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MODELING OF PHOTOCONVERTER PARAMETERS BASED ON CdS/porous-CdTe/CdTe HETEROSTRUCTURE

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Abstract. *This article presents a comprehensive study of the fabrication and modeling of a CdS/porous-CdTe/CdTe heterostructure aimed at improving solar cell efficiency. The research focuses on two critical processes: the electrochemical etching for producing porous-CdTe substrates and the chemical surface deposition method for applying CdS films. The structural and optical characteristics of the fabricated heterostructure were analyzed using SEM and EDAX methods, confirming the formation of a continuous CdS layer over a porous-CdTe layer. The thickness of the porous-CdTe and CdS layers was 1.0 and 2.0 μm, respectively. The obtained thick values of the manufactured structure were used to model the CdS/porous-CdTe/CdTe heterostructure in the PC1D-program in order to find the optimal solar cell parameters. The photoconverter current-voltage curve was obtained from the PC1D-program. The theoretically calculated efficiency was 21.6%. The study further explored the impact of varying the thickness of the CdS window layer and the porous-CdTe buffer layer on photoconverter performance. The efficiency of the CdS/porous-CdTe/CdTe photoconverter reaches maximum values at a thickness of 2.3-2.4 μm and 1.9 μm for CdS and porous-CdTe layers, respectively. Additionally, the buffer layer's porosity enhanced light absorption, contributing to higher carrier generation rates. In order to increase the CdS/porous-CdTe/CdTe photoconverter efficiency, the single-layer and double-layer antireflective coatings used, which are most often in the CdS/CdTe solar cells production, was investigated. To further optimize the photoconverter, anti-reflective coatings were investigated using the matrix method. The results showed that the best reflectance is observed for the ITO/ZnO double anti-reflective coating. The solar cell efficiency with this coating was 22.8% at 50/30 nm thicknesses. Additional research in the modifying the porosity of the substrates and its effect on the photoconverter characteristics may lead to the discovery of new opportunities increasing their efficiency and stability. The findings underscore the potential of CdS/porous-CdTe/CdTe heterostructures as efficient photovoltaic devices.*

Keywords: electrochemical etching, chemical surface deposition, anti-reflective coating, modelling

MODELOWANIE PARAMETRÓW FOTOPRZETWORNIKA OPARTEGO NA HETEROSTRUKTURZE CdS/porowaty-CdTe/CdTe

Streszczenie. *W artykule przedstawiono kompleksowe badanie wytwarzania i modelowania heterostruktury CdS/porowate-CdTe/CdTe w celu poprawy wydajności ogniw słonecznych. Badania koncentrują się na dwóch krytycznych procesach: trawieniu elektrochemicznym w celu wytworzenia porowatych podłoży CdTe oraz chemicznej metodzie osadzania powierzchniowego w celu nałożenia warstw CdS. Właściwości strukturalne i optyczne wytworzonej heterostruktury zostały przeanalizowane przy użyciu metod SEM i EDAX, potwierdzając tworzenie ciągłej warstwy CdS na porowatej warstwie CdTe. Grubość porowatych warstw CdTe i CdS wynosiła odpowiednio 1,0 i 2,0 μm. Uzyskane wartości grubości wytworzonej struktury zostały wykorzystane do modelowania heterostruktury CdS/porowate-CdTe/CdTe w programie PC1D w celu znalezienia optymalnych parametrów ogniwa słonecznego. Charakterystyka prądowo-napięciowa fotokprzetwornika została uzyskana z programu PC1D. Teoretycznie obliczona sprawność wyniosła 21,6%. W badaniu zbadano również wpływ zmiany grubości warstwy okiennej CdS i porowatej warstwy buforowej CdTe na wydajność fotoprzetwornika. Wydajność fotoprzetwornika CdS/porowate-CdTe/CdTe osiąga maksymalne wartości przy grubości 2,3-2,4 μm i 1,9 μm odpowiednio dla warstw CdS i porowate-CdTe. Dodatkowo, porowatość warstwy buforowej zwiększyła absorpcję światła, przyczyniając się do wyższych szybkości generowania nośników. W celu zwiększenia wydajności fotoprzetwornika CdS/porowate-CdTe/CdTe zbadano stosowane jedno- i dwuwarstwowe powłoki antyrefleksyjne, które są najczęściej stosowane w produkcji ogniw słonecznych CdS/CdTe. W celu dalszej optymalizacji fotoprzetwornika zbadano powłoki antyrefleksyjne przy użyciu metody matrycowej. Wyniki pokazały, że najlepszy współczynnik odbicia obserwuje się dla podwójnej powłoki antyrefleksyjnej ITO/ZnO. Sprawność ogniwa słonecznego z tą powłoką wyniosła 22,8% przy grubości 50/30 nm. Dodatkowe badania w zakresie modyfikacji porowatości podłoży i jej wpływu na charakterystykę fotoprzetworników mogą doprowadzić do odkrycia nowych możliwości zwiększających ich wydajność i stabilność. Wyniki badań podkreślają potencjał heterostruktur CdS/porowate-CdTe/CdTe jako wydajnych urządzeń fotowoltaicznych.*

Słowa kluczowe: trawienie elektrochemiczne, chemiczne osadzanie powierzchniowe, powłoka antyrefleksyjna, modelowanie

Introduction

In the modern world, photoconverters based on the CdS/CdTe heterostructure are one of the most promising technologies for the efficient solar cell production. Compared with commercial silicon CdS/CdTe panels, the panels still have lower conversion power, but solar cell CdS/CdTe have received much attention due to their high light absorption coefficient, low manufacturing cost, and high stability in a wide range of operating conditions [18, 40]. The unique properties of these materials make it possible to achieve significant improvements in the photovoltaic field.

The substrate porosity, adding unique properties to the systems, can open up ways to further efficiency and stability improvement of photodevices [6]. Obtaining CdS films on porous substrates made by electrochemical etching plays a key role in the development of thin-film solar cells and other electronic devices [7]. However, obtaining CdS films on porous CdTe substrates requires careful control of the synthesis process.

Thus, research in the synthes direction of CdS films on porous CdTe substrates and further photoconverter optimization based on the manufactured structures remain relevant.

The CdS window layer formation in the solar cell CdS/CdTe can be done using various methods: electrodeposition, chemical deposition in a bath, spray pyrolysis, thermal evaporation, solution growth, etc.

In research [13] an electrodeposited CdTe nucleation layer was introduced on a chemical bath deposited CdS layer prior to close-spaced sublimation of the CdTe absorber layer to improve the solar cell CdS/CdTe efficiency. It provided the highest efficiency rate 9.12% at an open-circuit voltage (V_{OC}) 640 mV.

It was shown in [24] that films grown by vacuum evaporation (VE) have better crystallinity than films grown by chemical bath deposition (CBD). VE-CdS films showed a higher transmittance and a larger band gap compared to CBD-CdS films. However, CdTe solar cells with these low-quality CBD–CdS layers provide higher and more stable performance.

CdS films were deposited on transparent conductive oxide (TCO)/glass substrates by the metal organic chemical vapor deposition (MOCVD). As a quality control CdS film result, a photoelectric conversion efficiency rate 10.5% was achieved for the size 1376 cm^2 solar cells in AM1.5 conditions [41].

CdS/CdTe cells with an efficiency rate 3.76% and an external quantum 70% were manufactured using the thermal evaporation technique [23]. The highest efficiency rate was observed for the CdS film grown at a substrate temperature 175°C, which was confirmed by SCAPS-1D simulations.

The authors report on [39] the change in the CdTe/CdS solar cell parameters made by depositing CdS window layers on soda lime, indium doped tin oxide (ITO), fluorine-doped tin oxide (FTO), glass substrates by CBD. A high-quality single-grain CdS layer ensured homogeneous CdS and CdTe mixing at the junction interface. A short-circuit current up to 25.1 mA/cm^2 was obtained for a CdS/CdTe solar cell single-grain. The corresponding solar battery efficiency rate was 14.6%.

An effective obtaining CdS method films with high quality and uniformity is the chemical surface deposition method [14, 16]. This method is characterized by simplicity and relative cheapness, which makes it attractive for industrial applications. However, achieving optimal synthesis conditions, controlling process parameters, selecting the best substrate, applying anti-reflective coatings, etc., are important challenges for researchers in this field.

The solar cell CdS/CdTe efficiency standards is ~10%, but in [15], the use of a two-layer ZnS/CdS film as an improved window layer for CdTe during annealing allowed to reach 10.3%. Subsequently, solar cells with the structure glass/FTO/n-ZnS/n-CdS/n-CdTe/Au were manufactured and characterized with the open-circuit voltage parameters $V_{OC} = 670$ mV, short-circuit current density $J_{SC} = 41.5$ mA/cm^2, the fill factor FF = 0.46 and the efficiency ~12.8% when measured at room temperature under AM1.5 lighting conditions [30].

Good results were obtained by Alvin D. Compaan and others [3] in the manufacture of highly efficient (14% at AM1.5) CdS/CdTe cells with ZnO:Al sputtering on aluminosilicate glass. The authors proved that the films have not only high optical quality, but also an excellent service life of the media.

The work [33] reports on obtaining CdS/CdTe thin-film solar cells with high efficiency from 14% to 14.6%. The procedure consists in sequentially depositing several layers on a glass substrate configured as glass/ITO/ZnO/CdS/CdTe/Cu/Mo using radio frequency sputtering and close space sublimation (CSS).

An efficiency rate about 16-17% was achieved by adding and optimizing an extended CdTe electron reflector layer on the back Schottky contact [12]. In the cell CdS/CdTe optimization, an extended region of the electron reflector with a barrier height 0.1 eV and a doping density $7 \cdot 10^{18}$ cm^{-3} was used. At an optimal thickness 100 nm, this leads to the best cell efficiency rate 19.83% compared to experimental data.

To predict the solar cell efficiency, optimize design and materials, reduce production costs and time, as well as to identify potential problems and improve technological processes, computer simulations are carried out before their direct manufacture.

According to computer simulations [21], a ZnO/CdS double-layer window with a combination 250/50 nm thickness and a 2.5 µm CdTe absorber layer demonstrated an efficiency rate 17.66% with a fill factor 73.7% due to the larger band gap and lower ZnO absorption.

In [28], a conversion efficiency rate 13.2% in the SnO_2/CdS/CdTe structure was achieved by reducing the thickness of the cadmium sulfide window layer to 60 nm along with the zinc oxide ZnO or zinc stannate Zn_2SnO_4 introduction as a buffer layer to prevent direct leakage current. The maximum conversion efficiency rate (using the AMPS1D simulator) reached rate 18.3% when using a CdTe absorber layer, a 60 nm CdS window layer, and a 100 nm ZnO or Zn2SnO4 buffer layer.

Modeling of the CdTe/CdS/ZnO photostructure using SCAP 1D performed in [37] changing the band gap and thickness of the absorber layer shows an increase in the filling factor, current density, and open-circuit voltage from 83.74–84.77; 26.26–28.85 mA/cm^2, 0.71–0.73 V, resulting in a solar cell efficiency rate ~17.82%. The research shows that the large absorber layer thickness and the low band gap contribute to the optimization.

Later, performance heterostructure FTO/TiO_2/ZnO/CdS/CdTe/V_2O_5/Au modeling as a solar cell (SCAPS-1D) showed $V_{OC} = 0.811$ V, short circuit current density, $J_{SC} = 38.51$ mA/cm^2, fill factor, FF rate 80% with bi-layer anti-reflection coating and back surface field [22].

Optimizing photovoltaic parameters by modifying the thickness of HTL, TCO and the absorber layer is proposed in [34]. Using the SCAPS-1D simulator, the authors managed to achieve an efficiency rate 23.59%, an open-circuit voltage $V_{OC} = 0.949$ V, a short-circuit current density $J_{SC} = 28.48$ mA/cm^2, and a fill factor FF = 87.27%. However, optimization due to the acceptor/donor density ($1 \cdot 10^{18}$ cm^{-3}) of the HTL/TCO material leads to an increase in efficiency rate to 24.48% at an operating temperature of 285 K, and the use of Pt as the back contact metal increases the efficiency rate to 28.11%.

That is, the computer modeling result indicates the efficiency dispersion of solar batteries, helping to identify and analyze the factors that affect their working efficiency.

In this article, we will consider the obtaining CdS filming process on porous-CdTe substrates by chemical surface deposition and consider potential directions for further improvement of these devices to maximize their efficiency and wide application in modern technologies.

The purpose of this research is to obtain a CdS/porous-CdTe/CdTe heterostructure and further photovoltaic parameter optimization of the manufactured photoconverters.

The task is as follows:

1. CdS/porous-CdTe/CdTe heterostructure fabrication and to study its structural parameters;
2. Conducting a numerical one's solar cell study using PC1D software;
3. Optimization of one's photoconverter design by selecting the most effective anti-reflective coating.

1. Materials and methods of the research

Porous CdTe was obtained by the standard method of electrochemical etching [6]. After cleaning the traces of the herbivore and drying the substrates, CdS films were applied to their surface by chemical surface deposition [10], applying an aqueous cadmium chloride $CdCl_2$, thiourea CH_4N_2S, and ammonium hydroxide NH_4OH solution to the substrate. The morphology and cross-section of the resulting structure was investigated using a JSM-6490 scanning electron microscope.

The PC1D program was used to calculate the CdS/porous-CdTe/CdTe photoconverter parameters. They were used for the calculations (table 1), the CdS filming parameters and the porous-CdTe and CdTe layers were obtained from the scientific literature (table 2). The simulation was carried out at room temperature (T = 300 K). Modeling and analysis of anti-reflective coatings was performed using the matrix method.

2. Researching the composition and properties of the structure

The porous CdTe substrates after the deposition of CdS over the entire working surface were covered with a solid film with a characteristic yellow-green color of cadmium sulfide, which confirms the EDAX results (Fig. 1). In the SEM photomicrograph (Fig. 2b) of the cross-section fabricated heterostructure, an intermediate layer between the CdS film and the CdTe substrate is observed – a porous CdTe layer. The columnar CdS structure in the initial growing stage turns into a continuous layer (Fig. 2a), penetrating into the pores.

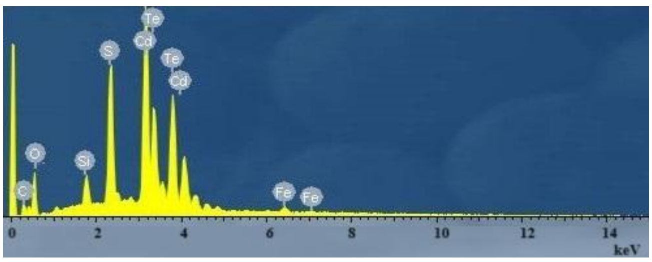
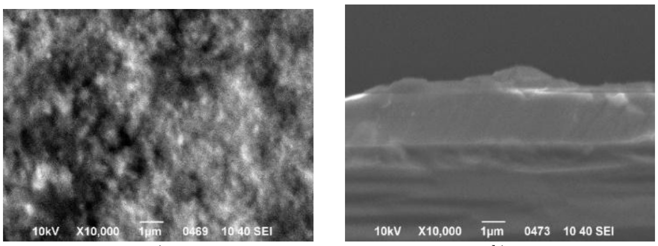


Fig. 1. EDAX spectrum of the CdS/porous-CdTe/CdTe heterostructure



a) b)

Fig. 2. The SEM-image surface (a) and cross-section (b) of the CdS/porous-CdTe/CdTe heterostructure

According to the SEM results, the thicknesses of each heterostructural layers were determined (table 1), which will be used in the future for solar cell photoconverter modeling in PC1D.

Table 1. Layer CdS/porous-CdTe/CdTe heterostructure thicknesses

parameter	value
CdTe layer thickness, μm	500,0
CdTe layer thickness, μm	1,0
CdS layer thickness, μm	2,0

3. Simulation results and it's discussion

Various tools are available for solar cell modeling: wxAMPS, Silvaco ATLAS, SCAPS-1D, GPVDM, etc. [1, 29, 42]. Each of the listed tools has its advantages and limitations. We chose the PC1D program because of its simplicity and the large number of available photoconverter models [17]. We have already shown in our works [9, 11] that this program can be used to calculate the porous-Si/Si photoconverter characteristics and make it possible to analyze and optimize various photovoltaic element parameters, such as semiconductor structure, impurities, light absorption depth, texturing surfaces, etc.

The investigated photoconverter model is shown in the Fig. 3, the parameters of each proposed modeling layers are given in the table 2.

Table 2. Parameters used in solar cell simulation [19, 25, 27]

parameter	CdS	porous-CdTe	CdTe
Bandgap, eV	2.4	1.46	1.5
Electron affinity, eV	4.3	4.28	4.28
Dielectric constant	10	9.4	9.4
Electron mobility, cm^2/Vs	100	150	320
Hole mobility, cm^2/Vs	25	40	40
Carrier concentration, cm^{-3}	$1\cdot10^{18}$	-	-
Carrier concentration, cm^{-3}	-	$1\cdot10^{14}$	$2\cdot10^{14}$

In Fig. 4 shows the current-voltage the CdS/porous-CdTe/CdTe photoconverter characteristics.

The CdS/porous-CdTe/CdTe photoconverter efficiency is calculated according to the formula [10]:

$$\eta = V_{OC} \cdot I_{SC} \cdot FF$$

where V_{OC}, I_{SC} are the open-circuit voltage and short-circuit current, respectively, obtained from the simulation results, $FF = \frac{I_{max} \cdot V_{max}}{V_{OC} \cdot I_{SC}}$ – fill factor.

According to calculations, the efficiency rate was 21.6%.

The thickness of the window layer significantly affects the efficiency of the photoconverter due to several key aspects. These include light absorption, recombination protection, electrical resistance, optical properties, and others.

In the case of the CdS/porous-CdTe/CdTe heterostructure, the thickness of the CdS window layer must be chosen to provide maximum light transmission, minimum recombination loss, and optimal electrical and optical properties to achieve high photoconverter efficiency.

To study the influence of the CdS layer thickness on the efficiency of the photoconverter, modeling was performed by changing the layer thickness from 0.1 to 3.0 μm. Other device parameters remained unchanged, as indicated in tables 1 and 2. From the analysis of the simulation results, the efficiency of the CdS/porous-CdTe/CdTe photoconverter changes by 0.9% when the layer thickness changes, reaching a maximum value at a thickness of 2.3–2.4 μm. The dependence of efficiency on the thickness of the porous layer is presented in Fig. 5.

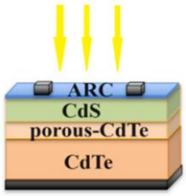


Fig. 3. Engineered and simulated solar cell structure

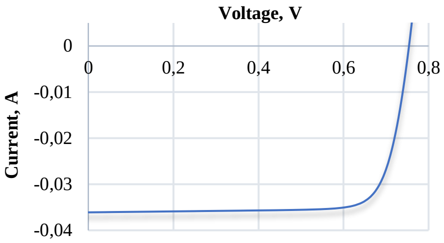


Fig. 4. The current-voltage CdS/porous-CdTe/CdTe photoconverter characteristics

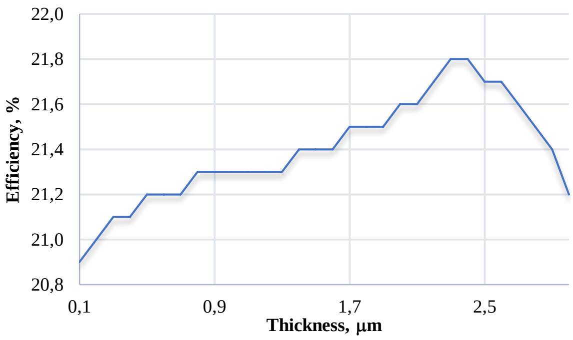


Fig. 5. Dependence of the efficiency of photoconverters based on the CdS/porous-CdTe/CdTe heterostructure on the thickness of the CdS layer

The buffer porous layer in CdS/porous-CdTe/CdTe-based photoconverters plays several important roles that significantly affect the efficiency and stability of these devices. A higher effective surface area leads to an increased probability of photon absorption. This helps increase the number of charge carriers generated, which increases the overall efficiency of the photoconverter.

Simulation was carried out by changing the thickness of the porous-CdTe layer from 0.1 to 2.5 μm. The influence of the thickness of the porous-CdTe layer on the value of the efficiency of the solar cell is shown in Fig. 6.

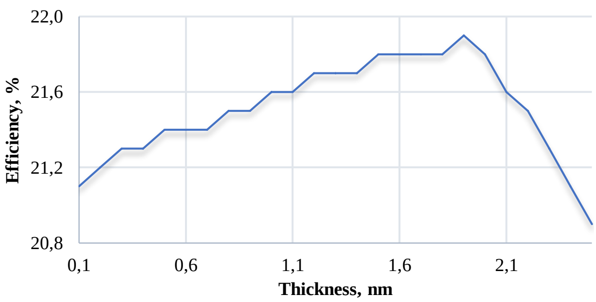


Fig. 6. Dependence of the efficiency of photoconverters based on the CdS/porous-CdTe/CdTe heterostructure on the thickness of the porous-CdTe layer

It was found that at a thickness of 1.9 μm, the efficiency of the solar cell takes on a maximum value, but with a further increase in the thickness of the porous layer, a decrease in the efficiency of the solar cell is observed. A decrease in the efficiency of solar cell with increasing thickness of the porous layer most likely occurs due to an increase in the recombination of generated carriers at deep centers, which are located at the interface between CdS and CdTe.

4. Research of anti-reflective coatings

A powerful tool for modeling and analyzing optical systems is the matrix method [32, 35]. The matrix method allows you to accurately determine the transmission and light reflection in optical systems that consists of several material layers with different properties.

The reflectivity of the structure, when the incident light falls normally on the heterostructural covered surface with a layer of one anti-reflective coating, can be found using the formula [36]:

$$R = \frac{r_1^2 + r_2^2 + 2r_1r_2\cos 2\theta_1}{1 + r_1^2r_2^2 + 2r_1r_2\cos 2\theta_1}$$

where

$$r_1 = \frac{n_0 - n_1}{n_0 + n_1}, \qquad r_2 = \frac{n_1 - n_2}{n_1 + n_2}$$

and

$$\theta_1 = \frac{2\pi n_1 d_1}{\lambda}$$

In case of double anti-reflective coating, the reflectivity can be calculated using the expression [8]:

$$R = \frac{\begin{matrix} r_1^2 + r_2^2 + r_3^2 + r_1^2r_2^2r_3^2 + 2r_1r_2(1 + r_3^2)\cos 2\theta_1 + \\ +2r_2r_3(1 + r_1^2)\cos 2\theta_2 + 2r_1r_3\cos 2(\theta_1 + \theta_2) + \\ +2r_1r_2^2r_3\cos 2(\theta_1 - \theta_2) \end{matrix}}{\begin{matrix} 1 + r_1^2r_2^2 + r_1^2r_3^2 + r_2^2r_3^2 + 2r_1r_2(1 + r_3^2)\cos 2\theta_1 + \\ +2r_2r_3(1 + r_1^2)\cos 2\theta_2 + 2r_1r_3\cos 2(\theta_1 + \theta_2) + \\ +2r_1r_2^2r_3\cos 2(\theta_1 - \theta_2) \end{matrix}}$$

where

$$r_3 = \frac{n_2 - n_3}{n_2 + n_3}$$

and

$$\theta_2 = \frac{2\pi n_2 d_2}{\lambda}$$

The anti-reflective coating choice may depend on the specific requirements for the photoconverter (spectral operation range, efficiency, resistance to ultraviolet radiation, technological limitations, etc.). In this work, coatings were used, which, according to research by other authors [19, 22, 31], showed better CdS/CdTe photoconverter efficiency (table 3).

Table 3. Materials of anti-reflective coatings with their refractive indices

material	refractive index
ITO	1.8270 [37]
ZnO	1.9268 [38]
SiO_2	1.4443 [39]
ZnS	2.2719 [40]
TiO_2	2.4538 [41]
AZO	1.8284 [42]

Table 4. Efficiency of CdS/porous-CdTe/CdTe photoconverters with anti-reflective coatings

material	ITO	ZnO	ZnO/TiO_2	ITO/ZnO
Efficiency, %	21.7	21.6	21.8	22.8

The ARC layer thickness was chosen equal to 50 nm. The wavelength was set in the range from 250 to 1200 nm.

In Fig. 7 shows the dependence of the reflection coefficient on the wavelength for the CdS/porous-CdTe/CdTe structure covered with different layers of ARC and DLARC under normal incident radiation.

The peak energy in the solar spectrum is at 500 nm, while the peak relative spectral CdS/CdTe cell response is in the wavelength range 650-800 nm, so the wavelength range of the best anti-reflection is in the range 500-700 nm. According to the results in the Fig. 7, the minimum antireflection value in this range is achieved for ARC ITO/ZnO. Further research was aimed at investigating the effectiveness of ARC and DLARC on CdS/porous-CdTe/CdTe, shown in the Fig. 4, and in the PC1D program (table 4).

The best result was obtained for ITO/ZnO, which agrees with the results regarding the coating obtained above (Fig. 7). However, it is worth noting that these values are given exactly for the ARC layer thickness 50 nm. As you know, solar cellefficiency can vary depending on the anti-reflective coating thickness. To find the optimal ITO, ZnO, ZnO/TiO_2, ITO/ZnO coatings thickness, simulations were carried out in PC1D for coating thickness values in the range 10–140 nm (Fig. 8).

According to the simulation results, it was established that the highest efficiency for ITO/ZnO is achieved at thicknesses 50/30 nm. Reducing the thickness of the anti-reflective coating helps reduce light loss due to reflection from the solar cell surface by increasing the number of photons that reach the active solar cell layer.

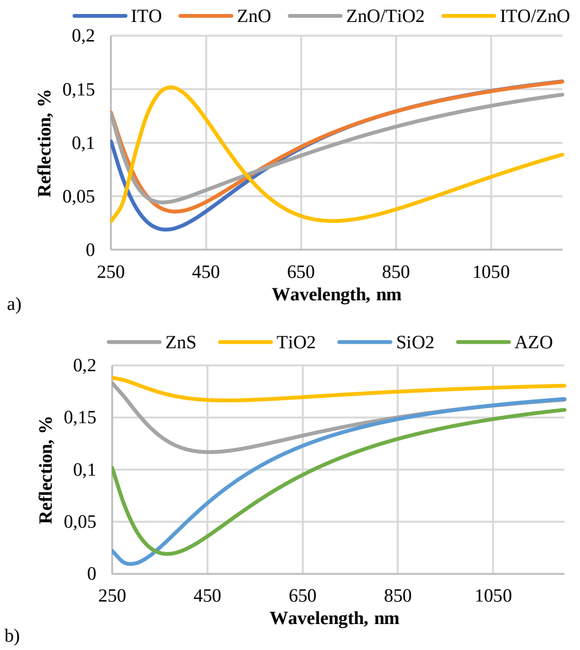


Fig. 7. Variation of reflectance as a wavelength function for ARC and DLARC on CdS/porous-CdTe/CdTe

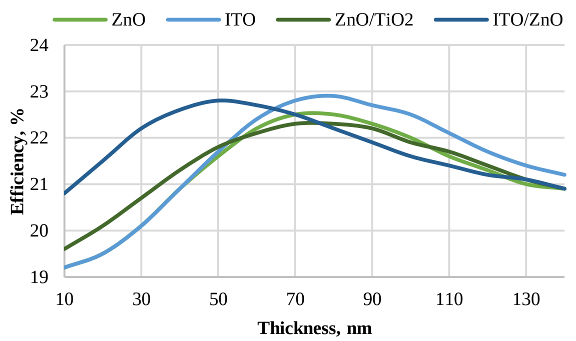


Fig. 8. Dependence of the photoconverter efficiency to the CdS/porous-CdTe/CdTe heterostructure on the antireflective layer thickness

5. Conclusion

This article examines the CdS/porous-CdTe/CdTe photoconverter prospects. These heterostructures were produced by applying CdS films to porous-CdTe/CdTe substrates by chemical surface deposition. To increase the solar cell efficiency, it is proposed to use single- and double-layer anti-reflective coatings. Using the matrix method and the PC1D program, the optical coating properties were modeled.

The results of the research indicate the importance of optimizing the anti-reflective coating thickness increasing the solar cell efficiency based on the CdS/porous-CdTe/CdTe heterostructure and can serve as a basis for further research in this direction and contributing to the more efficient solar cell development Additional research in the field of modifying the substrate porosity and its effect on the photoconverter characteristics may lead to the discovery of new opportunities increasing their efficiency and stability. Such studies play a key role in the further solar cell development based on CdS/porous-CdTe/CdTe heterostructures and their introduction into industrial production.

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