Research Article / Araştırma Makalesi GU J Sci, Part A, 9(2): 164-172 (2022) https://doi.org/10.54287/gujsa.1129794

Gazi University
Journal of Science
PART A: ENGINEERING AND INNOVATION
http://dergipark.org.tr/gujsa

Theoretical Evaluation of Angle-Dependent Optical Properties of a Thin Film Solar Cell including One-Dimension Photonic Crystals

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Keywords

Photonic Crystal
CdTe Solar Cell
Light Management Engineering
Transfer Matrix Method
Angular Dependent Optical Properties

Abstract

The effective use of photonic-based integrated systems, whose optical properties can be tuned through light management engineering in optoelectronic devices, constitutes the backbone of today's technology. Especially in systems such as CdTe-based solar cells with well-known and high efficiency, one-dimensional photonic crystal designs emerge as an effective way to provide an electronic or optical improvement. With this intention, in this study, the optical spectra of the MgF_2/MoO_3 one-dimensional photonic crystal integrated into the CdTe solar cell to improve photon harvesting were investigated theoretically under both bottom and top illumination according to the incidence angle of the electromagnetic wave. The transfer matrix method was used to calculate the angle dependent optical spectra. Since the electromagnetic wave interacts directly with the photonic crystal, it has been observed that the optical properties are more dependent on the angle under the top illumination compared to the bottom one. For top illumination, up to 30°, there is no significant change in reflection in the photonic band gap, but reflection drops significantly at incidence angles greater than 30°. Also, increasing the angle indicates that the low wavelength tail of the photonic band gap shifts to shorter wavelengths and enters the visible region. In the photonic band gap, for angles greater than 45°, the probability of absorption increases significantly as more electromagnetic waves enter the structure. For the bottom illumination, there is no serious dependence on the angle of incidence. For 75°, there is an increase in reflection for all wavelengths and, therefore, a decrease in absorption.

Cite

Cetinkaya, C. (2022). Theoretical Evaluation of Angle-Dependent Optical Properties of a Thin Film Solar Cell including One-Dimension Photonic Crystals. *GU J Sci, Part A*, *9*(2), 164-172.

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Article Process

Submission Date	12.06.2022
Revision Date	18.06.2022
Accepted Date	27.06.2022
Published Date	28.06.2022

1. INTRODUCTION

Photonic crystals (PC) are structures in which structures with different dielectric constants are spatially arranged in any direction (Liu et al., 2019). These structures are a hot topic of research in the field of photonics for optical fibers, light emitting diode (LED), sensors, photovoltaic devices, lasers, discrete and integrated optical components, illumination, and quantum computing (Lova et al., 2018). The propagation of the electromagnetic wave is modified by the periodic regulation of the dielectric constant and hence the index of refraction in a PC. During the propagation of the electromagnetic wave in a particular direction, Bragg scattering occurs, and thus the propagation of the electromagnetic wave in a particular frequency or wavelength range can be prohibited by the PC (Liu et al., 2019). This gap where the electromagnetic wave is not allowed to pass is called the photonic band gap (PBG) (Yablonovitch et al., 1991; Liu et al., 2019).

PCs are classified into 1-dimensional (1D), 2-dimensional (2D), and 3-dimensional (3D) depending on the number of spatial orientations in which the periodic dielectric constant changes. 1D-PCs are structures in which the dielectric constant changes periodically in only one direction, and they consist of structures with two or more dielectric constants that are superimposed or deposited in a single direction (Liu et al., 2019). Therefore, 1D-PCs have a PBG for the propagation of photons in only one direction. By integrating PBG created with

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PCs into solar cell (SC), the optical properties of SC can be changed significantly. These changes can be made to increase photovoltaic performance, improve semi-transparent (ST) properties, provide selective transmittance or color modification. Especially with the integration of 1D-PCs into ST organic SC (ST-OSC), structures showing improvement in cell performance have been designed (Hu et al., 2018). Although initial studies were aimed at improving cell performance, more recently 1D-PCs have also focused on modifying the optical properties of ST-OSCs (Hu et al., 2018; Zhang et al., 2019).

The integration of PCs into structures such as CdTe-based SCs with high efficiency of 22.1% (Green et al., 2020) and whose electrical properties are well known is very important in terms of improving optical properties. CdTe-based SCs are notable for their high absorption and direct optical band gap very close to 1.45eV. The absorber layer CdTe forms a heterojunction with a thin n-type CdS. The production of CdS/CdTe-based SCs for technological applications is highly advantageous in terms of their mechanical functionality, long-term thermal and mechanical stability, high efficiency and light weight. While the CdTe absorption coefficient is quite high for the visible region, it is quite low for wavelengths of 800 nm and longer. Therefore, SC structures in which CdTe is used as the absorber layer do not absorb photons efficiently in the near-infrared region (NIR). Therefore, in order to increase the photovoltaic performance in CdTe-based SCs, it is very important to carry out light management applications that will improve re-harvesting in the NIR region and to design functionally designed photonic crystals for this purpose. It is important to examine the optical characteristics and photon absorption properties depending on the angle of incidence of the light in SC structures with photonic crystal integration, especially for practical applications other than the ideal situation where the sun rays are perpendicular to the SC structure.

In this study, the optical spectra and photocurrent densities (J_{ph}) of the CdTe-based SC, in which a 4-period magnesium fluoride/molybdenum trioxide (MgF_2/MoO_3) photonic crystal with a PBG in the NIR region are integrated, are theoretically investigated. MgF_2 is transparent over a wide range of wavelengths and is therefore used in windows, lenses and prisms. MoO_3 is transparent in the visible region and is used as an electron transport layer in many optoelectronic devices. Optical spectra such as transmittance, reflection and absorption were calculated using the Transfer Matrix Method (TMM). Calculations were made depending on the angle of incidence of the electromagnetic wave according to the state of CdTe base SCs under upper and lower illumination, and bi-surface operating conditions were discussed optically.

2. MATERIAL AND METHOD

The structure of the CdTe-based SC in which the 4 period MgF_2/MoO_3 photonic crystal examined in the study is integrated is given in Table 1. Fluorine Tin Oxide (FTO), which is very transparent in the visible region and offers excellent conductivity, is used as the bottom contact in SC structures (Çetinkaya et al., 2021a; 2021b). SnO_2 is located on the bottom contact as the electron transport layer (ETL), which provides selective electron transmission in the structure. SnO_2 also has a wide band gap value, so that most of the photons from the bottom side can be transferred to the active site (Xiong et al., 2018). In the SC structure, CdS is included as the window layer. Here, CdS is n-type and has a relatively thick p-type CdTe with an absorber layer on it. The free carriers formed as a result of photoproduction are collected by the internal electric field formed at the CdS/CdTe heterojunction. Finally, the MoO_3 BSF layer was added to limit the movement of minority carriers around the pn junction, to collect more efficiently under the effect of the internal electric field and to reduce recombination. Thanks to the convenient work function of MoO_3, the electrons released as a result of photo-generation in the SC are prevented from reaching the top contact, and selective transport for the cavities can be achieved (Lin et al., 2010; He et al., 2020). Therefore, MoO_3 acts as a hole transport layer (HTL) in the SC structure. Au metal may be present on the BSF for direct ohmic contact. However, in the SC structure presented in the study, only a SC structure that allows the modification of optical characteristics with photonic crystal has been investigated. For experimental studies, thin and strip metal contact can be made right next to the photonic crystal with appropriate masking in the CdTe-based SC to be produced. By designing the PBG in the NIR region in CdTe-based SC, MgF_2 and MoO_3 with different refractive indices were used to improve the absorption by re-harvesting.

Table 1. *Structure of a CdTe-based SC with a 4 period MgF_2/MoO_3 photonic crystal*

One-dimension Photonic Crystal	$(MgF_2/MoO_3)^4$	155/100 nm
BSF-Hole transport layer	MoO_3	30 nm
Absorber layer	CdTe	600 nm
Window layer	CdS	50 nm
Electron transport layer	SnO_2	100 nm
Transparent bottom contact	FTO	--

Optical spectra such as absorption, reflection and transmittance of the CdTe-based SC in which the 4 period MgF_2/MoO_3 photonic crystals examined in the study were integrated were calculated using the Transfer Matrix Method. TMM is a very effective method that examines the propagation of electromagnetic waves in multilayer material systems and is used to calculate the optical properties of the structure (Nguyen et al., 2012; Li et al., 2014; Wang et al., 2014; Çetinkaya et al., 2022). The application of TMM to the SC structure is achieved by connecting the electric and magnetic field components of the electromagnetic wave to each other with a transfer matrix in each layer. In addition, optical calculations of the structures formed as a result of the integration of conductive contacts in the SC structure with different dielectric materials can be made. The calculation method used in the study and the equation sets included in TMM is given in our previous study (Çetinkaya et al., 2021b).

3. RESULTS AND DISCUSSION

Currently, studies focused on material modification are not preferred for more efficient cell designs in systems with high efficiency such as CdTe/CdS SCs. In particular, approaches such as effective photonic crystal designs that will increase photon harvest by making more use of electromagnetic radiation, and the use of bifacial configuration by modifying the orientation of the light have been preferred. In this direction, with a suitable optical engineering method, increasing the absorption in this region may be an effective approach since the absorption of CdTe, which acts as the absorber layer in CdTe/CdS SC as the first target, is very weak in the long wavelength region of AM1.5G. The variation of the absorption coefficient of CdTe depending on the wavelength is given in Figure 1.

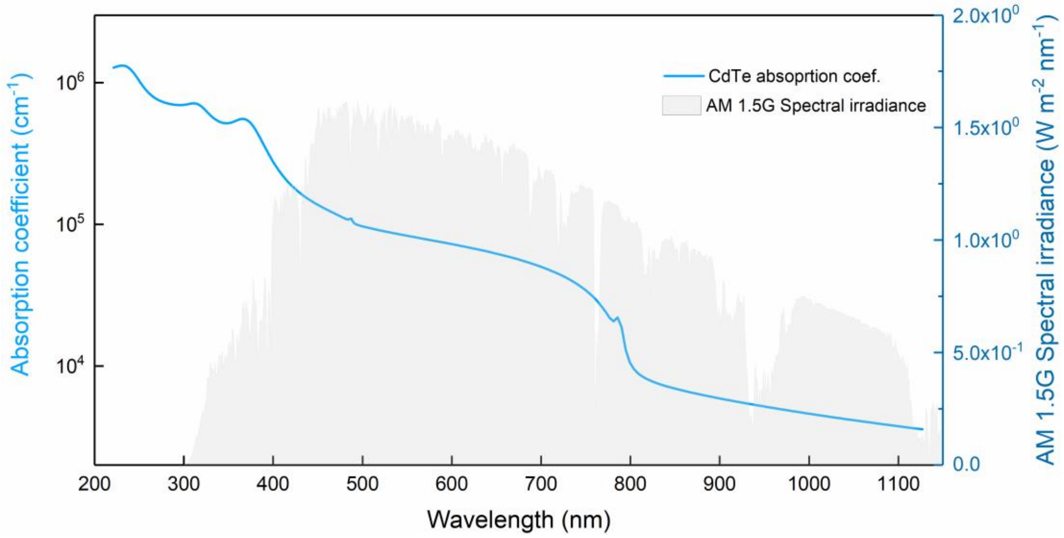

Figure 1. *Variation of CdTe absorption coefficient with wavelength*

When Figure 1 is examined, it is seen that the absorption characteristic of the absorber layer CdTe has decreased considerably in the NIR region. It is quite possible that photons in this region will pass through the CdTe-based SC without being absorbed. Therefore, in order to increase the absorption probability in this region, the photons can be reflected back into the structure and converted into efficient harvesting, which can positively affect the photovoltaic performance of the cell. Therefore, within the scope of the study, we started to analyze the angle dependence by first integrating it into the CdTe/CdS SC system of a 4 period MgF_2/MoO_3 1D-PC with a PBG center at λ_B=850 nm. Theoretical analysis was made over optical spectra calculated according to the incidence angle of the electromagnetic wave on CdTe/CdS SC with MgF_2/MoO_3 1D-PC under top and bottom illumination. Firstly, optical spectra of SC under top illumination were studied. Because with the top illumination, the electromagnetic wave will first interact with the MgF_2/MoO_3 1D-PC system and the PBG characteristic can be observed directly in the optical spectra. The reflection, transmittance and absorption spectra calculated by TMM of CdTe/CdS SC with MgF_2/MoO_3 1D-PC under top illumination are given in Figure 2a, b and c, respectively.

In the reflection spectrum of the CdTe-based SC, the direct effect of PBG at λ_B=850 nm formed with MgF_2/MoO_3 1D-PC is seen. In the case of perpendicularity of the electromagnetic wave (θ=0°), the reflection characteristic of PBG, which has a center at 850 nm and a width of about 300 nm, shows itself. For θ=0° top illumination, wavelengths longer than 700 nm are directly reflected from the surface and electromagnetic waves cannot enter the SC. Therefore, a decrease in reflection and absorption spectra is observed in this region. This causes a serious decrease in photovoltaic performance by preventing sufficient foton harvesting in the SC's top illumination condition. Therefore, the integration of MgF_2/MoO_3 1D-PC with PBG at λ_B=850 nm to the CdTe/CdS SC system may not be an effective approach for top illumination.

For top illumination, when the optical spectra are examined according to the incidence angle of the electromagnetic wave, there is no serious change in the reflection intensity in the region where the PBG is formed, up to θ=30°, but the reflection intensity drops significantly at incidence angles greater than θ=30°. Also, the increase in θ indicates that the low wavelength tail of the PBG shifts to shorter wavelengths and enters the visible region. This situation can be explained by the shift of the central wavelength at which λ_B is adjusted in the PBG design, to short wavelengths, as seen in Equation 1, together with the angle of incidence. Therefore, it is seen that the wavelength range for which the PBG is designed and the intensity of reflection are directly dependent on the incidence angle of the electromagnetic wave.

$$\frac{\lambda_B}{4\cos\theta} = n_i d_i \tag{1}$$

where, λ_B is the Bragg wavelength which is the central wavelength corresponding to the resonance wavelength of the PBG formed by the PC, n_i is the real part of the refractive index, and d_i is the layer thickness of each layer.

As a remarkable feature, the increase in the angle of incidence of the electromagnetic wave decreases the reflection intensity but increases the transmittance and especially the absorption intensity of the SC in the designed PBG. Especially in PBG, with incidence angles greater than θ=45°, the probability of absorption increases significantly as more electromagnetic waves enter the SC. At the same time, the shift of the PBG center to shorter wavelengths with increasing incidence angle reduces the absorption characteristic in the visible region.

As a general comment for top illumination, it is undesirable that the electromagnetic wave cannot penetrate the SC, especially for wavelengths longer than 700 nm. However, this disadvantage can be encountered as an effective way to increase photon harvest in the case of under-illumination. The reflection, transmittance and absorption spectra calculated by TMM of CdTe/CdS SC with MgF_2/MoO_3 1D-PC under bottom illumination are given in Figure 3a, b and c, respectively.

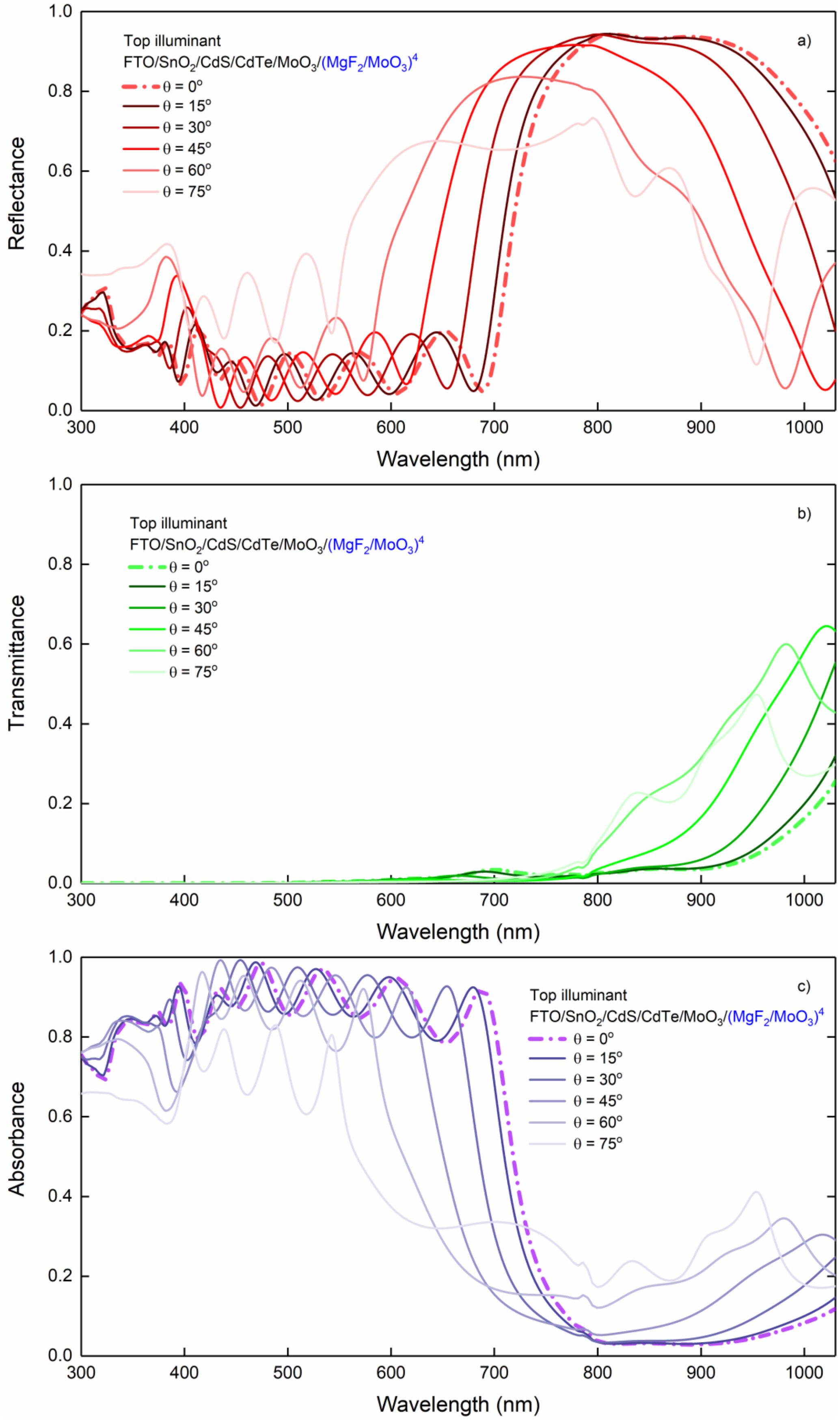

***Figure 2. a)** The reflection, **b)** transmittance and **c)** absorption spectra of a CdTe/CdS SC with MgF_2/MoO_3 photonic crystal under top illumination are calculated depending on the angle of incidence of the electromagnetic wave*

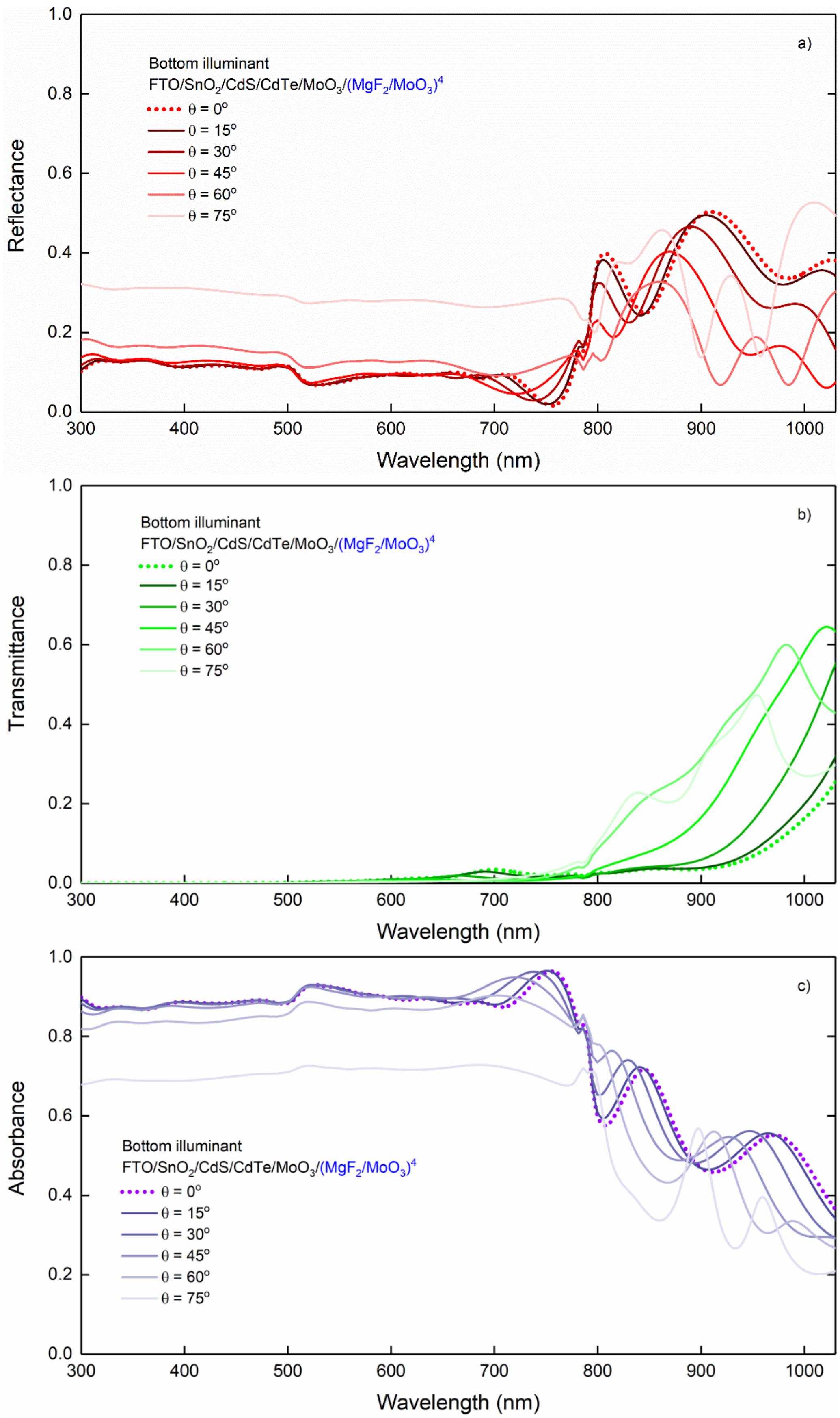

Figure 3. a) *The reflection,* ***b)*** *transmittance, and* ***c)*** *absorption spectra of a CdTe/CdS SC with MgF_2/MoO_3 photonic crystal under bottom illumination, calculated depending on the angle of incidence of the electromagnetic wave*

When the reflection spectrum is examined under bottom-illumination in Figure 3a, it shows the effect of PBG designed at λ_B=850 nm. However, this effect is not as effective and dominant as in top illumination. Also, there is no serious dependence on the angle of incidence of the electromagnetic wave. This is due to the fact that the MgF_2/MoO_3 PC is the last system to interact with the electromagnetic wave under the bottom illumination, as opposed to the top illumination. In the bottom illumination, when the electromagnetic wave enters the SC, especially the interaction with the absorber CdTe layer first ensures that the effect of MgF_2/MoO_3 PC on the angle-dependent optical spectra is not much. However, for θ=75°, there is an increase in reflection for all wavelengths and, therefore a decrease in absorption. This shows that a critical angle is formed, especially for angles greater than 60°. As the most important feature, the PBG effect is designed at λ_B=850 nm is effective in the absorption spectrum for all angles and the weak absorption property of the CdTe absorber layer can be improved with MgF_2/MoO_3. Because most of the electromagnetic waves in the PBG could be reflected back into the SC.

For the evaluation of effective photovoltaic properties according to the angle of incidence of the electromagnetic wave in a CdTe-based SC, we calculated the absorption characteristic of SC and J_{ph} over $S_{AM1.5G}$ using Equation 2. Because for this examination, the AM1.5G spectral irradiance distribution must also be taken into account.

$$J_{ph} = \int \frac{e\lambda}{hc} S_{AM1.5G}(\lambda)\, A(\lambda)\, d\lambda \qquad (2)$$

where e is the electron charge, h is the Planck constant, c is the speed of light, $S_{AM1.5G}$ is the photon flux, and $A(\lambda)$ is the absorption coefficient. When calculating J_{ph}, it is assumed that each photon creates an electron and a hole in the structure (Çetinkaya et al., 2021b). This situation provides a relative evaluation and allows us to understand how the flow mechanisms in the structure change relatively. The variation of J_{ph} values in CdTe/CdS SC with MgF_2/MoO_3 1D-PC according to the angle of incidence of the electromagnetic wave under the top and bottom illumination are given in Figure 4.

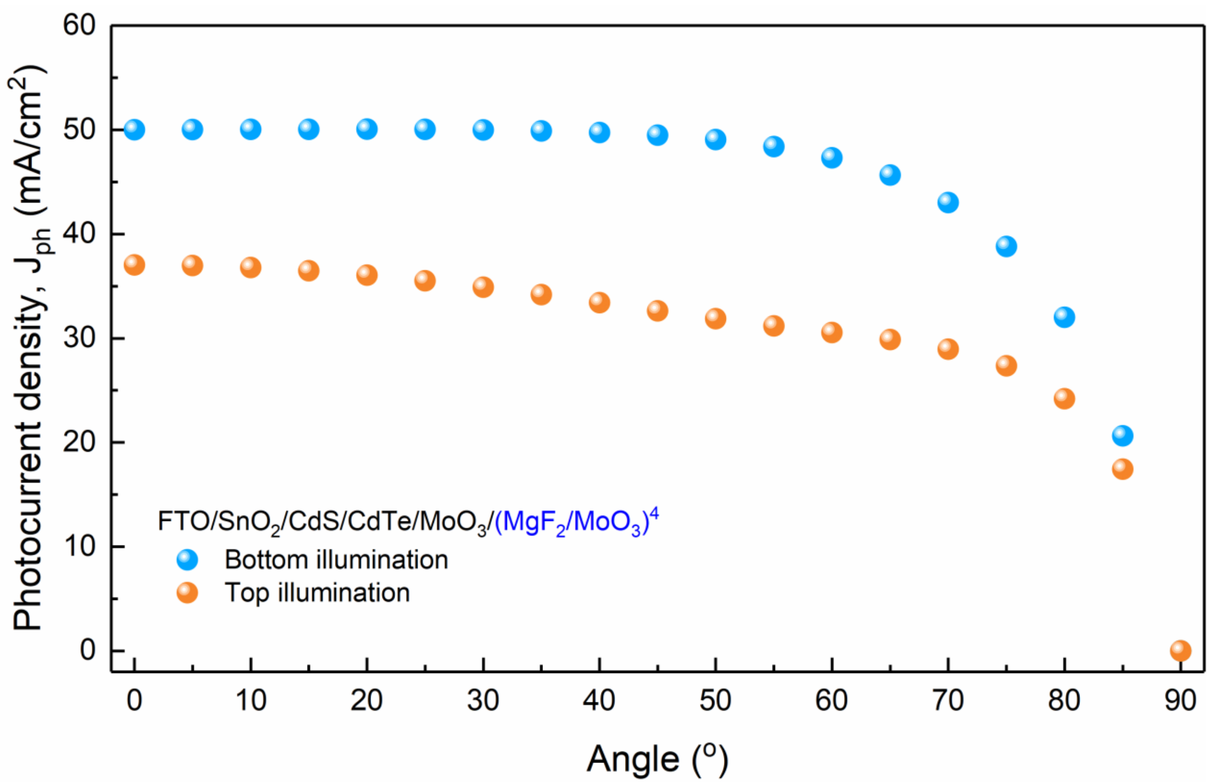

Figure 4. *The variation of J_{ph} values in a CdTe/CdS SC with MgF_2/MoO_3 photonic crystal according to the angle of incidence of the electromagnetic wave under the top and bottom illumination*

In cases where the electromagnetic wave comes to the SC from the top and from the bottom, since the first interaction of the electromagnetic wave in the top interaction is PC, the electromagnetic wave in the PBG is directly reflected from the surface, so sufficient photon harvesting cannot be achieved in the SC and J_{ph} decreases significantly compared to the bottom illumination situation. For top illumination, as previously discussed, the absorption characteristic increased in the NIR region, especially at angles greater than θ=30°, as the reflection decreased. However, since the increase in incidence angle shifts the center of PBG to shorter wavelengths, a reflection characteristic occurs in the visible region, and the absorption weakens in the region of the CdTe absorber layer with high absorption. This results in a deterioration in J_{ph} for angles greater than θ=30°. For bottom illumination, no significant change in J_{ph} is observed directly due to a specific angle. Because in the bottom illumination, since the electromagnetic wave MgF_2/MoO_3 interacts with the PC system last, the dependence on the angle disappears. In addition, after θ=60° for the bottom illumination and θ=80° for the top illumination, there was a serious increase in the reflection spectrum of the SC, especially in the visible region, and there was a deterioration in J_{ph}.

4. CONCLUSION

In this paper, we examined the interaction of the structure formed by the integration of the MgF_2/MoO_3 1D-PC system with PBG, which is designed with a central wavelength at 850 nm to improve photon harvesting in the CdTe/CdS heterojunction SC system, which can already be achieved with high efficiency, with the electromagnetic wave depending on the angle. We evaluated the optical properties by calculating the reflection, transmittance and absorption spectra theoretically with TMM. We presented and discussed all optical spectra for bifacial working conditions depending on the angle under both top and bottom illumination.

It was aimed to increase photon harvesting in the region where the absorption of CdTe, which is the absorber layer, is weak with PBG with a central wavelength at 850 nm, and we determined that the characteristic of PBG significantly changes the optical spectrum of the entire SC structure, especially under top illumination, depending on the angle. For θ=0°, under top illumination, wavelengths longer than 700 nm are directly reflected from the surface, thus preventing sufficient photon harvesting of the SC, causing a serious decrease in photovoltaic performance. For top illumination, the reflection intensity drops drastically at incidence angles greater than θ=30°. As the most important feature, as a typical PC feature, the increase of θ shifts the center wavelength of PBG to shorter wavelengths. Increasing the incidence angle of the electromagnetic wave increases the transmittance and especially the absorption intensity of the SC in the designed PBG. In PBG, for θ>45°, the probability of absorption increases significantly with the introduction of more electromagnetic waves into the SC.

For bottom illumination, the PBG effect is not as effective as for top illumination and there is no serious dependence on the angle of incidence of the electromagnetic wave. For θ=75°, an increase in reflection for all wavelengths and thus a decrease in absorption is observed. In addition, a critical angle occurs, especially for angles greater than 60°. The PBG effect designed at λ_B=850 nm is effective in the absorption spectrum for all angles and the weak absorption property of the CdTe absorber layer can be improved with MgF_2/MoO_3.

For J_{ph}, sufficient photon harvesting can not be achieved in the SC, since the electromagnetic wave is directly reflected from the surface in the top interaction, and J_{ph} is significantly less than in the case of bottom illumination. In top illumination, there is a deterioration in J_{ph} for angles greater than θ=30° and there is no drastic change in J_{ph} directly due to a specific angle. In addition, after θ=60° for bottom illumination and θ=80° for top illumination, a significant increase occurred in the reflection spectrum of SC, especially in the visible region, and weakening of J_{ph}' values was observed.

CONFLICT OF INTEREST

The authors declare no conflict of interest.

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