International Journal of Nanoelectronics and Materials
Volume 16 (Special Issue) December 2023 [43-49]

Design Simulation of Multilayer Structures for the Development of Biosensor Based on Transverse Matrix Method

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ABSTRACT

Simulation of electromagnetic wave propagation on layered metal-dielectric structures using analytical methods is a study that continues to be developed because it involves strict mathematical equations with exact results. In this study, the transfer matrix method was developed to analyze the dielectric-metal-metal-dielectric structure through the reflection profile. The emergence of the Surface Plasmons Resonance (SPR) phenomenon causes a minimum reflectance whose changes are analyzed through variations in optical and physical parameters. The simulation shows that the minimum reflectance angle occurs at an angle $\theta = 85^0$*, indicating the existence of the SPR phenomenon in the condition* $\omega/\omega_0 = 0.9$*. The choice of metal materials, namely gold and silver, resulted in a shift in the reflectance curve, and an increase in the thickness of the adhesive layer caused a shift in the reflectance curve towards a smaller angle. Changes in the refractive index of the upper dielectric material are important for biosensor development, namely a shift in the reflectance curve with a linear response at the interval of refractive index* $2.61 - 2.91$*.*

Keywords: Multilayer structure, transverse matrix method, biosensor

1. INTRODUCTION

The study of metal-dielectric structures using optical analysis remains an active research area, as evidenced by ongoing investigations [1,2]. Simultaneously, advancements in both hardware and software play a pivotal role in the evolution of optical devices. Researchers have devised various analytical [3] and numerical techniques [4] to elucidate optical phenomena through mathematical models from a theoretical perspective. In general, numerical methods are favored for their simplicity and efficiency in terms of execution. However, numerical methods come with their share of challenges, including issues related to resolution [5], stability [6], and calculation errors [7]. On the other hand, analytical methods yield precise solutions and can unveil optical phenomena within metal-dielectric structures without introducing errors. Analytical approaches can establish the presence of the Surface Plasmon Resonance (SPR) phenomenon by examining the transmittance or reflectance of waves post-interaction with these structures [8].

In this study, we employed the Transfer Matrix method to analyze a multilayer structure comprised of alternating dielectric-metal-metal-dielectric layers. This particular multilayer configuration was designed to exhibit the Surface Plasmon Resonance (SPR) phenomenon. SPR is a resonance phenomenon resulting from the interaction between light waves and electrons on a metal surface, leading to quantized electron oscillations on the metal surface. Previous research has demonstrated that the transmittance spectra of SPR sensors are wavelength-dependent [9]. Optical properties, including reflectance, can be examined concerning the presence of SPR and factors such as the angle of incident light waves and the refractive index of the structural layer.

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These parameters also influence the wavelength at which SPR occurs. It's worth noting that the shift in the reflectance peak associated with SPR exhibits a linear behavior, as observed in previous studies, making it a widely adopted feature for optical biosensors [10]. Selecting the appropriate metal layer and determining its thickness are crucial considerations in developing fabrication processes. Our simulations' outcomes can potentially inform the construction of optical biosensor devices.

2. MATERIAL AND METHODS

2.1 Finite Difference Method

This study used the Transfer Matrix Method [11,12], which provides an exact numerical solution to the proposed structural model and is relatively easy to modify if there is a change in the structural model. The reflectance of the structure was calculated using the following equation:

$$\begin{pmatrix} E_i/E_r \\ E_r/E_t \end{pmatrix} = \tau^{-1}\begin{pmatrix} 1 \\ 0 \end{pmatrix} \tag{1}$$

Where E_i, E_r, and E_t are the incident, reflected, and transmitted electric fields, respectively. The matrix τ is a transfer matrix that connects the electric fields of each layer.

$$\tau = P_0^{-1}(\ldots.Q_{n+1}P_{n+1}Q_nP_n)P_0 \tag{2}$$

Matrix P and Q according to Transverse Electric (TE) dan Transverse Magnetic (TM) polarization

$$P_j^{TE} = \begin{pmatrix} 1 & 1 \\ k_j cos\theta_j & -k_j cos\theta_j \end{pmatrix} \tag{3}$$

$$P_j^{TM} = \begin{pmatrix} cos\theta_j & cos\theta_j \\ k_j cos\theta_j & -k_j cos\theta_j \end{pmatrix} \tag{4}$$

$$Q_j^{TE} = \begin{pmatrix} e^{ik_j d_j cos\theta_j} & e^{-ik_j d_j cos\theta_j} \\ k_j cos\theta_j e^{ik_j d_j cos\theta_j} & -k_j cos\theta_j e^{-ik_j d_j cos\theta_j} \end{pmatrix} \tag{5}$$

$$Q_j^{TM} = \begin{pmatrix} cos\theta_j e^{ik_j d_j cos\theta_j} & cos\theta_j e^{-ik_j d_j cos\theta_j} \\ k_j e^{ik_j d_j cos\theta_j} & -k_j e^{-ik_j d_j cos\theta_j} \end{pmatrix} \tag{6}$$

where k_j is the wave number and θ_j is the angle of incidence at each layer. The reflectance of the electric field is given by

$$R = \left|\frac{E_r}{E_i}\right|^2 \tag{7}$$

The wavelength shift is a function of the change in the refractive index of the material, and thus, the sensitivity can be defined as [13,14]

$$S = \frac{d\lambda_p}{dn_d} \tag{8}$$

where λ_p is the peak wavelength of the reflectance and n_d is the refractive index of the dielectric material.

2.2 Design Structure

A multilayer layer is a dielectric or metal layer arranged alternately with a certain thickness. Using MATLAB software, a multilayer layer design is formed with parameters and sizes according to the design that has been made

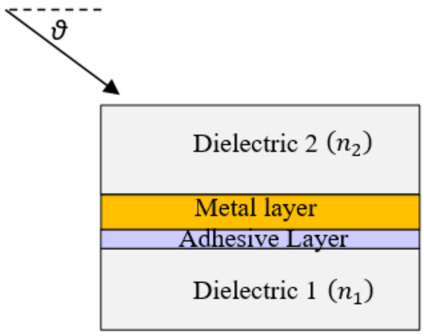


Figure 1. Multilayer structure.

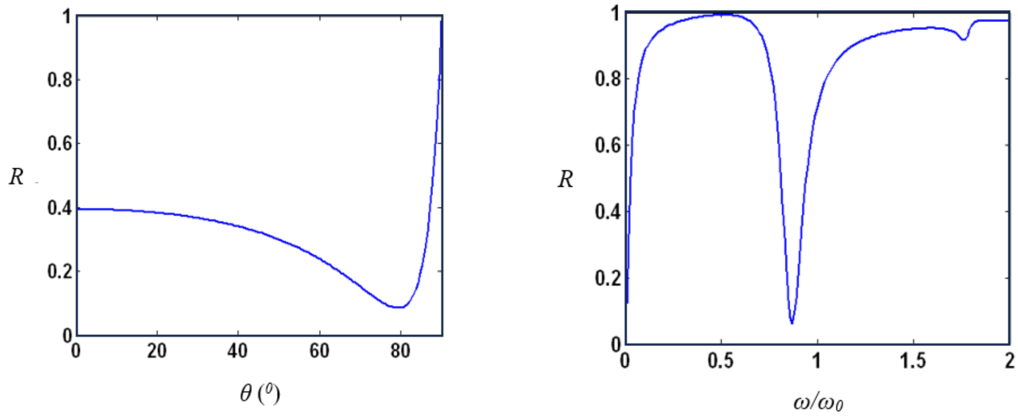
The structural design to be investigated consists of two dielectric layers separated by two metal layers, namely, the adhesive layer and the metal layer, as shown in Fig. 1. n_1 and n_2 show the refractive indices of dielectric 1 and dielectric 2, which are $n_1 = 2.61$ (TiO_2) and $n_2 = 3.61$ (GaAs) with the appropriate thickness $d_1 = d_2 = 58\ nm$. The adhesive layer is a titanium material with a refractive index $n_a = 2.611 + 3.6024i$ [15] and thickness $d_a = 29\ nm$. The metal layer can use gold and silver with a refractive index of refraction that follows the Drude-Lorentz formulation [16]:

$$n(\lambda) = \sqrt{\varepsilon(\lambda)} = \sqrt{1 - \frac{\lambda^2 \lambda_c}{{\lambda_p}^2(\lambda_c + i\lambda)}} \tag{9}$$

where λ_p denotes the plasma wavelength, while λ_c the collision wavelength. The values of λ_p and λ_c for gold were $1.6826 \times 10^{-7} m$ and $8.9342 \times 10^{-6} m$ respectively. The thicknesses of the dielectric layer and the gold layer were the same, namely400 nm. The wavelength was set in the visible light range of : $\lambda_0 = 580\ nm$. The simulation was performed 6the Transfer Matrix method. The use of metal materials among dielectric materials is the reason for the appearance of SPR, and the shift in the SPR wavelength is very sensitive to changes in the refractive index of the dielectric material (n_1), as reported in previous studies [17].

3. RESULTS AND DISCUSSION

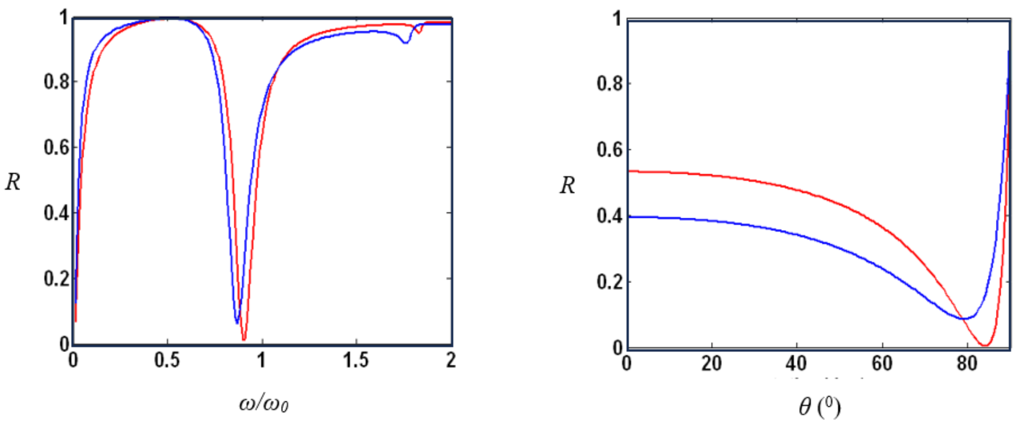
From the simulation results, the reflectance of the multilayer structure shows varying reflectance values for incident angles in the range of incident angles $0^0 - 90^0$. An angle of incidence of 85^0 °indicates the existence of a minimum reflectance value of $R = 0.09$ (Fig. 2a). The reflectance profile against the normalized frequency at an angle of incidence 85^0 °proves that the minimum reflectance falls at the normalized frequency $\omega/\omega_0 = 0.9$ (Fig. 2b). The minimum reflectance at this frequency value indicates that the field is transmitted because there is an increase in field localization between the dielectric and metal layers, which is called surface plasmon resonance (SPR), so that the angle 85^0 can be referred to as the SPR angle (θ_{spr}) for the proposed structure.



(a) (b)

Figure 2. (a) Relation of reflectance to incident angle (b) Normalized reflectance profile to frequency in a multilayer structure.

The use of metal layers in the dielectric multilayer structure is the main factor in the occurrence of SPR because of the localization of the field on the contact surface of the dielectric and metal. Therefore, resonance occurs when the frequency of the electromagnetic waves matches the oscillation frequency of electrons on the surface of the dielectric and metal. The metal materials commonly used in multilayer structures are Au and Ag. The simulation results for the gold and metal layers show different reflectance profiles. For the metal layer, silver showed a more negligible (minimum) reflectance than gold at normalized frequencies $\omega/\omega_0 = 0.9$ (Fig. 3a). Also, using different metal layers resulted in a shift of the SPR angle, as shown in Fig. 3b.



(a) (b)

Figure 3. Differences in the use of metal materials, namely gold (blue) and silver (red) (a) Normalized reflectance profile to frequency (b) SPR reflectance dip.

In multilayer structures, an adhesive layer is used on top of the substrate to adhere to the top layer. Generally, the adhesive layer uses titanium material with a refractive index $n_a = 2.611 + 3.6024i$ and is thin (thinner than the metal layer). The thickness of the adhesive layer can affect the reflectance profile, that is, the shift in the SPR angle and minimum reflectance value, as shown in Fig. 4. The thickness of the adhesive layer in the simulation is chosen: $d_a = 2.9\ nm$ (red), $d_a = 3.86\ nm$ (green), $d_a = 5.80\ nm$ (black), $d_a = 11.6\ nm$ (blue) produces a shift in the SPR angle and a minimum reflectance value

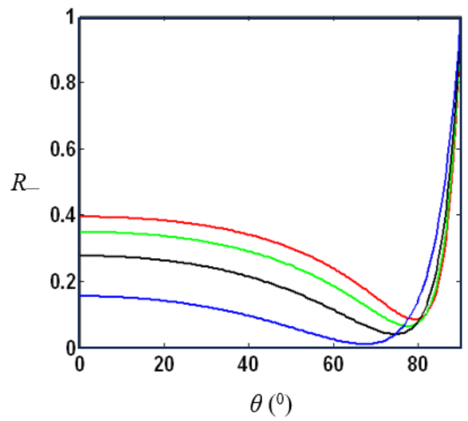


Figure 4. Relationship of angle of incidence and dip reflectance for variations in adhesive layer thickness: $d_a = 2.9\ nm$ (red), $d_a = 3.86\ nm$ (green), $d_a = 5.80\ nm$ (black), $d_a = 11.6\ nm$ (blue).

Variations in the top dielectric layer produce the same characteristics, that is, a shift in the reflectance curve, as shown in Fig. 5a. If the change in the refractive index of the upper dielectric layer is plotted, it produces a nonlinear reflectance value between the refractive index values $2.61 - 3.61$ (Fig.5b). Changes in the refractive index of the upper dielectric are important for the development of biosensor devices because they respond to biorecognition activity in detecting changes in objects (environment) outside the structure.

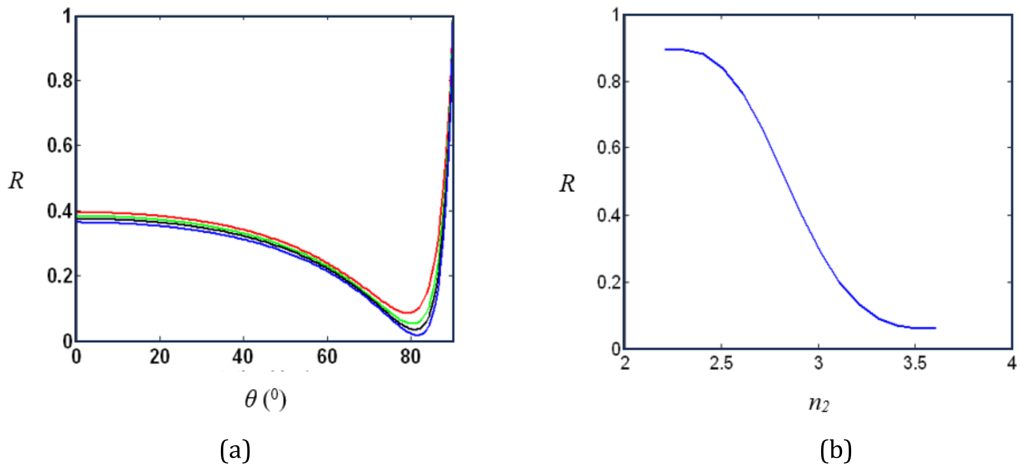


Figure 5. (a) SPR reflectance profile against variations n_2:3.61 (red), 3.41 (green), 3.31 (black), 3.21 (blue) (b) Plot of the relationship dip reflectance for the variation of the refractive index n_2.

If the range of refractive index changes is smaller, namely $2.61 - 2.91$ (Fig. 6), it will produce a linear change in reflectance with a sensitivity of

$$\frac{dT}{dn_2} = 2 \tag{10}$$

These results can be used as a standard for building biosensor devices that can sense sensitive changes in objects (environment) over a range of refractive indices $2.61 - 2.91$.

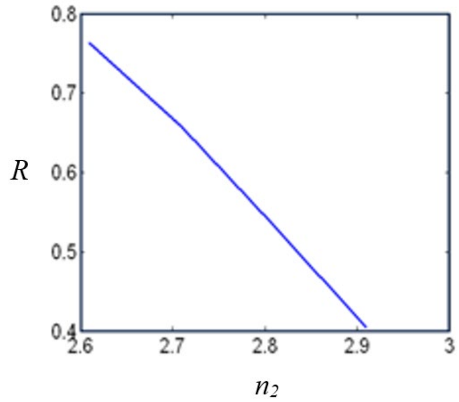


Figure 6. Plot of the relationship dip reflectance for the variation of the refractive index n_2: $2.61 - 2.91$.

4. CONCLUSION

Simulation of electromagnetic wave propagation in circular photonic crystal structures with dielectric-metal-metal dielectric layers has been carried out using transverse matrix methods. Output analysis was carried out through changes in reflectance due to changes in optical and physical parameters. The simulation results show that the minimum reflectance angle occurs at an angle $\theta = 85^0$ which indicates the existence of the SPR phenomenon in the condition $\omega/\omega_0 = 0.9$. The choice of metal materials, namely, gold and silver, resulted in a shift in the reflectance curve, and an increase in the thickness of the adhesive layer caused a shift in the reflectance curve toward a smaller angle. Changes in the refractive index of the upper dielectric material are important for biosensor development, namely, a shift in the reflectance curve with a linear response at the refractive index interval of $2.61 - 2.91$. Changes in the refractive index of the upper dielectric are important for developing biosensor devices because they respond to biorecognition activity in detecting changes in objects (environment) outside the structure.

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