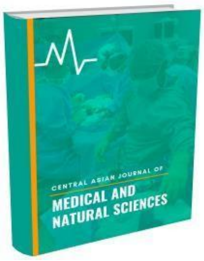

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Article

Optical Energy Management in $MAPbI_3$ Perovskite-Based Smart Windows Using TiO_2 Interlayers: A Transfer Matrix Study

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Abstract: The Optical multilayer perovskite thin films were integrated as a basic structure with smart window systems for Green buildings to to develop energy outputs, and the structure was numerically simulated due to its strong light–matter interaction and tunable optical and physical properties. We propose the Transfer Matrix Method (TMM), which was implemented in MATLAB. We used fixed constants and selected variables in order to study the differences. The variable was represented by the addition of a TiO_2 layer to the structure under study. First, we studied structure without TiO_2. After that, we studied the multilayer structure where we used three thicknesses for TiO_2 (20, 50, and 100 nm) For each case, we analysed important optical properties such as spectral stability, solar energy regulation, rejections of unwanted reflection, and transmission behaviour. The study was carried out in the visible spectral range. We calculated absorbance, reflectance, and transmittance for each case. From all of the above, we observed the enhanced performance of perovskite thin films highlighted their effectiveness in optical energy management. This can help thin-film researchers in the field of optics and photonics to design multilayer structures that can confine light efficiently through rapid, scalable, and optimizable modelling processes.

Keywords: $MAPbI_3$; multilayer structure ;TiO_2 interlayer ; Transfer Matrix Method ; smart windows

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1. Introduction

Perovskite thin films have been extensively researched recently, primarily because to their high absorption capacity and strong light interaction [1-3]. Furthermore, their physical characteristics can be modified based on the intended use. For these reasons, they have become attractive materials for optoelectronic and photonic devices. More recently, researchers have explored their use in smart window systems and energy-efficient buildings. In such cases, managing incoming solar radiation is essential to improve indoor thermal conditions and to lower energy consumption.[4].

In multilayer perovskite structures, titanium dioxide (TiO_2) is commonly used as an electron transport layer [5]. However, in addition to its electrical function, TiO_2 also plays an important optical role by modifying the distribution of the electromagnetic field through refractive index contrast and interference effects [6,7]. Several studies have reported that introducing TiO_2 layers can significantly influence the absorption behavior of perovskite films [8,9].

Most previous works mainly focused on enhancing optical absorption for photovoltaic applications and did not consider the full optical response of the multilayer system. The simultaneous control of reflectance, transmittance, and absorbance is particularly important for smart window applications, where optical energy management rather than absorption maximization is required [10].

Therefore, this work investigates a Glass / TiO_2 / $MAPbI_3$ / Air multilayer structure using the transfer matrix method. The optical response (R, T, and A) is calculated in the UV–Visible range, and the effect of TiO_2 interlayer thickness on light distribution and energy balance is systematically analyzed. This study introduces a new application-oriented perspective for perovskite thin films as optical energy management layers for smart window systems.

2. Theoretical Model

The optical response of the multilayer structure can be described using the Transfer Matrix Method (TMM) [11]. Light propagation in stratified optical medium is frequently modeled using this method. It is formulated on the basis of Maxwell's equations, where the tangential components of the electromagnetic field are assumed to remain continuous at each interface between adjacent layers. Due to its accuracy and computational simplicity, the TMM has been widely adopted in the analysis of multilayer optical systems and thin-film structures.[12,13].

Each layer in the stack, defined by its refractive index n_j and thickness d_j, is represented through a characteristic matrix M_j :

$$M_j = \begin{bmatrix} cos(\delta_j) & sin(\delta_j \frac{i}{\eta_j}) \\ i\eta_j \sin(\delta_j) & \cos(\delta_j) \end{bmatrix} \ldots\ldots\ldots(1)$$

where δ_j represents the phase term associated with the optical path inside the layer:

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

When several layers are combined, the overall transfer matrix is constructed through the successive multiplication of the individual layer matrices. In the present configuration, the structure consists of Glass / TiO_2 / $MAPbI_3$ / Air, and the global matrix is formed accordingly.

$$M_{tot} = M_{TiO2} \times M_{MaPbI3} \ldots. (3)$$

The reflection and transmission coefficients are determined using the components of the total matrix.

$$r = \frac{B-C}{B+C} \ldots\ldots\ldots\ldots\ldots\ldots\ldots (4)$$

$$t = \frac{2}{B+C} \ldots\ldots\ldots\ldots\ldots\ldots\ldots(5)$$

Where

$$B = M_{11} + C \ \ldots\ldots\ldots(6)$$

$$M_{12}Y_s = M_{21} + M_{22}Y_s \ldots\ldots(7)$$

and Y_s=n_s is the optical admittance of the substrate.

The reflectance R and transmittance T are then obtained from:

$$R = | r |^2 \ldots\ldots\ldots\ldots\ldots\ldots (8)$$

$$T = | t |^2 \cdot Re(\frac{Y_s}{Y_0}) \ldots\ldots\ldots\ldots (9)$$

The absorption coefficient (α) is used to describe optical absorption in the perovskite layer as follow.

$$A = \frac{4\pi k}{\lambda} \ldots\ldots\ldots\ldots\ldots\ldots (10)$$

where k is the material's related extinction coefficient.

The following formula is used to get the appropriate effective absorbance:

$$A_{eff} = \left(1 - e^{-\alpha d}\right)(1 - R) \ldots \ldots (11)$$

The earlier formulation gives a realistic representation of light absorption in the multilayer structure by taking into consideration both the intrinsic material absorption and the optical losses brought on by surface reflection. By incorporating these features, the model can be effectively applied in the analysis of optical systems and thin-film structures based on perovskite materials.[14–16].

3. Structure and Simulation Parameters

The perovskite-based multilayer structure was investigated using the configuration Glass / TiO_2 / $MAPbI_3$ / Air. It was designed to function as a single optical energy management layer for smart window applications. The simplicity of this architecture was intentionally chosen to minimize structural complexity while enabling effective control of light distribution through interference effects [17].

Based on previously published literature, the refractive index of the glass substrate was taken as (1.5) , while the TiO_2 interlayer was assigned a refractive index of (2.4). The perovskite layer was modeled using a complex refractive index, where the real and imaginary components were adopted from experimentally reported optical data in earlier studies [18]. The surrounding medium was considered to be air with a refractive index of (1).

All simulations were performed in the UV–Visible spectral range from **300 to 800 nm**, which covers the most relevant part of the solar spectrum for smart window and photonic applications. Different thickness values were used for the TiO_2 layer (20, 50,100) nm in order to examine the effect of thickness on the optical energy distribution within the multilayer stack. The thickness of the $MAPbI_3$ layer was kept fixed at the value adopted in the base structure to allow for a meaningful comparison between the investigated thickness conditions.

The optical calculations were carried out under normal incidence using the transfer matrix method as described in the theoretical model section. The reflectance (R), transmittance (T), and effective absorbance (A) were calculated for each case. These parameters were then used to evaluate the optical energy management performance of the proposed smart window system.

4. Results and Discussion

4.1 Optical response of the single-layer structure

Figure 1 shows the calculated reflectance (R), transmittance (T), and absorbance (A) spectra of the Glass / $MAPbI_3$ / Air structure in the UV–Visible region.

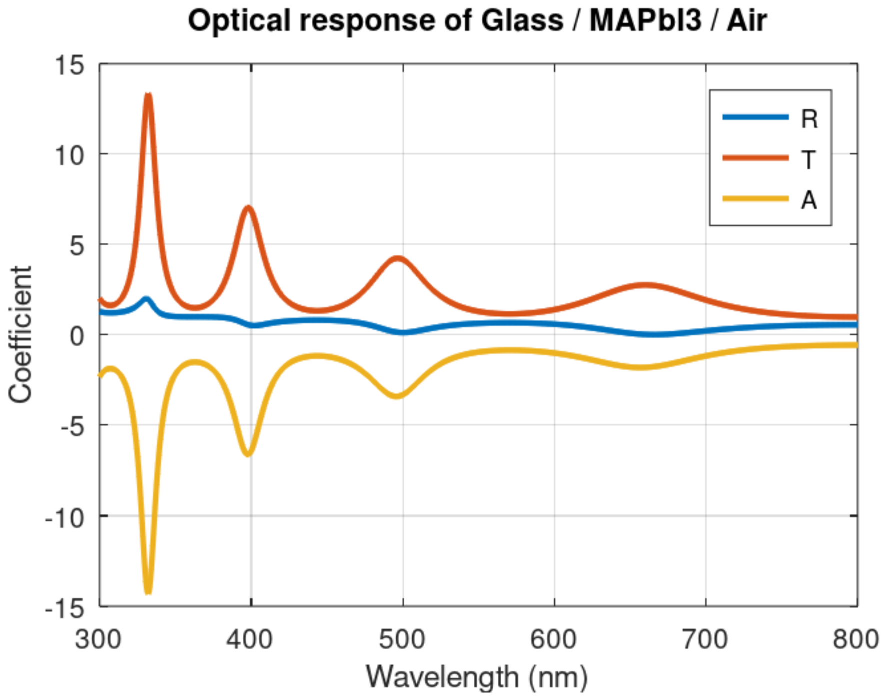

Figure 1. Reflectance (R), transmittance (T), and absorbance (A) spectra of the single-layer Glass / $MAPbI_3$ / Air structure in the UV–Visible region.

As shown in Figure 1, the $MAPbI_3$ layer exhibits strong absorption in the visible region due to its direct bandgap and high absorption coefficient. The reflectance and transmittance values exhibit oscillations as a result of the Fabry–Pérot interference that takes place inside the thin layers. These oscillations are a useful sign that the optical field is tightly contained within the perovskite layers, which strengthens the bond between matter and light. The overall energy utilization efficiency of this design is lowered, however, because a discernible amount of the incident light is still reflected or transmitted.

4.2 Role of TiO_2 Thickness in Optical Energy Control

The following figure shows the multilayer configuration's effective absorbance behavior at thicknesses of 20, 50, and 100 nm.

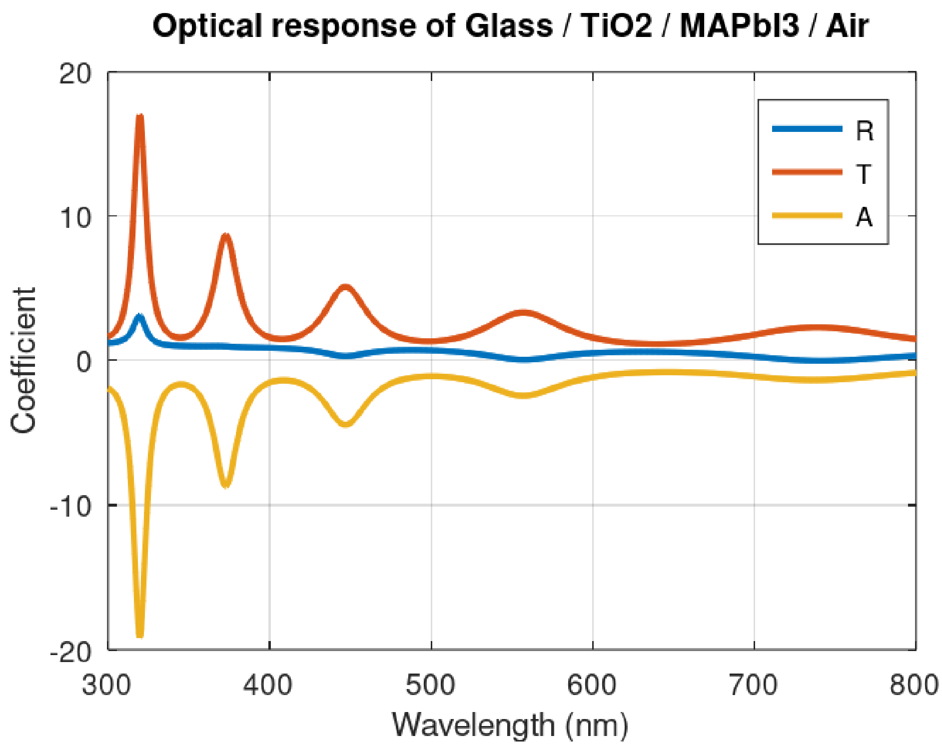

Figure 2. ***Wavelength-dependent optical properties of the Glass/TiO_2/$MAPbI_3$/Air bilayer structure in the UV–visible spectrum.***

As can be seen from the above picture, the addition of the TiO_2 interlayer causes a discernible difference in absorbance when compared to the single-layer structure (picture 1). The main cause of this notable improvement is the difference in refractive index between TiO_2 and $MAPbI_3$, which modifies the phase conditions and causes the optical field to be redistributed inside the multilayer structure. The variations observed for the three TiO_2 thicknesses can be interpreted as follows:

A reduced light confinement effect results from the phase shift being too modest to create constructive interference for the 20 nm thickness.

The structure gets closer to a resonant condition at 50 nm, which strengthens field localization inside the perovskite layer and increases absorbance as a result.

Phase mismatch causes partial destructive interference when the thickness approaches 100 nm, lowering the effective absorbance.

4.3 Comparative numerical evaluation

Table 1 displays the calculated mean absorbance values for the examined TiO_2 thicknesses.

Table 1. The results obtained from the analysis of effective absorbance values for different TiO_2 thicknesses.

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

The 50 nm layer is the ideal thickness for attaining increased absorbance, according to the values shown in the above table. These findings support the existence of an ideal thickness at this value and show that interference effects and optical path length are additional governing elements that affect the optical response in addition to intrinsic material absorption.

It is clear by comparing the statistics of the single-layer and multilayer structures that the multilayer structure offers more effective light confinement than the single-layer equivalent. Because of this fact, a multilayer design-based energy management strategy is proposed, in which light is managed by controlled interference as opposed to only optimizing absorption.

5. Conclusion

Significant differences in optical behavior were found by numerically analyzing the crystalline structure, which included the addition of a TiO_2 interlayer of varying thickness. The 50 nm layer yielded the best result out of all the tested values, exhibiting greater light confinement within the visible range and higher effective absorbance.

The comparison of thicknesses shows that optical performance is not exclusively dependent on the materials' inherent absorption. Rather, the total response is shaped by phase-related interference within the multilayer stack. Modifying the TiO_2 layer alters the internal field distribution, which simultaneously influences absorption, transmission, and reflection.

Specifically, by reducing reflection losses while preserving enough transmission and improving absorption, the 50 nm design offers a more evenly distributed energy. This behavior demonstrates that the TiO_2 layer is not just an extra absorbent layer but also an optical control element.

The current findings are in line with past research on light confinement in multilayer systems of perovskites and TiO_2. However, this work examines the structure from an energy-regulation standpoint, in contrast to many other research that focused on photovoltaic absorption increase. As a result, the multilayer configuration is regarded as a programmable optical system appropriate for controlling solar radiation in applications including smart windows and integrated buildings.

Overall, the results indicate that well-tuned perovskite-based multilayers may help with the realistic design of smart window devices and might operate as functional coatings for energy-efficient glazing systems.

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