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Nonlinear Angular and Polarization-Dependent Reflectance Sensitivity in $MAPbI_3$ Thin-Film Structures: Thickness-Tuned TiO_2 Interlayer Effects

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Abstract: This study presents a theoretical investigation of the angular and polarization-dependent reflectance sensitivity of $MAPbI_3$-based thin-film structures using the Transfer Matrix Method (TMM). Two configurations were considered: a single-layer structure ($Air/MAPbI_3/Glass$) and a bilayer structure incorporating a TiO_2 interlayer ($Air/MAPbI_3/TiO_2/Glass$). The analysis was performed within the 300–800 nm spectral range under oblique incidence conditions. The results show that the reflectance sensitivity exhibits a clear nonlinear dependence on the angle of incidence. Under TE polarization, the sensitivity increases significantly with angle and reaches its maximum at 60°, indicating strong angular amplification driven by interference-induced phase modulation. In contrast, TM polarization demonstrates a gradual reduction in sensitivity, accompanied by a sign reversal at higher angles due to impedance matching effects near Brewster-related conditions. The introduction of a TiO_2 interlayer preserves the overall angular trend while enabling moderate structural tuning. Thickness optimization reveals polarization-dependent optimal values, with peak TE sensitivity obtained near 80 nm and peak TM sensitivity around 50 nm. However, quantitative comparison between single- and bilayer configurations confirms that angular control plays a more dominant role in sensitivity enhancement than thickness adjustment alone. Overall, the findings highlight the effectiveness of polarization-engineered angular modulation as a practical approach for enhancing reflectance-based sensing performance in perovskite multilayer systems, offering simplified design guidelines for angle-selective photonic coatings and optical sensors.

Keywords: Reflectance Sensitivity, Angular Modulation, Perovskite Thin Films

Introduction

Perovskite, based thin films have recently been identified as promising new materials for an up, to, date optoelectronic application due to efficient light, matter interaction, theoretically adjustable bandgap and their high absorption rate in the visible range of spectrum (Kojima et al, 2009) (De Wolf et al, 2014).

Especially, $MAPbI_3$ continues to attract considerable interest not only in the field of solar cells but also as an effective material for various types of optical coatings, devices based on interference, sensors of refractive index, where the delicate control of reflection as well as phase modulation is necessary (De Wolf et al, 2014) (Snaith, 2013).

Electromagnetic wave propagation in multilayer optical structures is a phenomenon determined by multiple reflections, phase accumulation, and impedance mismatch at the interfaces of different materials. At the scale of advanced nanometer thin films, where variations in thickness, refractive index, or angle of incidence are minimal, these interference effects are greatly amplified such that they affect the spectral response to a large extent (Yeh, 2005).

The Transfer Matrix Method (TMM) offers a rigorous and efficient way to model wave propagation in stratified planar media, and it has been extensively used to study optical multilayer structures at both normal and oblique incidences (Macleod, 2010) (Katsidis & Siapkas, 2002) (Sayed et al, 2025).

In many previous studies, researchers have investigated the optical properties of perovskite-based thin films onto which light is incident at a perpendicular angle (Sayed et al, 2023) (Ma et al, 2025). However, practical optical devices rarely operate under perfectly perpendicular illumination. In real-world configurations-such as photonics, smart coatings, and angular-selective reflectors, the incident light typically arrives at oblique angles, causing significant changes in the effective optical path length, phase state, and polarization-dependent boundary behavior (Machleod, 2010) (Tene et al, 2025). The angular variation of reflection can play a dominant role in determining the device's sensitivity and spectral controllability.

Moreover, polarization effects introduce an additional degree of control in multilayer systems. The optical admittance differs for transverse electric (TE) and transverse magnetic (TM) polarizations, resulting in distinct angular responses and, in some cases, sign reversal behavior near Brewster-related conditions (Machleod, 2010) (Sayed et al, 2025) (Tene et al, 2025). Despite its importance, systematic investigations that combine angular variation, polarization dependence, and structural optimization in perovskite-based multilayers remain relatively limited in the recent literature.

Titanium dioxide (TiO_2) is commonly used as an interlayer in perovskite structures because of its optical stability, high refractive index and good match with perovskite films (Mischok et al, 2024) (Chen, 2024) (Salah, 2023). Along with its traditional purposes of charge transport and interface engineering, TiO_2 may be used as a phase layer in optical multilayers, thereby changing interference conditions and possibly increasing angular sensitivity. On the other hand, how much TiO_2 thickness influences angular and polarization, dependent reflectance sensitivity has not been thoroughly explained.

Here, we theoretically explore the problem of angular and polarization, dependent reflectance sensitivity of $MAPbI_3$- based thin, film structures through the Transfer Matrix Method (TMM) . The study covers both single, layer (Air/$MAPbI_3$/Glass) and bilayer (Air/$MAPbI_3$/TiO_2/Glass) systems at nonnormal incidences. The work mainly addresses (i) nonlinear angular boost of sensitivity, (ii) different types of polarized light and (iii) careful selection of TiO_2 thickness. It was found that angular tuning is most responsible for reaching the highest sensitivity, whereas TiO_2 thickness only hints at a secondary and measurable fine, tuning. Such insights can be directly translated into polarization, engineered optical sensors and angle, selective photonic coatings based on perovskite thin films.

In order to obtain better results and to be different from the prior studies which mainly focused on normal light incidence or on the improvement of a single optical parameter, we unified nonlinear angular enhancement analysis in this work. Besides, we studied the polarization dependent properties and controlled the thickness of multiple interlayers of the $MAPbI_3$ composite.Angular amplification and polarization sensitivity were studied, and a quantitative comparison was performed between single-layer and double-layer compositions. All of the above was done to understand the effect of angular light incidence in order to implement appropriate structural modifications for optimal use in interference-based optical sensing platforms.

Methodology

We analyzed the optical response of the simulated thin films using the Transfer Matrix Method (TMM), which accurately describes Maxwell's equations for electromagnetic wave propagation in layered structures (Yeh, 2005) (Katsidis & Siapkas, 2002). This method is particularly suitable for this complex system, as interference and phase accumulation at the layers play a key role in determining the type and behavior of the reflection.

In this study, we examined two formations:

1. Single-layer structure:

Air / $MAPbI_3$ / Glass

2. Bilayer structure:

Air / $MAPbI_3$ / TiO_2 / Glass

Assuming a monochromatic wave of wavelength λ strikes the structure from the first medium (air) at an angle θ_0, we can determine the internal propagation angle between the layers using Snell's law:

$$n_0 \sin\theta_0 = n_j \sin\theta_j \ldots\ldots(1)$$

Where n_0 is the refractive index of the incident medium , n_j is the refractive index of the j-th layer.

Phase Thickness

The phase thickness is defined as (for each layer) :

$$\delta_j = \frac{2\pi\, n_j d_j \cos\theta_j}{\lambda} \ldots\ldots(2)$$

Where d_j is the physical thickness of the layer.This actual condition governs the interference state within the multilayer group and strongly illustrates the angular dependence of the reflection spectrum (Yeh, 2005) (Machelod, 2010).

Optical Admittance - Polarization Dependence

The optical impedance cannot be matched for transverse electric polarization (TE) and transverse magnetic polarization (TM).

For **TE polarization**:

$Y_j^{TE} = n_j \cos\theta_j$……(3)

For **TM polarization**:

$Y_j^{TM} = \frac{n_j}{\cos\theta_j}$ ……(4)

This difference in permittivity results in a distinctive angular behavior of TE and TM waves, especially in the case of oblique fall, where the effects of impedance mismatch depend on polarization (Machelod, 2010) (Sayed et al, 2025).

Characteristic Matrix of a Layer

Each layer can be described by a 2×2 matrix:

$$M_j = \begin{bmatrix} \cos(\delta_j) & \sin\left(\delta_j \frac{i}{Y_j}\right) \\ iY_j \sin(\delta_j) & \cos(\delta_j) \end{bmatrix} \text{….(5)}$$

If a multi-layered structure contains m layers, the total transfer matrix can be obtained by multiplying the matrices:

$M_{tot} = \prod_{j=1}^{m} M_j$…..(6)

In the bilayer case:

$M_{tot} = M_{MAPbI3} \times M_{TiO2}$…..(7)

Reflectance and reflectivity coefficient

The overall transfer matrix can be used to calculate the composite reflection coefficient:

$r = \frac{Y_0 B - C}{Y_0 B + C}$…….(8)

Where:

$$B = M_{11} + M_{12} Y_s$$
$$C = M_{21} + M_{22} Y_s$$

And Y_s is the optical admittance of the substrate (glass).

The reflection is obtained from:

$R = |r|^2$…..(9)

Angular Sensitivity Definition

In order to determine the sensing performance, the sensitivity of reflection to changes in the refractive index is defined as follows:

$S = \frac{\Delta R}{\Delta n}$ ….(10)

Where

$$S(\theta) = \frac{R(n+\Delta n) - R(n)}{\Delta n} \text{……(11)}$$

Where Δn represents a slight disturbance in the refractive index of the incident medium. The sensitivity is expressed in RIU⁻¹. We evaluated the sensitivity at the wavelength corresponding to the lowest reflection which ensures maximum modulation response under angular changes.

This definition allows us to compare the effect of angular optimization (based on polarization) with the improvement of interlayer thickness.

The sign of the sensitivity indicates whether the reflectance increases or decreases with refractive index variation, while the magnitude determines the strength of modulation.

3. Simulation Parameters and Modeling Assumptions

The optical simulations were carried out over the wavelength range of 300–800 nm, covering the ultraviolet–visible region relevant to $MAPbI_3$-based photonic applications. A monochromatic coherent plane wave was assumed to be incident from air onto the multilayer structure.

Refractive index of air was taken as $n_0 = 1.00$, $n_{\mathrm{MAPbI3}} = 2.3$, $n_{\mathrm{TiO2}} = 2.4$, and the glass substrate as $n_{\mathrm{glass}} = 1.5$.

The refractive indices were assumed constant within the investigated spectral range. Although $MAPbI_3$ exhibits noticeable dispersion in the visible region, constant refractive indices were adopted in order to isolate angular interference effects and polarization-dependent phase modulation.

These parameters were chosen in accordance with the most common literature data for optical modeling studies [9-15]. During angular investigations, the thickness of the $MAPbI_3$layer was kept at 150 nm, whereas for structural optimization analysis, the TiO_2 interlayer thickness was changed within the range of 30, 110 nm. Both transverse electric (TE) and transverse magnetic (TM) polarizations were treated separately.

To measure the sensitivity, a tiny change of $\Delta n=0.01$ was made to the surrounding refractive index. The reflectance sensitivity was determined at the wavelength where the minimum reflectance was observed for each angle condition.

Surface roughness, dispersion effects, and material absorption losses were not considered in order to focus on interference, driven phase modulation and polarization, dependent boundary effects. In order to confirm the numerical stability and physical consistency of the transfer matrix implementation, energy conservation was tested for all simulated angles and polarizations. The calculated reflectance (R), transmittance (T) fulfilled the relation

$$\mathrm{R} + \mathrm{T} = 1$$

Since all refractive indices were assumed real-valued, the multilayer system was treated as lossless. Under this assumption, energy conservation reduces to R+T=1, which was verified numerically for all simulated angles and polarizations. Material absorption and dispersion were neglected in order to isolate angular interference effects and polarization-dependent phase modulation.

To within numerical precision (error < 10^{-6}). This proves that the numerical model is both accurate and stable even at oblique incidence.

Result and Discussion

Reflectance Behavior of the Single-Layer Structure

To check the accuracy of the numerical implementation of the Transfer Matrix Method (TMM), the reflectance spectra of the single, layer Air/$MAPbI_3$/Glass structure were first computed for different perovskite thicknesses at normal incidence.

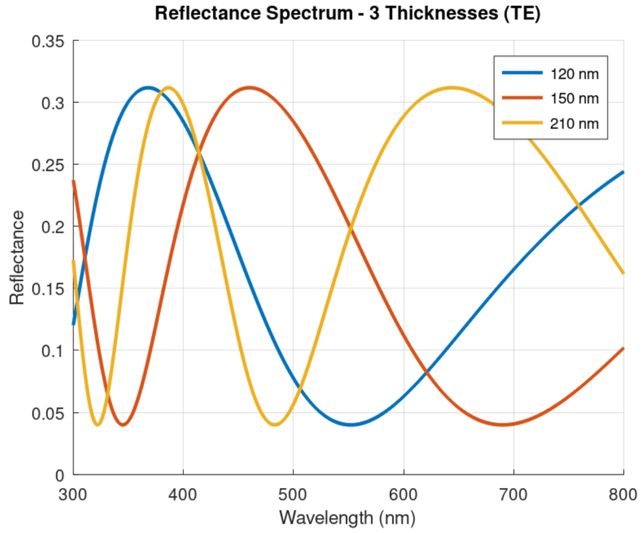

Figure 1. Reflectance spectra of the single, layer Air/ $MAPbI_3$/Glass structure for different $MAPbI_3$ thicknesses under normal incidence (θ = 0°).

Figure 1 demonstrates that the increase of thickness from 120 nm to 210 nm causes the reflectance minima to shift clearly in their spectral position to longer wavelengths. Such behavior follows the phase condition

$$\delta \propto nd$$

Which means that an increase in the optical thickness results in a change of the interference condition inside the film. The shift that has been observed confirms the validity of the phase accumulation model and proves the correctness of the numerical implementation of the transfer matrix formulation.

4.

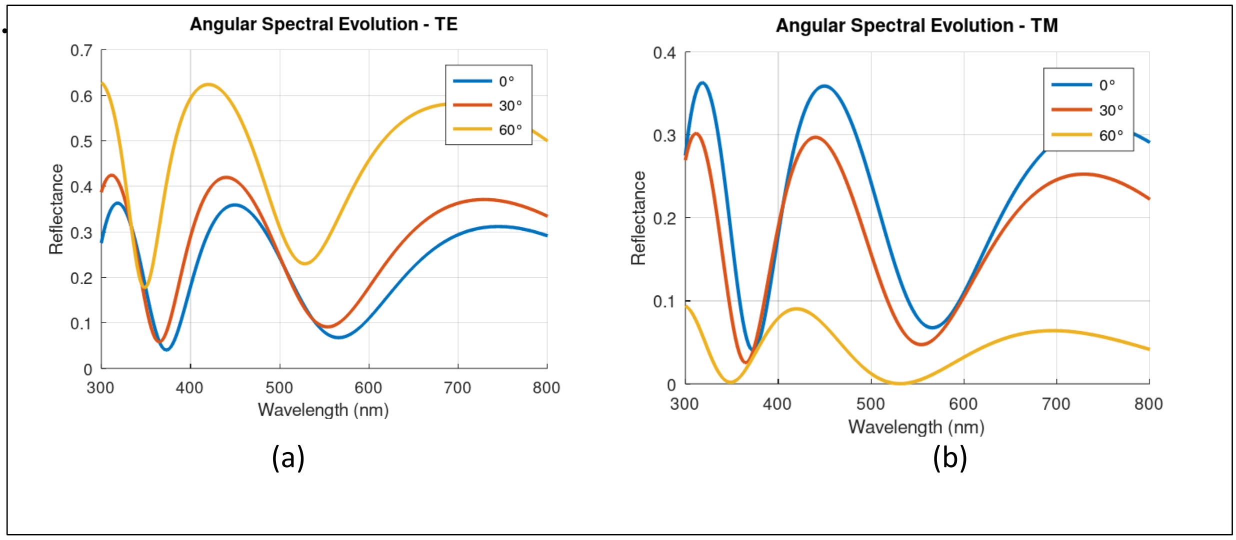

Figure 2. Angular evolution of reflectance spectra for the bilayer Air/MAPbI$_3$/TiO$_2$/Glass structure under (a) TE and (b) TM polarization.

Figure 2 shows how the reflectance spectra change in angular dependence for TE and TM polarizations. Reflectance under TE polarization (Figure 2a) shows a gradual raise to the incidence angle, along with major changes in the spectral minima caused by the phase accumulation in the multilayer stack, which changes with the angle. This increase in the spectral modulation at higher angles is, in fact, the physical basis of the nonlinear sensitivity amplifier, which is explained later.

On the other hand, TM polarization (Figure 2b) reveals a dramatic decrease in reflectance with the increase in the angle of incidence, especially at 60°. This kind of behavior is related to impedance matching and Brewster, type effects that lead to the vanishing of Fresnel reflection when light is incident at an oblique angle. Hence, the decrease in baseline reflectance is a major element in the observed polarization, dependent sensitivity nature and eventual sign change at high angles.

Such angular spectral changes serve as a basis for quantitatively analyzing the sensitivity behavior in the next subsection.

Polarization-Dependent Angular Sensitivity (Single Layer)

In order to study the angular effects, the reflectance sensitivity was determined in relation to the angle of incidence for both TE and TM polarizations.

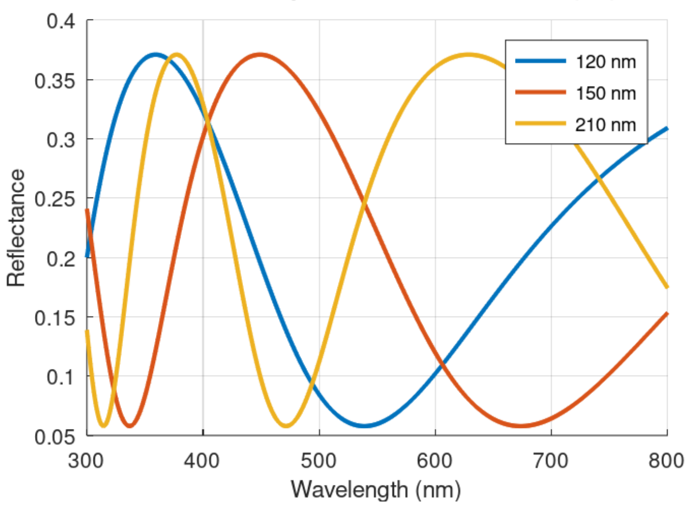

Figure 3. *depicts the nonlinear angular variation of sensitivity for both polarizations.*

As shown in Figure 3, the sensitivity varies greatly with polarization. The sensitivity magnitude for TE polarization increases in a nonlinear manner with the angle and reaches a maximum at 60°. On the other hand, TM polarization shows a decreasing trend as the angle increases and changes the sign near the large angles. The reason for this is polarization, dependent optical admittance and by being close to Brewster, related conditions, which drastically changes impedance matching under oblique incidence. Polarization, engineered reflectance modulation has recently been the focus of angle, selective photonic coatings and sensing applications [19, 20].

The comparison shows that angular tuning is the main factor responsible for enhancing reflectance modulation, especially under TE polarization.

Table 1. Angular Sensitivity (Single Layer)

Angle (°)	**S_TE** (RIU^{-1})	**S_TM** (RIU^{-1})
0	-0.1889	-0.1889
30	-0.2514	-0.1329
60	-0.5142	+0.0216

The sign of the sensitivity indicates the direction of reflectance variation with refractive index, while its magnitude determines the strength of modulation.

Table 1 illuminates the fact that maximum sensitivity is obtained at 60° for TE polarized light, showing nonlinear angular amplification.

Effect of TiO_2 Interlayer on Angular Response

To investigate the effect of structural engineering, a TiO_2 interlayer was inserted between $MAPbI_3$ and the glass substrate.

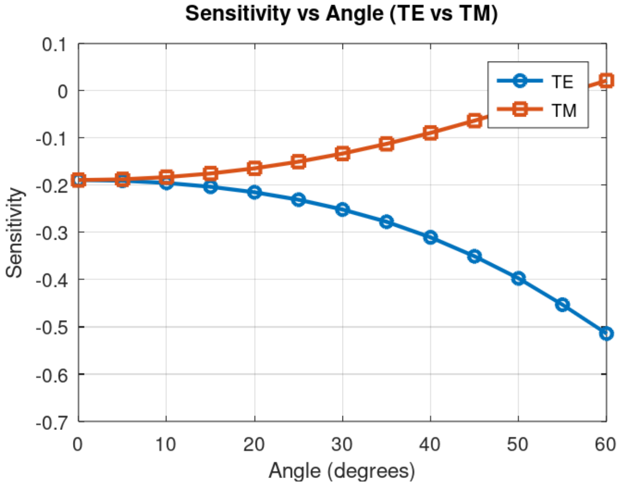

Figure 4. *juxtaposes TE and TM sensitivities for the bilayer setup.*

According to Figure 4, the total polarization, dependent pattern is retained after the incorporation of TiO_2. Nevertheless, sensitivity values show only minor quantitative shifts. The angular amplification is still largely due to TE polarization, whereas TM maintains the sign, reversal trend. Recent optical sensing investigations (Aliqab, 2023) (Tene at al, 2025)

(Mishra, 2025) have reported similar nonlinear angular amplification in multilayer platforms for sensing.

These findings suggest that the TiO_2 interlayer essentially plays the role of a phase, tuning layer, instead of being a main amplification mechanism.

Thickness Optimization of the TiO_2 Interlayer

In order to examine the effects of thickness on sensitivity, the TiO_2 layer thickness was changed while keeping the incidence angle at 60°, which is the angle giving the highest angular sensitivity.

Table 2 . Effect of TiO_2 Thickness at 60°

TiO_2 (nm)	**S_TE** (RIU^{-1})	**S_TM** (RIU^{-1})
30	-0.4819	0.0260
50	-0.4859	**0.0371**
80	**-0.4928**	0.0237
110	-0.4863	0.0244

Table 2 shows that the best TiO_2 thickness for each polarization is different. For the TE mode, the highest sensitivity is achieved around 80 nm, while the peak TM sensitivity is reached around 50 nm.

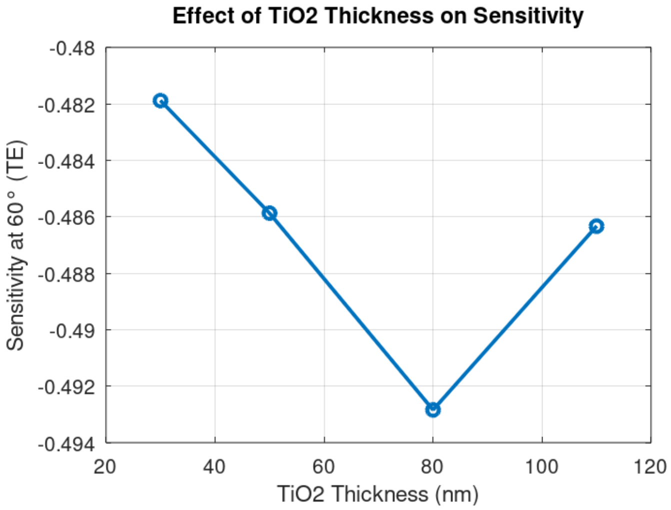

Figure 5. Effect of TiO_2 thickness on TE-polarized sensitivity at an incidence angle of 60°.

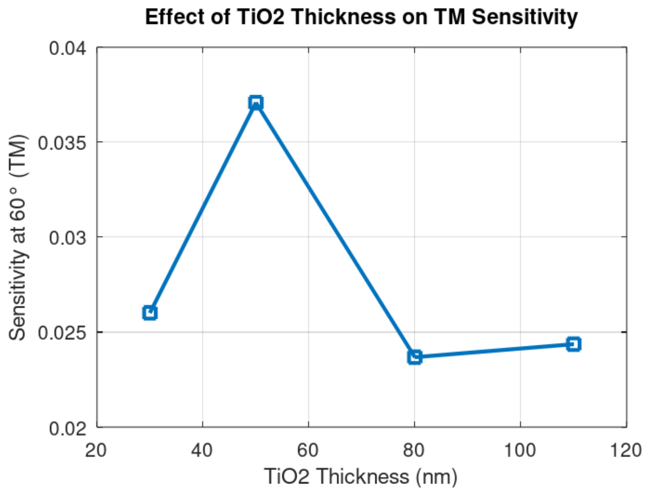

Figure 6. Effect of TiO_2 thickness on TM-polarized sensitivity at an incidence angle of 60°.

The findings reveal, first of all, that angular tuning the major factor that determines sensitivity. However, the thickness of TiO_2can still be used for a secondary fine adjustment. Also, the best thickness heavily depends on the polarization, thus opening the way for the design of polarization, engineered sensors.

Comparison Between Single and Bilayer Structures

Table 3. Comparison at 60°

Structure	**S_TE** (RIU^{-1})	**S_TM** (RIU^{-1})
Single Layer	-0.5142	0.0216
Bilayer (optimal TE)	-0.4928	0.0237

From the data in Table 3, it is clear that the incorporation of TiO_2 layer does not substantially improve the highest angular sensitivity but at the same time, it changes the polarization response. In fact, this is in line with the statement that optimizing the angle has a more significant effect on sensitivity than adjusting the thickness.

Conclusion

In this work, the angular and polarization-dependent reflectance sensitivity of $MAPbI_3$-based thin-film structures was theoretically investigated using the Transfer Matrix Method (TMM). Both single-layer (Air/$MAPbI_3$/Glass) and bilayer (Air/$MAPbI_3$/TiO_2/Glass) configurations were analyzed under oblique illumination in the visible spectral range.

The results revealed a pronounced nonlinear enhancement of sensitivity with increasing incidence angle under TE polarization, reaching a maximum at 60°. In contrast, TM polarization exhibited a gradual reduction in sensitivity accompanied by a sign reversal at high angles, attributed to Brewster-type impedance matching effects and polarization-dependent optical admittance.

The incorporation of a TiO_2 interlayer preserved the overall angular behavior while enabling secondary structural tuning. Thickness optimization demonstrated polarization-dependent optimal values, with peak TE sensitivity near 80 nm and peak TM sensitivity near 50 nm. However, quantitative comparison confirmed that angular control plays a more dominant role in sensitivity enhancement than thickness adjustment alone.

Numerical stability of the model was verified through energy conservation validation ($R + T = 1$) under all simulated conditions.

Overall, the findings demonstrate that polarization-engineered angular modulation provides an efficient and simplified strategy for enhancing reflectance sensitivity in $MAPbI_3$-based multilayer systems, offering practical design guidelines for angle-selective photonic sensors and optical coatings.

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