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Working Characteristics Simulation of p^+-CuO / p-ZnTe / n-CdSe / n-$MoSe_2$ / Mo Solar Cell

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In this paper it was carried out the simulation of the main working characteristics (light I-V curves, quantum yield spectral dependences) of CuO / ZnTe / CdSe / $MoSe_2$ / Mo solar cell (SC). As a study result, there were determined the open-circuit voltage U_{OC}, short-circuit current density J_{SC}, fill-factor *FF*, and device's efficiency depending on its constructive features (window, absorbing and near-contact layer thickness) and working temperature. There were estimated the SC's parameters with the maximum conversion efficiency of solar energy.

Keywords: Solar cell, p-ZnTe / n-CdSe heterojunction, Simulation, Fill factor, Solar cell efficiency.

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1. INTRODUCTION

The massive use of terrestrial photoelectric converters (PEC) of solar energy is one of the ways to overcome the global energy crisis [1, 2]. Solar cells based on silicon technologies are currently the most common ones [3]. Thin-film heterojunction PEC based on direct band semiconductors are their alternative. A particular scientific interest, due to the possibility to create on their basis highly efficient converters of solar energy, is devoted in this case to semiconductor compounds of A_2B_6 group [4]. Thus, films of cadmium selenide (CdSe) are widely used in solar power engineering as an absorbing (basic) layer of single-junction SC, since material's band gap (BG) is close to the optimal one (the Shockley-Queisser limit) (E_g = 1.50 eV) [1] and is equal to E_g = 1.70 eV [5]. We should note that at the same time, CdSe is a promising material of an absorbing layer of the first element of tandem SC, whose second element is PEC with $CuInSe_2$ (CIS) or Cu(In, Ga)Se_2 (CIGS) base layer [6-7].

Zinc telluride (ZnTe) with BG equal to E_g = 2.39 eV and p-type conductivity can serve in this case as a window layer of devices forming the heterojunction [8]. An important feature of p-ZnTe / n-CdSe heterojunctions is a proximity to ideal ones, since mismatch of the lattices of semiconductors with the cubic structure in this couple is less than 1 % [9]. This allows to reduce almost to zero the recombination losses of the light-generated charge carriers at the heteroboundary of the materials. Except the basic layers, SC always contain current-collecting contacts – frontal and back, to which a number of contradictory requirements is advanced [10].

Dichalcogenides of transition metals (WS_2, WTe_2, WSe_2, MoS_2, $MoTe_2$, $MoSe_2$) are considered as a new class of materials for producing the back contacts of SC [11-15]. These materials allow to obtain a good ohmic contact to absorbing layers of PEC, which has high temporal stability and provides their high adhesion to the substrate [16]. Moreover, because of the difference in the values of E_g between the absorbing layer and dichalcogenide film, the latter can play the role of an "electron mirror" that leads to the enhancement of the recombination level of electron-hole pairs on the junction boundary and provides high quality of the ohmic contact [17]. As a result, as shown in [18], this interlayer increases the SC efficiency. In a number of cases, layers of dichalcogenides at high temperatures are formed independently due to the mutual thermal diffusion of the components of semiconductor layers and molybdenum, which is traditionally used as the back contact of the majority of SC with the "substrate" structure [11].

Nowadays, efficiency of SC based on p-ZnTe / n-CdSe heterojunctions is equal to 10.8 % [19]. Further increase in the efficiency of such PEC is only possible by optimizing their design that is possible by simulating the physical processes occurring in devices under sunlight radiation. This conditioned the aim of the work, numerical simulation of the principal operating characteristics of PEC based on p^+-CuO / p-ZnTe / n-CdSe / n-$MoSe_2$ / Mo heterosystem depending on the structural characteristics of the device and temperature of its operation.

2. TECHNIQUE OF NUMERICAL SIMULATION

For the numerical simulation of the light current-voltage characteristics (CVC) and spectral dependence of the SC quantum yield, the following program packages are currently used: AMPS [20], wx-AMPS [21], PC-1D [22], ASA [23], SCAPS [24-26]. The last package, due to the possibility of taking into account both the individual properties of semiconductor layers and recombination processes occurring at the interface, was chosen for the calculation (SCAPS-3102). Moreover, SCAPS-3102 allows to model the physical processes in the structures composed of seven semiconductor layers with different doping profiles and arbitrary energy distribution of donors or acceptors in these layers and at the heteroboundary.

Such important parameters of photoconverters as the short-circuit current density J_{sc}, open-circuit voltage U_{oc}, filling factor *FF* of CVC and efficiency η of PEC were further determined from the light CVC [27].

Schematic representation of the PEC design with the p^+-CuO / p-ZnTe / n-CdSe / n-$MoSe_2$ / Mo structure, for which simulation is carried out, is illustrated in Fig. 1. Copper oxide (CuO), which is transparent in the visible spectral region and has p-type conductivity, was selected as the upper current-collecting contact to the p-ZnTe layer [28].

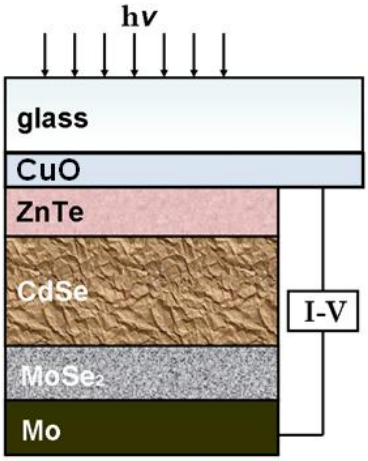

Fig. 1 – Schematic representation of the SC design with the structure p^+-CuO / p-ZnTe / n-CdSe / n-$MoSe_2$ / Mo

Before starting the simulation, it is necessary, first of all, to specify the input parameters of the materials entering into the PEC composition, such as window and absorbing layer thickness (d), BG of the materials (E_g), their electron affinity (χ), dielectric constants of semiconductors ($\varepsilon/\varepsilon_o$), mobilities of electrons and holes (μ), their effective masses m_e, m_h, densities of states in the conduction and valence bands N_C, N_V, etc. [29-30].

The main basic parameters, which we have used in the numerical simulation of the physical processes in SC, are given in Table 1.

In the majority of the cases, simulation was carried out under the conditions of AM 1.5 and room temperature (T = 300 K). Thickness of the window layer of ZnTe was varied in the range of d_{ZnTe} = (0.05-0.50) μm, of the absorbing layer – d_{CdSe} = (1.0-5.0) μm, of the $MoSe_2$ sublayer – d_{MoSe2} = (0.1-0.5) μm. Two simulation parameters were usually fixed, while the third one was changed.

Table 1 – The input parameters of the simulation

Layer	p-ZnTe	n-CdSe	n-$MoSe_2$
Parameters			
d, μm	0.05-0.50	1.00-5.00	0.05-0.50
E_g, eV	2.39	1.74	1.26
χ, eV	3.53	4.95	4.05
$\varepsilon/\varepsilon_o$	7.28	6.10	15.40
N_C, cm^{-3}	2.24×10^{18}	1.75×10^{18}	1.05×10^{18}
N_V, cm^{-3}	1.60×10^{19}	2.10×10^{19}	1.40×10^{19}
μ_n, cm^2/c	–	650	280
μ_p, cm^2/c	100	–	–
m_n/m_0	0.20	0.13	0.28
m_p/m_0	0.20	0.45	0.50

3. RESULTS AND DISCUSSION

Thickness of the absorbing layer is an important SC characteristic, which influences the amount of absorbed radiation (by the device), and, therefore, the study of its influence on the electrophysical characteristics of PEC is an urgent task.

In Table 2 and Fig. 2 we present the simulation results of the light CVC of SC with changing the absorbing layer thickness. Thickness of two other layers was taken to be equal to d_{ZnTe} = 0.10 μm, d_{MoSe2} = 0.2 μm.

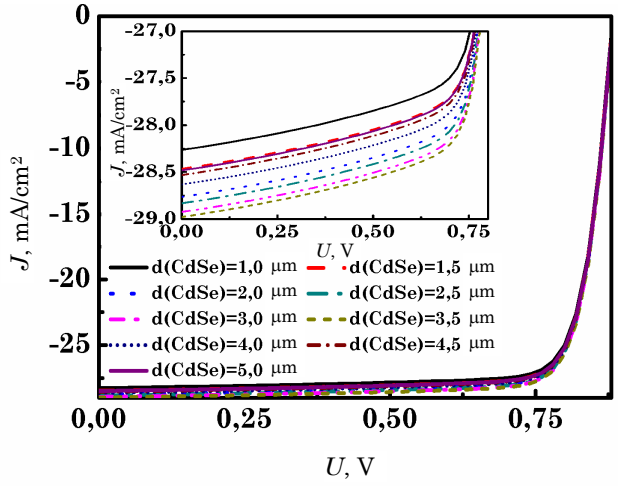

Fig. 2 – Light CVC of SC with the structure p^+-CuO / p-ZnTe / n-CdSe / n-$MoSe_2$ / Mo at different thicknesses of the CdSe absorbing layer

Table 2 – SC operating characteristics at different thicknesses of the CdSe absorbing layer

d_{CdSe}, μm	U_{OC}, V	J_{SC}, mA/cm²	FF, %	η, %
1.0	0.88	28.28	82.14	20.38
1.5	0.88	28.47	82.14	20.56
2.0	0.88	28.60	82.14	20.78
2.5	0.88	28.83	82.14	20.93
3.0	0.88	28.93	82.14	21.01
3.5	0.88	28.98	82.14	21.04
4.0	0.88	28.63	82.14	20.76
4.5	0.88	28.53	82.14	20.69
5.0	0.88	28.48	82.14	20.56

It is seen from the analysis of the simulation results that there is some increase in the SC efficiency to the level of 21.04 % with increasing absorbing layer thickness to d_{CdSe} = 3.5 μm. This is conditioned by the increase in the value of J_{SC} from 28.60 to 28.98 mA/cm² at constant values of U_{OC} = 0.88 V and FF = 82.14%. With further increase in the CdSe layer thickness, SC efficiency begins to decrease. This can be explained by the fact that the total light absorption by SC occurs at the absorbing layer thickness of 3.5 μm, and, correspondingly, a number of generated electron-hole pairs attains saturation. Further increase in the absorbing layer thickness d_{CdSe} leads to the increase in the series resistance of the device and removal of the carrier generation region away from the heterojunction. As a result, the total decrease in the device efficiency takes place.

Increased recombination of generated carriers on deep centers located at the absorbing layer/current-collecting contact interface influences the decrease in the SC efficiency at small absorbing layer thickness.

Thus, as a result of the performed calculations it is established that the value of d = 3.5 μm is the optimal absorbing layer thickness of SC based on ZnTe / CdSe heterojunction. We have used just this value in further calculations.

The window layer thickness in PEC is an important characteristic, since it determines the amount of radiation entering the absorbing layer of SC, and, therefore, optimization of its thickness is necessary.

Simulation results of light CVC of the devices with different thicknesses of ZnTe layer are given in Fig. 3 and Table 3.

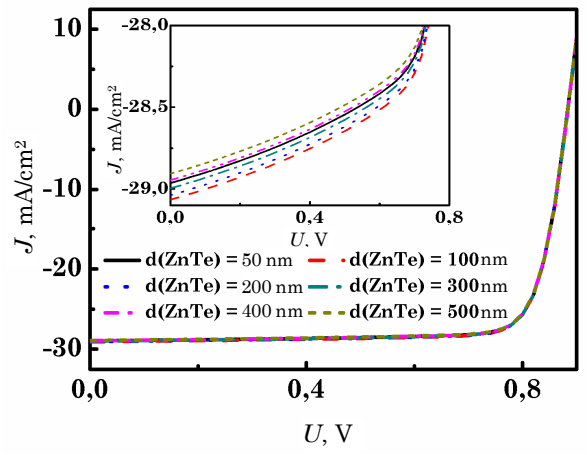

Fig. 3 – Light CVC of SC with the structure p^+-CuO / p-ZnTe / n-CdSe / n-$MoSe_2$ / Mo at different thicknesses of the ZnTe window layer

Table 3 – SC operating characteristics at different thicknesses of the ZnTe window layer

d_{ZnTe}, nm	U_{OC}, V	J_{SC}, mA/cm²	FF, %	η, %
50	0.88	28.63	82.14	20.78
100	0.88	29.07	82.14	21.10
200	0.88	29.02	82.14	21.07
300	0.88	29.00	82.14	21.04
400	0.88	28.91	82.14	21.02
500	0.88	28.89	82.14	20.98

As a result of the performed calculations, it was established that a slight decrease in the SC efficiency is observed with increasing window layer thickness from 0.10 to 0.50 μm. This is due to the fact that larger number of photons with energy $h\nu > E_g$ begins to be absorbed in ZnTe layer with increasing ZnTe window layer thickness. This leads to the decrease in the SC quantum yield in the radiation wavelength range of $\lambda < 530$ nm. The role of the recombination processes on the PEC surface significantly increases at small window layer thickness ($d = 0.05$ μm) resulting in the decrease in their efficiency. We should note that it is difficult to experimentally obtain the continuous ZnTe films of smaller thickness, and, therefore, simulation at smaller thickness of ZnTe layer has not been performed.

Simulation of the processes occurring in SC allowed to determine the optimal design characteristics of the real PEC, namely, the window layer thickness should be equal to 0.1 μm.

The change in the $MoSe_2$ near-contact layer thickness also can influence the SC efficiency. In Fig. 4 and Table 4 we present the simulation results of the light CVC of the heterosystem depending on the thickness of $MoSe_2$ layer.

It is seen from the analysis of the simulation results that the increase in the SC efficiency to 20.76 % is observed with increasing thickness of the intermediate layer. The corresponding increase in the values of U_{OC} from 0.83 V to 0.88 V and of J_{SC} from 24.78 to 28.60 mA/cm² takes place in this case.

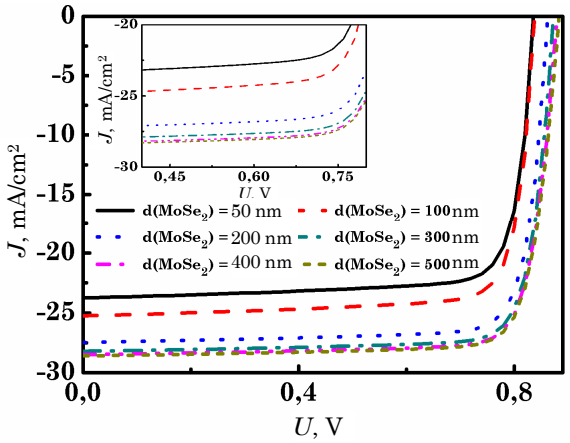

Fig. 4 – Light CVC of SC with the structure p^+-CuO / p-ZnTe / n-CdSe / n-$MoSe_2$ / Mo at different thicknesses of the $MoSe_2$ layer

Table 4 – SC operating characteristics at different thicknesses of the $MoSe_2$ layer

d_{MoSe2}, nm	U_{OC}, V	J_{SC}, mA/cm²	FF, %	η, %
50	0.83	24.78	80.29	16.56
100	0.84	25.25	81.28	17.20
200	0.86	27.46	82.75	19.59
300	0.87	28.21	82.68	20.37
400	0.88	28.50	82.39	20.65
500	0.88	28.60	82.14	20.76

SC can be warmed up in the operation under the action of solar radiation that can substantially influence their operating characteristics. In connection with this, we studied the influence of the operating temperature on the view of the PEC CVC. Simulation was carried out in the temperature range, which really can be realized during the SC operation, $T = 280$-320 K for the optimized values of the thickness of all layers. Calculation results of the main PEC characteristics depending on the operating temperature are given in Fig. 5 and Table 5.

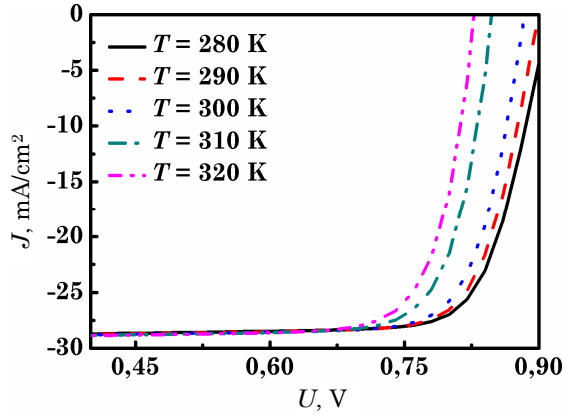

Fig. 5 – Light CVC of SC with the structure p^+-CuO / p-ZnTe / n-CdSe / n-$MoSe_2$ / Mo at different operating temperatures

It is established that SC efficiency decreased from 21.60 % (280 K) to 19.83 % (320 K) with increasing operating temperature from 280 K to 320 K. The result is physically clear, since with increasing T, BG of the material decreases, correspondingly, contact potential difference on the heterojunction decreases and leakage currents of the diode simultaneously increase.

Table 5 – SC operating characteristics at different operating temperatures

T, K	U_{OC}, V	J_{SC}, mA/cm^2	FF, %	η, %
280	0.91	29.03	81.64	21.60
290	0.90	29.07	81.87	21.41
300	0.88	29.00	82.14	21.06
310	0.85	29.15	82.25	20.33
320	0.83	29.18	82.05	19.83

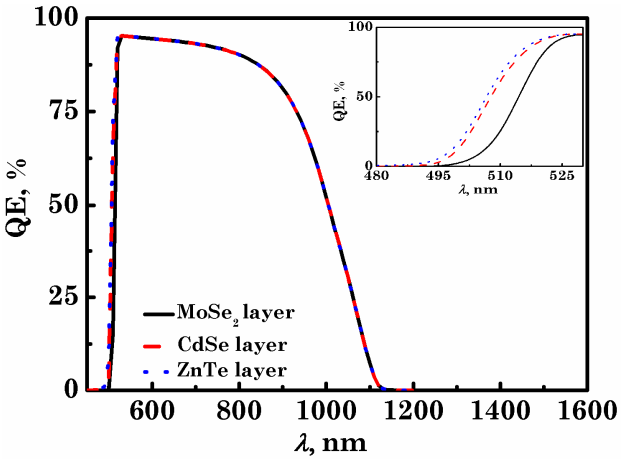

Fig. 6 – Dependences of the quantum yield of SC with the structure p^+-CuO / p-ZnTe / n-CdSe / n-$MoSe_2$ / Mo on the heterosystem layer thickness

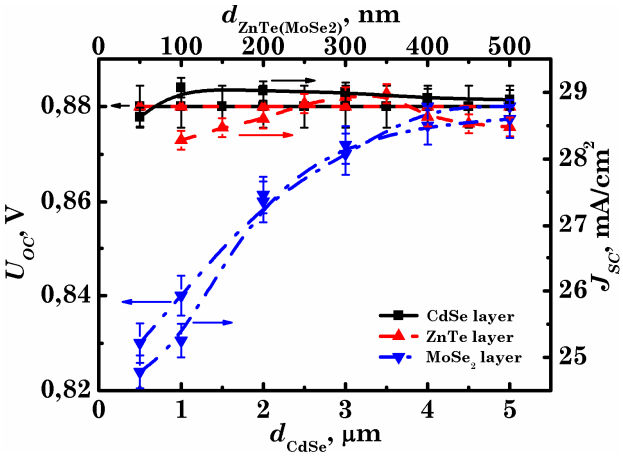

Fig. 7 – Dependences of U_{OC} and J_{SC} of the p^+-CuO / p-ZnTe / n-CdSe / n-$MoSe_2$ / Mo SC on the layer thickness

Dependences of the quantum yield of the p^+-CuO / p-ZnTe / n-CdSe / n-$MoSe_2$ / Mo SC taking into account different physical and technological methods for producing layers are illustrated in Fig. 6. As it was expected, PEC are photosensitive in the radiation wavelength range of 512-978 nm.

In Fig. 7 and Fig. 8 we show the generalized dependences of the open-circuit voltage U_{OC}, short-circuit current density J_{SC}, filling factor of CVC FF and efficiency of p^+-CuO / p-ZnTe / n-CdSe / n-$MoSe_2$ / Mo SC on the thickness of the absorbing (CdSe), window (ZnTe) and near-contact ($MoSe_2$) layers. They allow to finally determine the optimal thicknesses of these layers. They are equal to 3.5 μm for the absorbing CdSe layer, 0.1 μm for the window ZnTe layer, and 0.5 μm for the near-contact $MoSe_2$ layer.

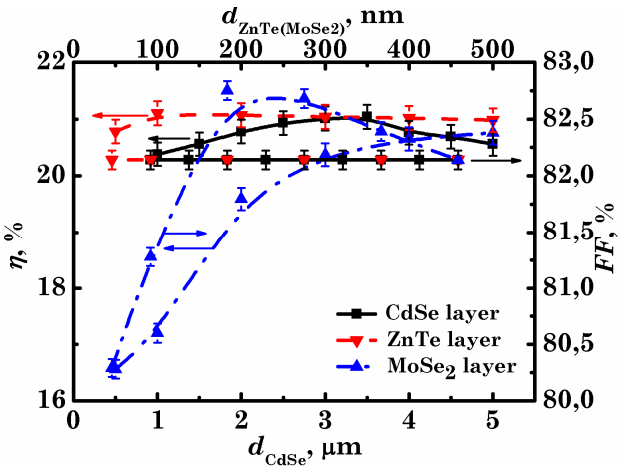

Fig. 8 – Dependences of FF and η of the p^+-CuO / p-ZnTe / n-CdSe / n-$MoSe_2$ / Mo SC on the layer thickness

4. CONCLUSIONS

Simulation of the light CVC as well as the spectral distributions of the quantum efficiency of SC with the ZnTe / CdSe / $MoSe_2$ / Mo structure has been performed in this work. As a result of the simulation, we have established the optimal design parameters of PEC, which provide their maximum efficiency at the temperature of 280 K, namely, the thicknesses of the absorbing CdSe layer – 3.5 μm, of the window ZnTe layer – 0.10 μm, of the intermediate $MoSe_2$ layer – 0.5 μm. The maximum efficiency of photoconverters based on the ZnTe / CdSe / $MoSe_2$ / Mo heterojunctions with an optimal design can reach the values $\eta = 21.60$ %, $U_{OC} = 0.91$ V, $FF = 82.05$ %, $J_{SC} = 29.03$ mA/cm^2. The corresponding devices on their basis can have a wide range of photosensitivity in the interval of $\lambda = 512$-978 nm.

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