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Thickness-Dependent Optical Confinement in Glass/TiO₂/Perovskite (MAPbI₃) Thin Films: A Spectral Integration Approach

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Abstract: In this study, we proposed a theoretical investigation of the optical interaction of multilayer thin films designed from glass/TiO₂/MAPbI₃ using the Transfer Matrix Method (TMM) in the range of 300–800 nm of visible light. The effect of TiO₂ interlayer thickness (20 nm, 50 nm, and 100 nm) on the confinement of interference light within a 400 nm-thick MAPbI₃ absorber layer was analyzed. Our results showed that adding a layer of TiO₂ modifies the phase conditions within the structure, leading to a redistribution of the optical field and a thickness-dependent absorption behavior. We also used spectral integration to determine the overall effective absorption across the visible light spectrum. We studied three layer thicknesses, but the 50 nm TiO₂ layer exhibited the highest average absorption (0.259), representing an improvement of approximately 5.3% compared to the 100 nm thickness. In the results obtained, we focused on the importance of improving the thickness of the multiple layers in perovskite systems that are designed as a crystalline structure, and cover important applications that work on developing the structure of thin-film photovoltaic structures.

Keywords: Perovskite thin films; Transfer matrix method; Optical confinement; Multilayer structures ;Spectral integration.

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1. Introduction

Perovskite materials are classified as high-efficiency semiconductors due to their high absorption coefficient, making them suitable for optoelectronic and photonic applications, their controllable and tunable direct bandgap, and their large charge carrier diffusion length [1-4]. Among them, the compound (MAPbI₃) exhibits strong absorption in the visible spectrum, enabling efficient light capture in thin films with thicknesses of less than a micron [2, 4].

In the inner core of multi-layered thin films, the optical response depends on many factors and is not limited to absorption alone, but is also affected by interference effects from the many reflections that occur at the contact surfaces of the materials [5], [6]. The difference in the refractive indices of the layers that make up the core, as well as the optical path length (that light travels within each material), are the differences that determine the conditions of constructive and destructive interference. Because of these conditions, any change in the thickness of the layer leads to significant changes in the reflection, transmission, and absorption spectra of the mediums of those layers [5,7].

The use of Titanium dioxide (TiO₂) is widely used as an electron transport layer in perovskite solar cells, due to its physical properties in terms of its bands and optical transparency in the visible light range [8]. In addition to its electrical role, the TiO₂ interlayer influences the optical field distribution within the device by altering phase matching conditions and adding extra interfaces [9, 10]. Although many studies have brought up the electrical and structural optimisation of TiO₂-based structures, theoretical research focused on thickness-based optical interference effects in simplified glass/TiO₂/MAPbI₃ multilayer systems is still limited.

The Transfer Matrix Method (TMM) provides a clear and precise analytical method for modeling electromagnetic wave propagation in layered media by solving Maxwell's equations under appropriate boundary conditions [5], [11]. Transfer Matrix Method has been widely used in optical simulation models, as it provides extremely accurate calculations for determining the magnitudes of reflection, absorption, and transmission spectra. Perovskite compounds have garnered significant attention for such simulations. [6,7]

The presented analysis offers practical guidance for improving optical thickness in perovskite-based multilayer structures and contributes to a clearer understanding of controlled light management in thin-film photovoltaic systems.

To understand the mechanisms of constructive and destructive interference, we conducted a theoretical analysis of the optical behavior of glass/TiO₂/MAPbI₃ multilayer thin films using the (TMM). The focus was specifically on how variations in the thickness of TiO₂ interlayer affect the absorption characteristics in the UV-Vis and visible ranges. The results indicated that thickness-dependent interference effects play a key role in enhancing the effective absorption figures. These findings contribute to improving the optical performance of perovskite-based multilayer devices.

2. Theoretical Model

We analyzed the optical response of the studied multilayer structure using the (TMM), which provides a clear model of wave propagation in different multilayer insulating media. by solving Maxwell's equations under appropriate boundary conditions [5,11]. The TMM is used in thin-film optics to assess the reflection, transmittance, and absorption spectra of multilayer systems due to its numerical stability and suitability for dielectric layer structures [6,7,12,14].

In this paper, we assumed the electromagnetic wave incident perpendicularly. We also considered all media to be non-magnetic ($\mu = \mu_0$). We proposed the crystal structure presented for study.:

Air / TiO₂ / MAPbI₃ / Glass

Where MAPbI₃ acts as an absorbent semiconductor, while TiO₂ acts as an interfacial layer that modifies the optical phase conditions within the structure.

From Eq. 1, the optical properties of each layer are described by a composite refractive index :

$$\hat{n} = n + ik \dots (1)$$

where n represents the real refractive index and k denotes the extinction coefficient. For simplicity, constant refractive indices were assumed within the 300–800 nm spectral range in order to isolate interference-driven effects from dispersion-related variations. Such approximations are commonly adopted in theoretical thin-film modeling studies when the focus is on phase-dependent optical confinement rather than material dispersion analysis [7,15].

For a homogeneous thin film of refractive index n_j and thickness d_j , the characteristic matrix is given by Eq. (2) [5]:

$$M_j = \begin{bmatrix} \cos(\delta_j) & \sin(\delta_j \frac{i}{\eta_j}) \\ i\eta_j \sin(\delta_j) & \cos(\delta_j) \end{bmatrix} \dots\dots(2)$$

Where the phase thickness δ_j is defined in Eq. 3 :

$$\delta_j = \frac{2\pi}{\lambda} n_j d_j \cos \theta_j \dots\dots(3)$$

and η_j is the optical admittance of the j-th layer. Through the process of multiplying the layers' matrices from Eq. 4, we were able to obtain the overall transport matrix of the multilayer system [5,14]:

$$M = \prod_j M_j \dots\dots (4)$$

The reflection coefficient r was calculated from the elements of the total matrix using Eq. 5, and the reflection is determined as follows:

$$R = |r|^2 \dots\dots\dots (5)$$

To extract absorption inside the MAPbI₃ layer, the absorption coefficient was calculated using the Beer–Lambert relation Eq. 6 [12,16]:

$$\alpha = \frac{4\pi k}{\lambda} \dots\dots(6)$$

After finding the effective absorption coefficient within the layer, we approximated it as follows:

$$A_{\text{eff}} = (1 - e^{-\alpha d})(1 - R) \dots\dots (7)$$

The above equation takes into account the absorption of the intrinsic material with the inclusion of reflection losses at the interfaces, which gives us a practical picture of light energy dissipation in multilayer thin films [6,7,17].

The thickness of MAPbI₃ was assumed to be fixed at 400 nm, while the thickness of the TiO₂ interlayer was varied (20 nm, 50 nm, and 100 nm) to study its effect on optical confinement resulting from interference and absorption enhancement.

3. Results and Discussion

3.1 Optical Response of the Single-Layer Structure

Figure 1 shows the wavelength-dependent reflectance (R), transmittance (T), and absorbance (A) spectra of the single-layer Glass / MAPbI₃ / Air structure within the 300–800 nm spectral range.

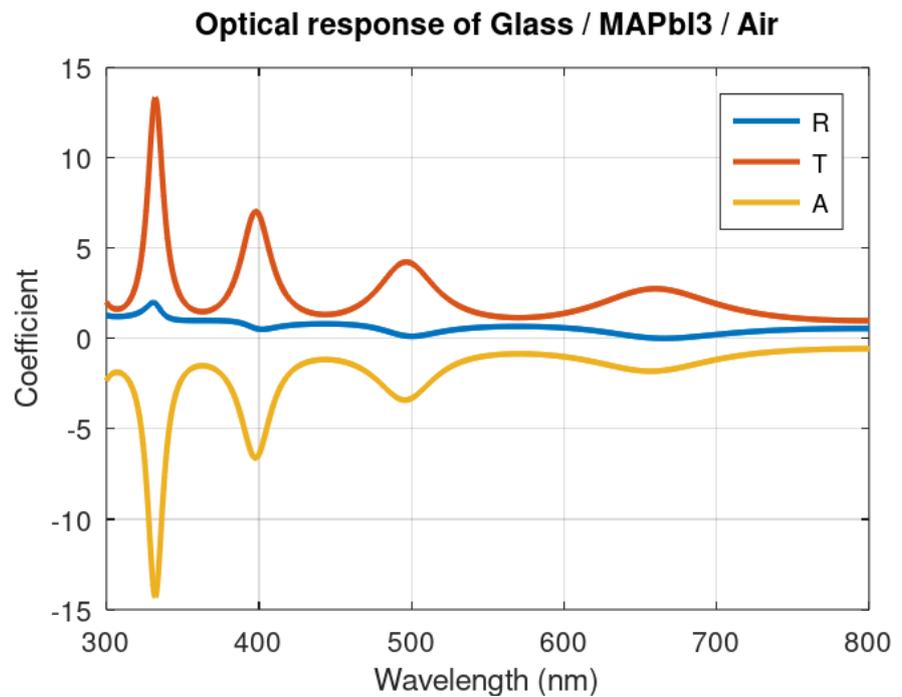


Figure 1. Reflectance (R), transmittance (T), and absorbance (A) spectra of the single-layer Glass / MAPbI₃ / Air structure in the UV–Visible region.

The results above show a striking oscillatory behavior in the optical parameters due to interference effects within a 400 nm thick MAPbI₃ layer. Reflection suffers moderate fluctuations across the visible light region, while absorption shows wavelength-dependent enhancement, and this enhancement is subject to phase-dependent optical confinement within the thin layer. These interference-induced oscillations are characteristic of thin-film semiconductor structures and are consistent with classical multilayer optics theory [14,18].

The numerical absorption values at specific wavelengths are listed in Table 1.

Table 1. Effective absorption values resulting from different thicknesses of TiO₂

Wavelength (nm)	Absorption (20 nm)	Absorption (50 nm)	Absorption (100 nm)
300.501	0.0	0.0	0.0
325.526	0.0	0.0	0.0
350.551	0.0	0.0	0.0
375.576	0.004	0.02	0.004
400.601	0.143	0.081	0.174
425.626	0.381	0.199	0.247
450.651	0.14	0.444	0.121
475.676	0.149	0.188	0.254
500.701	0.349	0.179	0.517
525.726	0.556	0.3	0.255
550.751	0.325	0.531	0.196
575.776	0.209	0.425	0.247
600.801	0.189	0.257	0.422
625.826	0.229	0.205	0.512

650.851	0.332	0.217	0.352
675.876	0.468	0.274	0.256
700.901	0.503	0.374	0.226
725.926	0.413	0.472	0.237
750.951	0.315	0.476	0.279
775.976	0.251	0.392	0.351

By observing the previous table, we can see that absorption values increase significantly in the visible light region compared to the near-UV range, where reflection losses are predominant.

3.2 Optical Response of the Bilayer Structure

Figure 2 explains the effect of introducing an intermediate layer of (TiO_2).

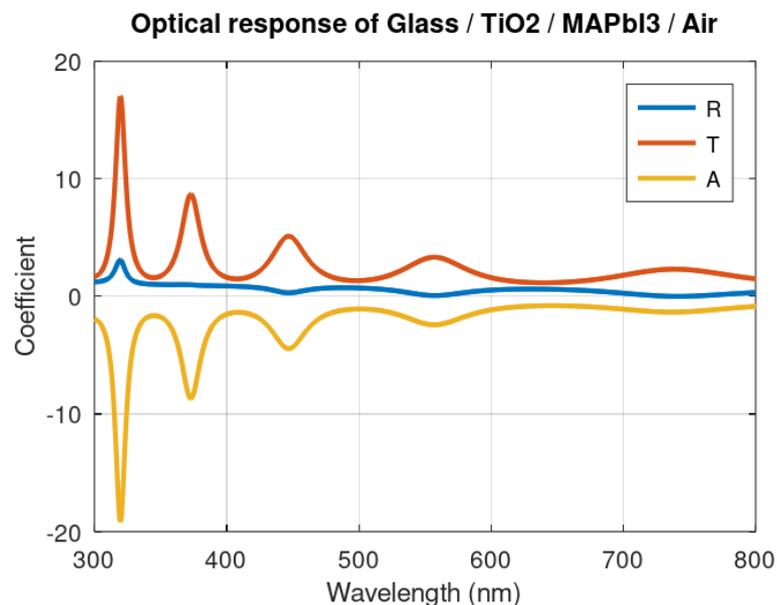


Figure 2. Optical response of the bilayer $\text{Glass} / \text{TiO}_2 / \text{MAPbI}_3 / \text{Air}$ structure in the UV-Visible region.

The introduction of TiO_2 layer causes a change in the phase conditions within the structure, resulting in a redistribution of the electromagnetic field within the MAPbI_3 layer. When the spectral peak positions and absorption spectral amplitude differ in the bilayer configuration, they differ from those in the bilayer structure, distinguishing it from a monolayer structure. The primary reason for these properties is the constructive and destructive interference behavior resulting from the optical path added by the TiO_2 layer. [14,17].

3.3 Influence of TiO_2 Thickness on Integrated Absorption

Using spectral integration, we were able to determine the effect of titanium dioxide layer thickness in order to calculate the effective absorption mean within the wavelengths (300 – 800)nm, and the results for the curves were shown in the following figure.

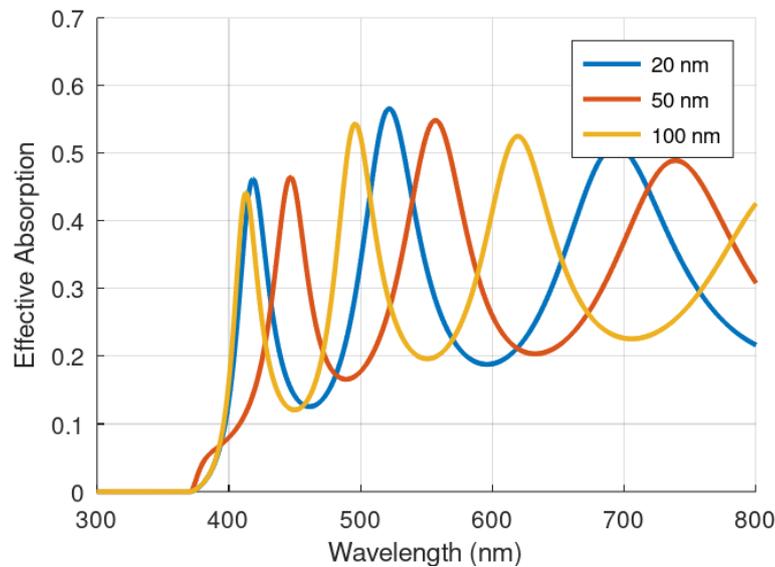


Figure 3. Effect of TiO₂ layer thickness on absorption of multilayer structure

After performing mathematical operations on the values resulting from the simulation process in the equations mentioned in the theoretical section, the absorption coefficients were listed in the table below.

Table 2. Average Absorption for Different Thicknesses of TiO₂

TiO ₂ Thickness (nm)	Average Absorption
20	0.254
50	0.259
100	0.246

The results clearly show that a 50 nm of TiO₂ layer achieves the highest integrated absorption (0.259). This represents an improvement of approximately 5.3% compared to a 100 nm layer and about 2% compared to a 20 nm layer.

The improved performance at 50 nm is attributed to more favorable phase-matching conditions, which increase the rate of constructive interference within the absorbing layer. Increasing the titanium dioxide layer thickness beyond this optimum value alters the interference pattern, slightly reducing the overall light-trapping efficiency [18-20].

3.4 Comparison with Previous Studies

Following up on the absorption behavior studied through thickness variation in previously studied interferometric multilayer photovoltaic systems, we found consistency in the results obtained as an improved transport layer thickness enhances light confinement efficiency.

At the same time, our results confirmed that small differences in interlayer thickness significantly affect optical confinement in perovskite-based thin-film structures.

4. Conclusion

In this study, the optical response of multilayer glass/TiO₂/MAPbI₃ thin films was systematically investigated using the Transport Matrix Method within the 300 – 800 nm spectral range. The results focused specifically on the absorption behavior induced by

interference rather than modeling electrical devices, thus isolating phase-dependent optical confinement effects.

Upon further examination, the addition of an intermediate titanium dioxide layer significantly modifies the optical field distribution within the absorbing MAPbI₃ material. Three thicknesses were investigated, with the 50 nm titanium dioxide layer exhibiting the highest mean effective absorption (MEA) (0.259), representing an increase of approximately 5.3% compared to the 100 nm layer.

This work utilizes spectral integration to provide a quantitative and physically significant assessment of absorption performance across the entire visible light spectrum, unlike studies that primarily focus on electrical simulations or spectral peak comparisons. The results confirm that small variations in interlayer thickness can significantly impact optical confinement through constructive interference mechanisms.

The presented analysis offers practical guidance for improving optical thickness in perovskite-based multilayer structures and contributes to a clearer understanding of controlled light management in thin-film photovoltaic systems.

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