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Application of Artificial Intelligence and Machine Learning in Surface Plasmon Resonance Sensor for Blood Sample Diagnosis

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ABSTRACT

In recent years, various optical biosensor technologies are used by researchers to evaluate the conformational changes of biomolecules and their molecular interactions in a wide range of biomedical diagnostic and analysis operations. One of the most widely used techniques among several optical biosensors is surface plasmon resonance biosensors, which are used for label-free, real-time monitoring with exceptional accuracy and precision. In this study, quick and extremely sensitive SPR biosensors based on artificial intelligence (AI) programmed and machine learning (ML) are proposed to optimize the concentration of hemoglobin, plasma, and platelets in blood cells. Prism N-FK51A, graphene, nickel, potassium niobate, silver metal, and glass make up the suggested SPR biosensor device. Kretschmann configuration is the basis for the device structure, and attenuated total reflection (ATR) is the basis for the device function. Blood samples have undergone numerical analysis of the performance characteristics, including angular sensitivity, quality factor, detection accuracy, limit of detection, and electric field. The suggested surface plasmon resonance biosensor can be used for blood sample diagnosis, which opens the new path in biomedical domain.

Keywords: Surface Plasmon, Artificial intelligence, Machine learning, Algorithms, Nickel.

I. INTRODUCTION

In order to facilitate complex model analysis, the rapid advancements in artificial intelligence (AI) and machine learning (ML) have led to the development of neural networks, pattern recognition, cognitive computing, and robotics. AI is working cooperatively in a number of fields by utilizing machine learning techniques. While requiring little in the way of human resources, an AI-driven application promotes knowledge, complicated programming, system improvement, and accuracy as well as long-term viability [1]. Applying real-time AI models to data analysis has recently been done with the goal of providing complicated datasets with decision support capabilities [2]. The development of AI system models takes human behavior into account, particularly when it comes to demonstrating cognitive thinking and reasoning skills that are similar to those of humans [3]. These models take data out of databases and turn it into knowledge that can be used. ML is used to carry out the transformative process through a collection of pre-established algorithms [4,5].

The collection of machine learning methods designed to enable AI models to process revolutionary tasks in real-time has attracted significant attention in recent years. It is noteworthy that the ML model is the core component of the spectroscopic method that uses emission spectra targeted at the material surface to quickly generate results for a variety of samples without requiring complex pre-processing steps. Robotics, healthcare, and computer vision are just a few of the industries that have greatly benefited from the AI and ML integrated systems [6–8]. By recognizing pertinent patterns in a large volume of data, these integrated systems can take advantage of an unmet demand. The systems are different from conventional statistical techniques in that they prioritize categorization and prediction based on high-dimensional data instead of inference [9]. These suggested approaches have mostly concentrated on creating a multilayer programmable AI model for multiplex expressions for simultaneous analysis, despite efforts to address particular resource restrictions in AI/ML for healthcare [9-11]. By incorporating Artificial Intelligence (AI) and Machine Learning (ML) into Surface Plasmon Resonance (SPR) sensor technology, researchers are attempting to enhance performance, sensitivity, and data interpretation. In order to swiftly and accurately differentiate between positive and negative samples, AI and ML systems categorize sensor responses. The proposed study uses reflecting light angles on the material surface to develop a novel AI model based on machine learning for biomedical application. Among the many benefits of the SPR-based optical biosensor are its high throughput, exact binding affinity, and affordability [12].

In order to further the development of future extremely precise and targeted biomedical devices, firstly examine the datasets identified using SPR-sensing for cancer detection and classification. The parameters are employed for the categorization and analysis, and the reflecting angles on the material's surface are identified. Although it takes a lot of work and money to generate reflecting angles for various surfaces and biomolecule deposition, the current study lays the groundwork for the creation of ML based models specifically suited to SPR-based biosensor. This model makes it possible to thoroughly test and forecast biosensor performance over a variety of parameter regimes. The model is powered by AI and ML. AI technologies will be used to accelerate the model's significant quantification and advancement. The system benefits from the synergistic effect of the bimetallic components, which include multiple layers of graphene, nickel, silver, and potassium niobate. The surface plasmon resonance model sensitivity is expected to increase with the addition of silver nanoparticles. According to this method, the addition of colloidal silver nanoparticles affects the attenuated total reflection curves by changing the angle of SPR reflectance, which lengthens the curve and increases the minimum reflectivity.

II. THEORETICAL MODELLING

2.1 Experimental Feasibility of Proposed SPR Sensor

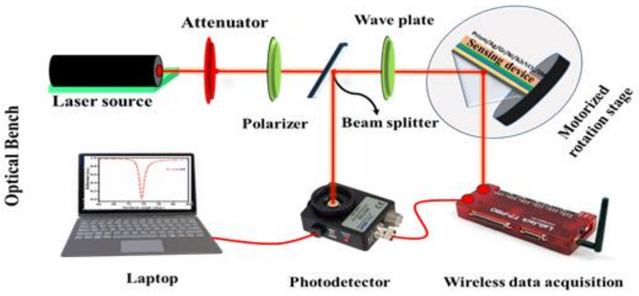

Fig:1 Experimental feasibility of surface plasmon resonance sensor.

Figure 1 depicts the experimentally possible arrangement of proposed SPR sensor. The components that helps to determine the operation and potential of the SPR biosensor include an optical source, attenuator, polarizer, beam splitter, wave plate, photodetector, and computer system. The following steps has been used to construct the SPR sensor chip. Initially, the NK51A prism surface has been cleaned by using acetone vapor and methanol before to connecting the Ag metal layer monolayer. The monolayer of Ag metal deposited on NK51A prism surface by physical vapor deposition (PVD) using a thermal evaporation technique. Similarly, graphene and nickel monolayers have been created using the liquid exfoliation process and placed on top of Ag metal. The chemical vapor deposition (CVD) creates the $KbNO_3$ monolayer, which is then chemically transferred to the nickel layer. In order to assess the performance of the SPR sensor, the chip has been lastly placed over the NK51A prism and linked for the testing setup.

2.2 Mathematical Modelling

MATLAB software has been used to mathematically simulate the suggested SPR sensor utilizing the Transfer Matrix approach (TMM) and finite element approach. When the propagation constant of the SPs wave and the propagation constant of the incoming photons match, the resonance condition will be met. The equation that follows needs to be met in the resonance condition:

$$K_X = \left(\frac{2\pi}{\lambda}\right) n_p \mathrm{Sin}\theta_i = K_{SPW} \qquad (1)$$

Here, the K_X stands for the horizontal component of the propagation constant of incident light, λ for wavelength, n_p for prism refractive index, θ_{inc} for incidence angle, and K_{SPW} for surface plasmon propagation constant. Two conditions must be met for surface plasmon resonance: first, the transverse magnetic (TM) or p-polarized light must be incident; second, the propagation constant of the incident light must match that of the surface plasmon.

The SPR curve reflectance is plotted against the incident angle of light after a dramatic dip is obtained when all of the photon energy is converted to surface plamons. For optimizing the optical sensor qualities, such as transmittance and reflectance, of multilayer layer stacked devices. The transfer matrix method (TMM) offers a number of benefits. This work takes into account the Fresnel equation, the transfer matrix technique, and the N-layer model analysis. The electromagnetic field's tangential component at the first and last surface boundaries follows the following relation:

$$[E_1.B_1] = X_{ij}[E_{N-1}.B_{N-1}] \quad (2)$$

Where, E_1, E_{N-1} and B_1, B_{N-1}, respectively, stand for the electric and magnetic field components of the first and last surfaces.

For an integrated structure, the characteristics matrix X_{ij} is described as follows:

$$X_{ij} = [X_{11}.X_{12}.X_{21}.X_{22}] = \prod_{K=2}^{N-1} X_K \qquad (3)$$

With

$$X_K = \left[\mathrm{Cos}\beta_K \frac{-i\mathrm{Sin}\beta_K}{q_K} - iq_K \mathrm{Sin}\beta_K \mathrm{Cos}\beta_K\right] \quad (4)$$

Where the elements of the transfer matrix are denoted by X_{11}, X_{12}, X_{21}, and X_{22} respectively. It is defined as follows: K is any arbitrary number, β_K is the phase thickness, and q_K is the refractive index of the corresponding layers.

Where, the components X_{11} , X_{12} , X_{21} , and X_{22} represent the transfer matrix elements respectively. K is any arbitrary number and β_K represents the phase thickness and q_K represents the refractive indices of corresponding layers and it is defined as:

$$q_K = \left[\frac{(\epsilon_K - n_1^2 \sin^2\theta)^{\frac{1}{2}}}{\epsilon_K}\right] \quad (5)$$

$$\beta_K = \left[\frac{2\pi d_K \ (\epsilon_K - n_1^2 \sin^2\theta)^{\frac{1}{2}}}{\lambda}\right] \quad (6)$$

Here n_1, θ and λ stand for the prism's refractive index, incident angle, and incident wavelength, respectively. In addition, d_K and ϵ_K are the K^{th} layer thickness and dielectric constant, respectively. The following formulas can be used to determine the reflectivity (R_P) and reflection coefficient (r) for incident p-polarized light.

The prism's refractive index, incident angle, and incident wavelength are represented by the symbols n_1, θ, and λ, respectively. Furthermore, the K^{th} layer thickness is denoted by d_K, and the dielectric constant by ϵ_K. The reflectivity (R_P) and reflection coefficient (r) for incident P-polarized light can be found using the following formula:

$$R_P = |r|^2 = \left[\frac{(X_{11}+X_{12}q_N)q_1-(X_{21}+X_{22}q_N)}{(X_{11}+X_{12}q_N)q_1+(X_{21}+X_{22}q_N)}\right] \quad (7)$$

2.3 Performance Parameters of SPR Sensor

There are a few important parameters that determine how well SPR sensors respond. These include detection accuracy (DA), detection limit (LoD), figure of merit (FoM), sensitivity (S), and full width at half maximum (FWHM) [13].

i. Detection Accuracy, DA= $\left[\frac{1}{FWHM}\right]$

ii. Detection Limit, LoD = $\frac{1}{S} \times 0.001°$

iii. Figure of Merit, FoM = $\left[\frac{S}{FWHM}\right]$

iv. Angular Sensitivity, S = $\left[\frac{\Delta\theta_{Res}}{\Delta n}\right]$

v. Electric Field Intensity Enhancement Factor, EFIEF = $\left|\frac{E\left(\frac{1}{l-1}\right)}{E\left(\frac{1}{2}\right)}\right|^2 = \left(\frac{\varepsilon_1}{\varepsilon_l}\right)|T|^2$

vi. Phase Angle, ϕ = arg (r)

vii. Full Width at Half Maximum, FWHM = $\frac{1}{2}(\theta_{Maxi} + \theta_{Mini})$

III.RESULT AND DISCUSSION

3.1 Application of SPR sensor for human plasma, platelets & hemoglobin dictation from blood samples or proteins

Figure 2 (a) illustrates how the resonance angle changed between 1.335-1.385 for different sensing medium RI, which is the region where both normal and diseased RI are situated. Fig. 2 (a) shows the variation of reflectance curve shift corresponding to the change in incident angle, also can be clearly witnessed that the maximum shift (blue color) is obtained for the proposed SPR sensor design for hemoglobin from blood sample. Similarly, Fig. 2(b) indicates the shift in incident angle that results from various blood sample cells (plasma, platelets & hemoglobin) with different RI of infected and normal cells.

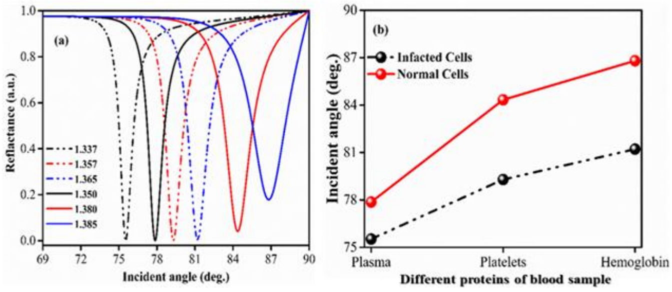

Fig.2 Optimized reflectance curve for various blood sample.

3.2 Optimized performance parameters for human plasma, platelets & hemoglobin dectation from blood samples

Figure 3 (a) and (b) display the most efficient parameters of the suggested SPR sensor for plasma, platelets, and hemoglobin in a human blood sample. For a blood sample, the suggested SPR sensor yields the best results for hemoglobin protein, having angular sensitivity (S) 280.00 deg/RIU, quality factor (Q.F) 273.00 RIU^{-1}, FWHM 1.026 deg, detection accuracy (DA) 0.975 deg^{-1}, LoD 3.565 x 10^{-6} and shift in resonance angle (δ_θ) 5.61deg . Similarly, for blood samples including infected and non-infected cells with different RI ranges of 1.335 to 1.385, Fig. 3 (c) and (d) define the electric field intensity enhancement factor (EFIEF) and change in phase shift. The figure shows maximum phase shift and EFIEF for hemoglobin blood sample with proposed SPR sensor. The optimized results have been shown in Table 1.

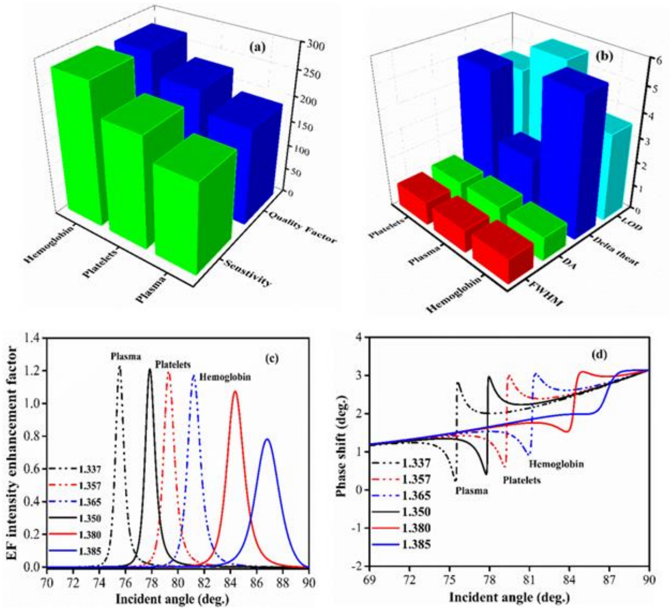

Fig.3 Optimized performance parameters of SPR sensor for blood sample.

Table 1. Optimized performance parameters for various proteins from blood samples.

Considered Protein Cells (Blood Sample)	Change in Resonance Angle (deg)	Angular Sensitivity (deg/RIU)	FWHM (deg)	Detection Accuracy (deg^{-1})	Quality Factor (RIU^{-1})	Limit of Dictation ($x10^{-6}$)
Plasma	2.32	178.46	0.935	1.069	190.77	5.603
Platelets	5.06	220.00	0.955	1.047	230.34	4.545
Hemoglobin	5.61	280.00	1.026	0.975	273.00	3.565

3.3 Comparative study of SPR Sensor

A comparison of proposed methods sensitivity to earlier surface plasmon resonance (SPR) technologies and the materials used in their constituent layers is shown in Table 2.

Table 2. Comparative study of SPR Sensor.

S. No.	Device Structure of the SPR Sensor	Sensitivity (°RIU^(-1))	References	
1.	Prism N-FK51A/Cu/BP	Prism N-FK51A/Cu/BP	124.0	[14]
2.	Prism CaF2/Cu/BaTiO3/Graphene	Prism CaF2/Cu/BaTiO3/Graphene	179.0	[15]
3.	Prism BK7/Ag/Si/BP/MXene	Prism BK7/Ag/Si/BP/MXene	245.00	[16]
4.	Prism N-FK51A/Ag/Gr/Ni/KbNO3	Prism N-FK51A/Ag/Gr/Ni/KbNO3	280.00	Proposed

IV. CONCLUSION

This study introduces an unconventional sensor created especially for the highly sensitive identification of plasma, platelets and hemoglobin form blood sample. The Transfer Matrix Method (TMM) with finite element method in MATLAB based simulation framework has been used to carefully optimize the SPR sensor. During the optimization phase, the prism and silver (Ag) layer thicknesses were systematically adjusted to reduce reflectance and increase angular sensitivity. The best result has been optimized for Hemoglobin having angular sensitivity (S) 280.00 deg/RIU, D.A 0.975 deg^{-1}, Q.F 273.00 RIU^{-1}, and LoD 3.565×10^{-6} within a refractive index interval of 1.335 to 1.385.

The proposed SPR sensor is well suited for early stage advanced biomedical diagnosis because of its low detection threshold and excellent angular sensitivity. The enhanced design not only significantly improves detection capacities but also facilitates early diagnosis of blood samples and the use of preventative measures in clinical settings.

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Author Contribution: Original draft writing and methodology: Shalini Srivastava, Software and conceptualization: Ramesh Mishra & Sachin Singh, Supervision: Shambhavi Mudra Shukla & Parimal Tiwari.

Declarations

Ethics Approval: Ethics approval is not needed for this theoretical investigation.

Conflict of Interest: The authors say they have no conflicting interests.

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