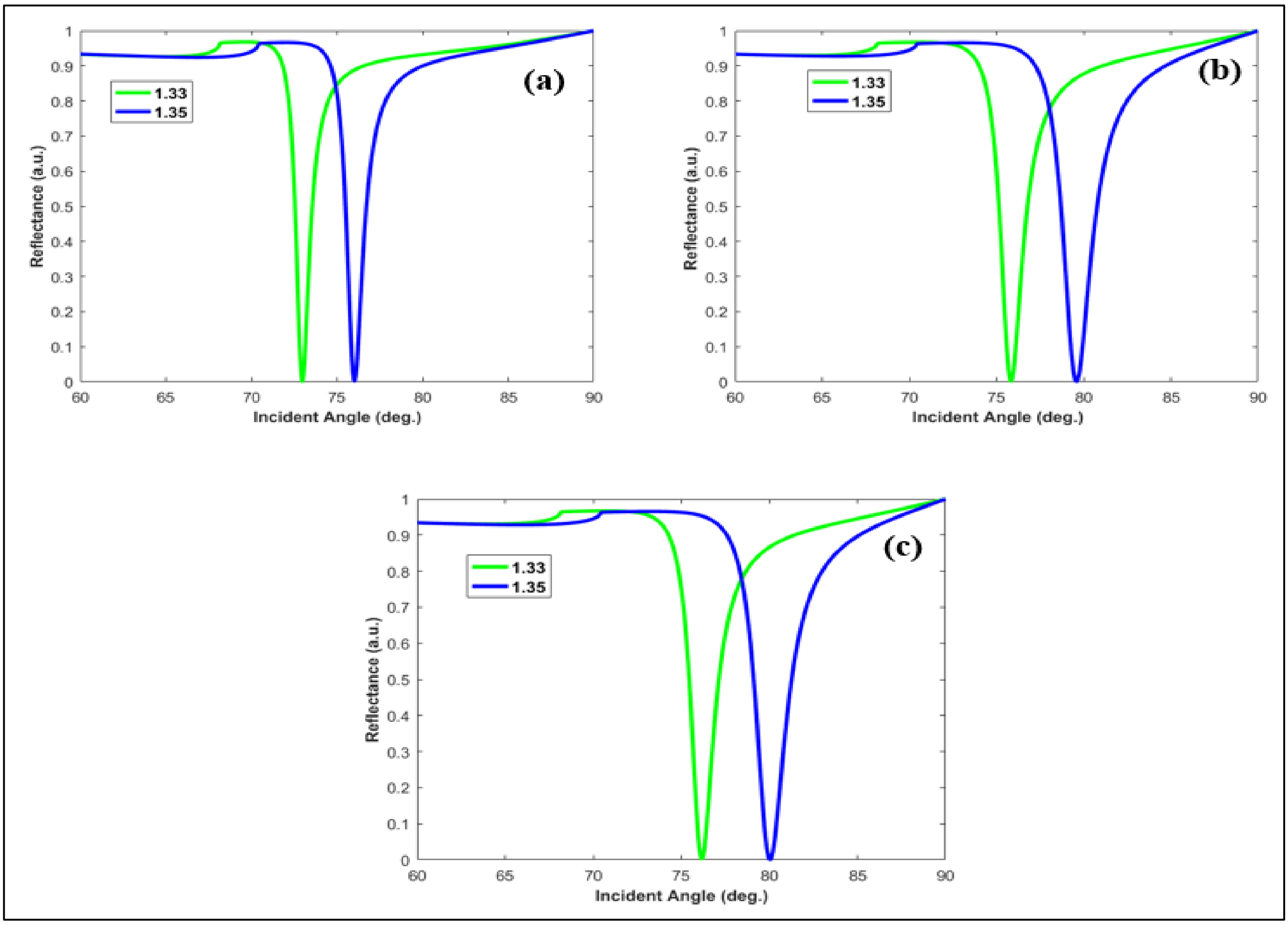

Fig 4 Performance Parameter of Various Proposed SPR Sensor.

IV. CONCLUSION

This research presents an innovative biosensor designed. The sensor structure was systematically optimized using the Transfer Matrix Method (TMM) within a MATLAB-based simulation framework. The optimization process focused on reducing reflectance and enhancing sensitivity through careful adjustment of the prism and silver layer thicknesses. The finalized design demonstrated an angular sensitivity of 193.50°/RIU, a detection accuracy (DA) of $0.59°^{-1}$, a quality factor (QF) of 114.3 RIU^{-1}, and a figure of merit (FOM) of 191.18.26114 RIU^{-1} across a refractive index range of 1.33 to 1.35.

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