APPLIED MECHANICS

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Cadmium telluride solar cells are among the most common devices for photovoltaic applications. However, the energy conversion efficiency of these elements remains insufficiently high. Using the SCAPS programming environment, research and optimization of a classical thin-film solar cell based on CdTe were carried out. The structure of this element consisted of ITO as a transparent conductive contact, a cadmium sulfide (CdS) layer, and a cadmium telluride (CdTe) absorber layer with a metal contact. To optimize this structure in terms of power conversion efficiency, the influence of the thickness and concentration of acceptor impurities in the CdTe absorbing layer, as well as the influence of the thickness and concentration of donor impurities in the CdS buffer layer, were considered. It was established that the optimal thicknesses for the CdS buffer layer and absorption CdTe layers are 50 nm and 3000 nm, respectively. An additional CdSeTe layer between the CdS and CdTe layers has been proposed as one of the optimization options to improve the device efficiency. The main photovoltaic parameters of such a solar cell were analyzed depending on the thickness of the CdSeTe layer and its selenium content. It has been demonstrated that adding CdSeTe solid solution to the 1500 nm thick CdTe absorber layer increases the efficiency of the solar cell by 6.84 %. The main photovoltaic characteristics of CdS/CdTe and CdS/CdSeTe/ CdTe solar cells were compared. The results showed that the simulated CdS/CdSeTe/CdTe structure provides better photoconversion efficiency in the AM1.5G light spectrum compared to the classical CdS/CdTe structure. Such elements can be used to form highly efficient solar panels

Keywords: solar cell, SCAPS, thin films, heterostructures, cadmium telluride, cadmium chalcogenide

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OPTIMIZATION OF THE SOLAR CELL BASED ON CADMIUM TELLURIDE BY ADDING THE CdSeTe ABSORBING LAYER (HETEROSTRUCTURE **SIMULATION)**

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1. Introduction

Solar energy is considered one of the most important renewable energy resources on Earth. Therefore, the market for photovoltaic devices has grown rapidly in recent decades. Different materials are used to design solar cells, among which silicon is the most common. Solar cells based on cadmium chalcogenides occupy an important place in the world market of photovoltaic energy. The use of CdTe-based solar cell (SC) is growing rapidly and it is the second most used type of SCs in the world after silicon. Cadmium telluride (CdTe) is considered the most competitive thin-film photovoltaic technology due to its low production cost and high module efficiency. SCs based on CdTe make it possible to obtain a conversion efficiency of more than 22 % [1].

The main advantage of this technology is that the panels can be manufactured at a lower cost than silicon-based solar panels. First Solar was the first cadmium telluride panel manufacturer to produce solar cells for less than USD 1.00 per watt [2].

CdTe panels have a number of advantages over conventional silicon technology. Firstly, they are easy to manufacture. Secondly, they have an optimal band gap, which makes it possible to absorb light at a wavelength close to the spectral maximum of solar radiation. Third, the presence of cadmium in nature is abundant, and it will not cause price fluctuations at the end product stage.

The layers of semiconductor materials used to make these photovoltaic devices are very thin – just a few micrometers. They are much thinner than crystal plates, several hundreds of micrometers thick. Moreover, the possibility of applying films on thin substrates makes it possible to construct flexible photovoltaic modules. These advantages can help reduce costs by using different deposition processes, such as magnetron sputtering, close-space sublimation, etc. [3].

Therefore, investigation on and search for optimal parameters of solar cells based on cadmium telluride remain relevant.

2. Literature review and problem statement

Typically, a CdTe-based SC device consists of a transparent conducting oxide (TCO), an optically transparent CdS semiconductor layer, a CdTe absorber layer, and a contact. It should be noted that the use of CdS as a buffer layer has been a standard practice in the design of CdTe-based devices since the beginning of their development [4–6]. Hence, improving the device efficiency by optimizing these layers is considered as an alternative approach.

Work [4] considers the search for optimal thicknesses of each CdS/CdTe layer, taking into account the effect of optical and recombination losses. It is shown that the proposed SC design provided about 18 % device efficiency. However, the thickness of the absorber layer was 8 µm. Studies [5] draw attention to the fact that the efficiency of classical SC depends on the methods of obtaining CdS and CdTe layers. The research results also show a SC efficiency of 18 % at a CdTe thickness of 10 µm. In [6], the main points of design that should be paid attention to when developing SC based on CdS/CdTe to improve its characteristics are considered. In particular, it is suggested to pay attention to the method of obtaining the CdTe absorber layer, determining the doping concentration and the mobility of charge carriers. And as one of the methods for increasing efficiency, it is proposed to design solar cells based on multilayer structures of devices with a graduated band gap. However, these studies do not consider the introduction of additional layers to improve the performance of the device.

This approach is considered in [7], in which it is proposed to introduce an additional layer of CdSe between the layers of CdS and CdTe in order to form a solid solution. As a result, such a structure showed better photovoltaic characteristics. However, the efficiency remained below 15 %. The reason for this may be the formation of solid solutions with a structure that is not photoactive. In [8], it is proposed to completely replace the CdS layer with CdSe. This made it possible to obtain a device with an efficiency of 18 %. The CdS layer used in high-efficiency CdTe SCs has a large lattice mismatch (by 11 %) compared to CdTe and a bandgap of 2.4 eV. In addition, interdiffusion occurs at the CdS/CdTe interface during heat treatment, which leads to the formation of CdS_vTe_{1-v} . And, as a result, the current density (I_{sc}) and open circuit voltage (V_{oc}) are reduced compared to what was predicted in the design. The solubility of selenium (Se) in CdTe is much higher than that of sulfur (S), and therefore it can easily diffuse from the CdSe layer into CdTe during growth and annealing. Diffusion of Se forms a CdSe_xTe_{1-x} layer, which reduces the band gap of CdTe.

In [9], it is noted that the thickness of the introduced CdSe layer is important for efficiency optimization. The interdiffusion between the CdSe and CdTe layers must be sufficient to avoid the existence of a separate CdSe layer. Residual CdSe can significantly degrade V_{oc} and J_{SC} , resulting in poor device performance. Work [10] reports the introduction of a CdSeTe (CST) layer in various ways but suggests replacing the CdS buffer layer with MgZnO. The smaller CST band gap explains the absorption of light at longer wavelengths [11, 12], and this leads to an increase in J_{sc} . An increase in the photocurrent under the mode of short-wave radiation indicates that the deposited CdSe layer completely diffuses into CdTe. During growth, a solid solution of CdSeTe is formed. The CdSe_xTe_{1-x} compound has a cubic structure of zinc blende for the composition $0 \le x < 0.4$, and for $0.6 < x \le 1$ it has a wurtzite structure, which is not photoactive and is not used in SC [13].

The width of the band gap of the CdSeTe solution depends on the Se content and, at a certain composition, has

a value lower than that of the binary compounds CdSe and CdTe from which it is formed. Therefore, adding a CST layer in the absorber layer can improve the SC efficiency. This is the approach used in works [8–10].

However, the influence of the solid solution of CST on the characteristics of the classical structure based on cadmium chalcogenides has not been fully studied. In particular, when changing the thickness of the absorbing materials Cd-SeTe and CdTe without changing the total thickness of the absorbing layer (and as a result, without changing the total thickness of SC). This gives reason to assert that it is reasonable to study the dynamics of changes in the main electrical parameters of the CdS/CdTe SC when a CdSeTe layer is introduced into the absorber layer. As well as the search for the optimal quantitative ratio between CdSeTe and CdTe layers at a constant thickness of the absorbing layer.

3. The aim and objectives of the study

The aim of our study was to find the optimal CdS/CdTe SC structure and improve its photovoltaic characteristics by introducing an additional CST absorber layer. This will make it possible to predict and obtain SC with higher efficiently.

To achieve the goal, the following tasks were set:

- to investigate the structure of CdS/CdTe depending on the thickness and concentration of carriers of the CdTe absorber layer and the CdS buffer layer;
- to investigate the influence of additional CST absorption layer on the photovoltaic characteristics of SC;
- to compare the characteristics of CdS/CdTe and CdS/ CST/CdTe structures.

4. The study materials and methods

One of the most common structures for solar cells based on cadmium telluride, CdS/CdTe, was chosen as the research object due to its low cost and high module efficiency. It is known that one of the ways to optimize the photovoltaic parameters of solar cells is to introduce an additional layer of $CdSe_xTe_{1-x}$ between the binary components [8–10]. In view of this, a hypothesis was proposed to study the influence of this layer on the properties of the element. The simulation was carried out using the software SCAPS (Solar Cell Capacitance Simulator) [14]. It provides a wide range of structure photovoltaic performance parameters such as charge carrier generation and recombination profile, spectral response, open circuit voltage (V_{OC}), current density (J_{SC}), fill factor (FF), and efficiency (η) of the solar cell.

With this program, the films used in solar cells were analyzed to understand the performance of CdS/CdTe thin film SCs and to produce the cells with the highest efficiency. The thickness of each layer was varied and adjusted to obtain the highest possible efficiency value.

Fig. 1 shows the schematics of CdTe solar cells. The first is a classical CdTe SC structure consisting of indium tin oxide (ITO), on top of which an n-type CdS layer is deposited, followed by a p-type CdTe absorber layer and a back contact. The second demonstrates that a $\text{CdSe}_x\text{Te}_{1-x}$ layer is added between the CdS and CdTe layers in order to increase the efficiency due to the expansion of the spectral range of photon absorption. In order to find out the dynamics of change

in photovoltaic parameters only due to the influence of the $CdSe_xTe_{1-x}$ layer, a simplification was accepted that does not take into account the interdiffusion at the boundary of the layers and the presence of defects.

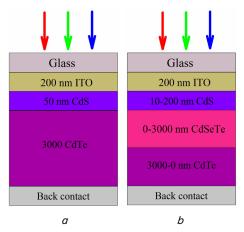


Fig. 1. Schematic diagrams of CdTe solar cells: a — with CdS/CdTe layers; b — with CdS/CdSeTe/CdTe layers

The AM 1.5 light spectrum with a radiation power of $1000~\text{W/m}^2$ and a temperature of 300~K was used for the study of the proposed SC structure in SCAPS.

5. Results of modeling photovoltaic parameters of solar cells

5. 1. Investigating the effect of thickness and concentration in the absorber layer and buffer layer on the parameters of the CdS/CdTe structure

One of the parameters that determines the efficiency and cost of SC is the thickness of the CdTe absorbing layer. In order to find its optimal thickness, simulations were carried out and the main photovoltaic characteristics of the CdS/CdTe solar cell were determined at a constant carrier concentration of N_A =2·10¹⁴ cm⁻³. The thickness of the CdS layer was 50 nm and remained unchanged during the simulation, while the thickness of the CdTe layer varied in the range of 500–6000 nm. The dependence of photovoltaic parameters of the CdS/CdTe structure on the thickness of absorber is shown in Fig. 2, a.

Similar dependences on the carrier concentration in the CdTe layer are shown in Fig. 2, b. The simulations were carried out at a constant thickness of d(CdTe)=3000 nm.

Fig. 3 shows the dependence of CdS/CdTe quantum efficiency on the thickness (Fig. 3, *a*) and concentration (Fig. 3, *b*) of the CdTe absorbing layer, respectively.

Fig. 4 shows the results of modeling the main photovoltaic parameters in the SCAPS program for the CdS buffer layer in the CdS/CdTe structure.

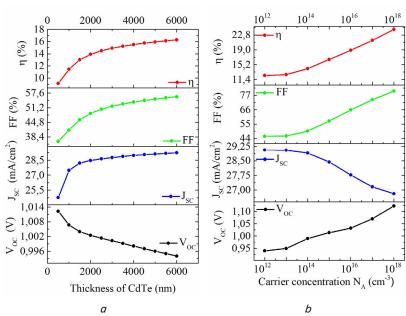


Fig. 2. Dependences of photovoltaic parameters of the CdTe layer: a — on thickness; b — on the concentration of carriers

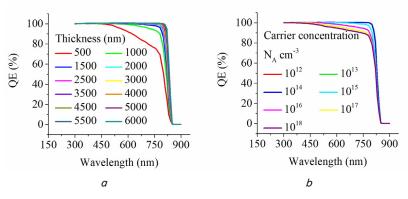


Fig. 3. Dependence of quantum efficiency in the CdTe layer: a- on thickness; b- on the concentration of carriers

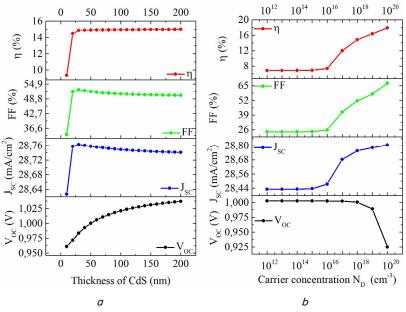


Fig. 4. Dependences of photovoltaic parameters of the CdS layer: a — on thickness; b — on the concentration of carriers

The layer thickness varied from 10 nm to 200 nm. The concentration of carriers varied from N_D =10¹² cm⁻³ to N_D =10²⁰ cm⁻³. The thickness of the CdTe absorbing layer remained unchanged and was 3000 nm.

5. 2. Influence of the additional CST absorption layer on the photovoltaic characteristics of the solar cell

To optimize the solar cell, more and more attention is paid to the modification of the layers of the CdS/CdTe structure. There are many studies where an additional layer of CdSe is introduced into these layers [8, 15] for interdiffusion and formation of solid solutions. However, in the manufacture of a CdTe solar cell, a thin layer of CdSe $_{\rm x}$ Te $_{\rm 1-x}$ is formed between the CdTe and CdSe layers because selenium Se has a high reactivity. Therefore, the study of the effect of the CdSe $_{\rm x}$ Te $_{\rm 1-x}$ layer on SC efficiency plays a significant role in the optimization of the solar cell.

Using the SCAPS program, the CdS/CdSeTe/CdTe structure was modeled depending on the Se content in the CST solution and its thickness. The initial data for modeling are given in Table 1.

Table 1
Simulation parameters used in the SCAPS program for CdS/CdTe and CdS/CdSeTe/CdTe solar cells

| Parameter | Material layer | | | | |
|--|----------------------|----------------------|----------------------|----------------------|--|
| Layer | ITO | CdS | CdSeTe | CdTe | |
| | [16] | [17, 18] | [8, 19] | [19, 20] | |
| Thickness (nm) | 200 | 10-200* | 0-3,000* | 500-6,000* | |
| Bandgap (eV) | 3.7 | 2.4 | 1.41 | 1.5 | |
| Electron affinity (eV) | 4.9 | 4.5 | 4.2 | 3.9 | |
| Dielectric permittivity (relative) | 9 | 10 | 9.4 | 9.4 | |
| CB effective density of states (cm ⁻³) | 2·10 ¹⁸ | $2.2 \cdot 10^{18}$ | 8 10 ¹⁷ | 8 10 ¹⁷ | |
| VB effective density of states (cm ⁻³) | 1.8·10 ¹⁹ | 1.8·10 ¹⁹ | 1.8·10 ¹⁹ | 1.8·10 ¹⁹ | |
| Electron/hole thermal velocity (cm/s) | 1·10 ⁷ | 1·10 ⁷ | 1·10 ⁷ | 1.107 | |
| Electron mobility (cm ² /Vs) | 30 | 100 | 320 | 320 | |
| Hole mobility (cm ² /Vs) | 5 | 25 | 40 | 40 | |
| Donor/acceptor density N_D/N_A (cm ⁻³) | 1.1019 | 1.1018 | 1.1014 | 2.1014 | |

Note: * - parameters that changed during simulation in the SCAPS program.

It is important to determine the optimal composition of $CdSe_xTe_{1-x}$ since the band gap (E_g) for pure CdSe and CdTe is $1.74 \, eV$ and $1.5 \, eV$, respectively. For the $CdSe_xTe_{1-x}$ ternary solution, the dependence of E_g is not linear and depends on the content of selenium Se. It has a deflection below the values for binary compounds $(E_g(CdSe)=1.74 \, eV \, and \, E_g(CdTe)=1.5 \, eV)$. The content of Se from x=0.1 to 0.6 can reduce the band gap compared to $1.5 \, eV$ of CdTe, expanding the range of the absorption spectrum. Changing the ratio of Se and Te will allow adjusting the width of the band gap. It should be noted that the $CdSe_xTe_{1-x}$ solution at x>0.6 has a wurtzite structure, which is not photoactive and is not suitable for use in SC.

Se can be introduced by depositing a thin film of CdSe precursor and then diffusing it into CdTe during annealing. However, during the fabrication of CdSeTe/CdTe devices, the thickness of CdSe must be precisely controlled to prevent the formation of a CdSe layer after the activation treatment

when not all of the CdSe has diffused into CdTe. Obtaining residual CdSe leads to a sharp decrease in device efficiency due to a decrease in current density and efficiency [21].

The smallest forbidden band gap is in the cubic structure of CST solid solution with Se content x=0.3, so the CdSe_{0.3}Te_{0.7} layer was used in our study. Since thin structures were investigated, it was decided not to increase the thickness of the absorbing layer, but to model it by adding a CST film, so that the total thickness of CST and CdTe remained 3000 nm. The results of SCAPS modeling are shown in Fig. 5, 6, where structures from CdS/CdTe without CST to complete replacement of CdTe with CST with a thickness of 3000 nm are considered.

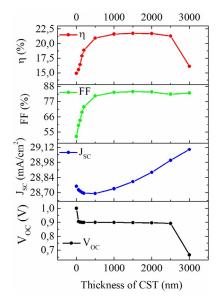


Fig. 5. Dependences of photovoltaic parameters on the thickness of CdSeTe layer

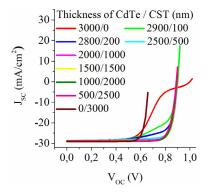


Fig. 6. Volt-ampere characteristics of a CdS/CST/CdTe solar cell

As the thickness of the CST layer increases, the exponential dependence of the current density on voltage is observed.

5. 3. Comparing the main characteristics between CdS/CdTe and CdS/CST/CdTe solar cell structures

A comparison of the characteristics of CdS/CdTe and CdS/CST/CdTe structures obtained using the SCAPS program is given in Table 2 and shows the differences in the main photovoltaic parameters. Fig. 7 demonstrates the *J-V* characteristics of unilluminated and illuminated structures.

These results show the superiority of SC with the addition of a CST layer over the basic CdS/CdTe structure.

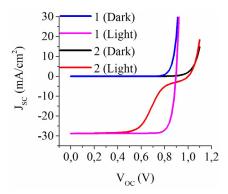


Fig. 7. Comparison of current-voltage characteristics of SC CdS/CST/CdTe (1) and CdS/CdTe (2)

Table 2

Main photovoltaic characteristics of CdS/CdTe and CdS/CST/CdTe structures

| Structure | $V_{OC}(V)$ | J_{SC} (mA/cm ²) | FF (%) | η (%) |
|--------------|-------------|--------------------------------|--------|-------|
| CdS/CdTe | 1.0003 | 28.757920 | 51.82 | 14.91 |
| CdS/CST/CdTe | 0.8971 | 28.800363 | 84.18 | 21.75 |

6. Discussion of results based on the simulation of CdS/CdTe and CdS/CST/CdTe structures depending on the parameters of layers

The results shown in Fig. 2, a demonstrate that the optimal layer thickness should be at least 1500 nm. This ensures device efficiency of more than 13 %. When the thickness of the CdTe absorber increases, a higher absorption efficiency of long-wave photons is observed, which increases the J_{sc} value (Fig. 3, a) and, therefore, the efficiency of the device.

However, analyzing the dependence of SC quantum efficiency on the thickness of CdTe (Fig. 3, a), its maximum value is observed at thicknesses above 3000 nm. Therefore, the thickness of the absorbing layer is 3000 nm, which provides η =14.9%. With a further increase in thickness, the efficiency increases within 1%, that is, it does not change significantly. Therefore, increasing the thickness of the absorbing layer does not significantly improve the efficiency of solar cells, but leads to an increase in the production cost of SC.

Fig. 2, b shows the dependence of acceptor concentration (N_A) in the absorber layer (CdTe) varying in the range from $1 \cdot 10^{12}$ cm⁻³ to $1 \cdot 10^{18}$ cm⁻³ at a constant thickness of 3000 nm.

A linear increase in the open circuit voltage V_{OC} from 0.94 V at N_A =10¹² cm⁻³ to 1.1 V at N_A =10¹⁸ cm⁻³ and a linear decrease in the current density J_{SC} , respectively, from 29.06 mA/cm² to 26.8 mA/cm² can be explained by an increase in the recombination of free charge carriers inside the volume [20]. On the other hand, the fill factor (*FF*) and hence efficiency (η) increase linearly with increasing hole concentration.

However, an increase in carrier density in the range of $(10^{15}-10^{18}) \, \mathrm{cm^{-3}}$ leads to a decrease in the quantum efficiency in the wavelength range of $500-850 \, \mathrm{nm}$ (Fig. 3, b). At high concentrations of carriers in the absorbing layer of CdTe, the scattering of impurities increases, therefore the rate of recombination of carriers also increases. And this negatively affects the transport of holes in the CdTe layer to the CdS buffer layer [17]. Taking this into account, the optimal level of carrier concentration in the layer of absorbing material CdTe was determined, which was $N_A = 2 \cdot 10^{14} \, \mathrm{cm^{-3}}$.

The decrease in quantum efficiency (QE) can be attributed to enhanced photon collection at longer wavelengths. The production of additional electron-hole pairs in thin-film SC results from the absorption of photons with a longer wavelength, which leads to an increase in J_{SC} at low concentrations of acceptor charge carriers (N_A) (Fig. 2, b). The increase in V_{OC} with increasing N_A shows that the open circuit voltage (V_{OC}) of the CdTe layer is significantly affected by the concentration of acceptor charge carriers (N_A) . The generated electric field in the depletion region changes when the concentration of the charge acceptor carrier of the CdTe layer is high. As a result, the recombination of free charge carriers decreases, increasing V_{OC} [20].

Analyzing the dependence of main photovoltaic parameters on the thickness of the CdS buffer layer (Fig. 4), it can be noted that its thickness should be at least 30 nm. Starting from a thickness of 40 nm, the J_{SC} , FF, and η parameters remain almost unchanged and are 28.75 mA/cm², 50.5 %, and η =14.9 %, respectively.

Since thick buffer layers contribute to lower SC efficiency, it is important to reduce their thickness to less than 100 nm to limit photon absorption losses. Therefore, in this work, the optimal thickness of the buffer layer was taken as 50 nm.

Typically, a buffer layer is used to reduce the recombination of charge carriers at the interface between different material layers in a solar cell (CdS/CdTe). Increasing the concentration of donors in the buffer layer can help reduce recombination and increase the efficiency of converting sunlight energy into electric current. However, a high concentration of donors can also lead to a deterioration of the electrical characteristics of SC due to an increase in resistance. Thus, optimizing the concentration of donors in the layer is also an important step in improving the efficiency of SC.

Fig. 4, b shows how a high donor concentration in the buffer layer improves the efficiency of the solar cell. Although J_{SC} , FF, and η increase, V_{OC} decreases. The explanation for this is the loss of photons in the buffer layer. When the concentration of the buffer layer (N_D) decreases, more incident photons generated by the CdS layer are absorbed, reducing the number of photons that can be absorbed by the absorber layer (CdTe) [20]. The optimal concentration of donor charge carriers is taken as N_D =10¹⁸ cm⁻³.

Adding a CST solid solution layer to the CdTe absorber layer increases the SC efficiency. This is due to the addition of selenium to form a film of $CdSe_xTe_{1-x}$ in the front part of the absorber. Next comes the CdTe layer. CST has a smaller band gap of about 1.41 eV compared to 1.5 eV for CdTe. Due to the reduced bandgap, the CST layer increases the absorption of long-wavelength photons in the solar spectrum, resulting in improved J_{sc} . Increasing the current density and maintaining the open circuit voltage lead to an increase in the efficiency of the device by more than 20 % [22].

In the presence of the CST layer, V_{OC} is almost independent of the thickness and remains approximately constant at 0.9 V. At the same time, when the CST layer thickness increases, the FF and η indicators increase and reach their maximum in the configuration of the absorbing layer: CST d=1500 nm and CdTe d=1500 nm. At the same time, their values are 84.18 % and 21.75 %, respectively. J_{sc} increases from 28.75 mA/cm² to 29 mA/cm² with increasing thickness. When the CdTe layer is completely replaced by a CST layer, the SC efficiency drops sharply to 16.11 %.

Fig. 6 shows the current-voltage characteristics of the CdS/CST/CdTe element depending on different thickness

of the CST/CdTe absorbing layer. For the CdTe-only absorber, the J-V curve has V_{OC} =1 V, and for the CST-only absorber, it is much smaller and equal to V_{OC} =0.66 V. For the double-layer absorber (CST/CdTe), the J-V characteristics acquire the correct exponential form. V_{OC} and J_{SC} change slightly and are about 0.9 V and 28.7 mA/cm², respectively.

A simple measurement of the J-V characteristics in the dark creates an exponential curve characteristic of a p-n junction. In the dark, it gives an extremely small value of the current coming from non-main charge carriers. After the solar cell is illuminated, the photoelectric process begins, and charge carriers are generated by absorbing incident photons and produce a photocurrent, therefore, the J-V curve shifts to a value equal to the photocurrent density J-SC (Fig. 7).

The efficiency of SC increased as a result of changing the configuration of the absorbing layer. Replacing the CdTe absorber with the CdSe $_{0.3}$ Te $_{0.7}$ (d=1500 nm)/CdTe (d=1500 nm) structure made it possible to increase the efficiency of the device by 6.84 %. At the same time, the fill factor increased significantly from 51.82 % to 84.18 %, and the current density increased from 28.76 mA/cm² to 28.8 mA/cm².

Therefore, the introduction of an additional layer of CST provides an increase in the efficiency of the device without changing the total thickness of SC. As mentioned above, this is achieved due to the smaller bandgap of the CST layer than CdTe. In contrast to the results reported in [8], in which the CdS layer is completely replaced by CdSe and an efficiency of 18 % is achieved, the introduction of an additional absorber layer ensures the efficiency of the device by more than 20 %. It should be noted that our results are for an ideal structure. In practice, recombination and mutual diffusion of carriers between layers of the element should be taken into account. However, the research results will be useful for establishing optimal thicknesses and carrier concentrations in cadmium chalcogenide layers for thin-film SCs. They could also become the basis for further studies on the influence of defects and interdiffusion at the layer boundaries.

7. Conclusions

1. During our studies, with the help of simulation, an optimized SC structure based on CdS/CdTe was obtained, which ensures maximum efficiency. When the absorber layer increases, the efficiency of SC increases, but with thicknesses from 3,000 nm to 6,000 nm, the efficiency does not increase significantly. At high concentrations of impurities in the CdTe layer, the scattering of charge carriers increases, therefore their recombination rate also increases. And this negatively affects the transport of holes in the CdTe layer to the CdS buffer layer. Therefore, the optimal thickness and concentration of impurities in the CdTe absorbing layer are taken as $d{=}3,000\,\mathrm{nm}$ and $N_A{=}2.10^{14}\,\mathrm{cm}^3$, respectively. The CdS

buffer layer helps reduce the recombination of electrons and holes at the interface between the different SC layers, which increases the efficiency of the device as more charge carriers reach the electrodes. Therefore, it is better to have a high level of impurities in the CdS thin film. The optimal thickness and concentration of donor charge carriers in the CdS buffer layer are taken as d=50 nm and $N_D=10^{18}\,\mathrm{cm}^{-3}$, respectively.

2. The effect of an additional CST absorption layer on the photovoltaic characteristics of SC based on CdTe was investigated. The optimized CdS/CdTe structure shows a solar energy conversion efficiency of 14.91 %. However, when a CdSeTe solid solution is introduced by replacing the CdTe absorber layer with CST/CdTe layers in equal proportions, an increase in efficiency is observed. The composition of the solid solution is taken as CdSe $_{0.3}$ Te $_{0.7}$ since its band gap is 1.41 eV. The optimal thickness of the CST layer is d=1,500 nm. The SC structure of CdS/CST/CdTe improves the efficiency up to 21.75 %, which is associated with a smaller band gap than that of CdTe. Thanks to this, the CST layer increases the absorption of long-wave photons in the spectrum, which leads to an improvement in the current density and increases the efficiency of SC.

3. We have compared the CdS/CdTe and CdS/CST/CdTe solar cell structures. Introducing a CST film with a thickness of $1,500\,\mathrm{nm}$ into the absorber layer, without changing the overall thickness of the absorber layer, increases the efficiency of the device by $6.84\,\%$.

Conflicts of interest

The authors declare that they have no conflicts of interest in relation to the current study, including financial, personal, authorship, or any other, that could affect the study, as well as the results reported in this paper.

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Data availability

All data are available, either in numerical or graphical form, in the main text of the manuscript.

Use of artificial intelligence

The authors confirm that they did not use artificial intelligence technologies when creating the current work.

References

- 1. Green, M. A., Dunlop, E. D., Hohl-Ebinger, J., Yoshita, M., Kopidakis, N., Hao, X. (2021). Solar cell efficiency tables (Version 58). Progress in Photovoltaics: Research and Applications, 29 (7), 657–667. https://doi.org/10.1002/pip.3444
- 2. Thompson, N., Ballen, J. (2017). First Solar. MIT Management Sloan School. Available at: https://mitsloan.mit.edu/sites/default/files/2020-03/First%20Solar.IC_.pdf
- Romeo, A., Artegiani, E. (2021). CdTe-Based Thin Film Solar Cells: Past, Present and Future. Energies, 14 (6), 1684. https://doi.org/10.3390/en14061684
- Mohamed, H. A. (2015). Optimized conditions for the improvement of thin film CdS/CdTe solar cells. Thin Solid Films, 589, 72–78. https://doi.org/10.1016/j.tsf.2015.04.081

- Morales-Acevedo, A. (2006). Thin film CdS/CdTe solar cells: Research perspectives. Solar Energy, 80 (6), 675–681. https://doi.org/10.1016/j.solener.2005.10.008
- 6. Dharmadasa, I. M., Alam, A. E., Ojo, A. A., Echendu, O. K. (2019). Scientific complications and controversies noted in the field of CdS/CdTe thin film solar cells and the way forward for further development. Journal of Materials Science: Materials in Electronics, 30 (23), 20330–20344. https://doi.org/10.1007/s10854-019-02422-6
- Yang, X., Liu, B., Li, B., Zhang, J., Li, W., Wu, L., Feng, L. (2016). Preparation and characterization of pulsed laser deposited a novel CdS/CdSe composite window layer for CdTe thin film solar cell. Applied Surface Science, 367, 480–484. https://doi.org/10.1016/j.apsusc.2016.01.224
- 8. Ibrahim, M., Chelvanathan, P., Miraz, M. H., Alkhammash, H. I., Hasan, A. K. M., Akhtaruzzaman, Md. et al. (2022). Comprehensive study on CdSe thin film as potential window layer on CdTe solar cell by SCAPD-1D. Chalcogenide Letters, 19 (1), 33–43. https://doi.org/10.15251/cl.2022.191.33
- 9. Li, C., Hu, G., Hao, X., Li, C., Tan, B., Wang, Y. et al. (2021). Performance improvement of CdS/CdTe solar cells by incorporation of CdSe layers. Journal of Materials Science: Materials in Electronics, 32 (14), 19083–19094. https://doi.org/10.1007/s10854-021-06425-0
- Lingg, M., Buecheler, S., Tiwari, A. N. (2019). Review of CdTe_{1-x}Se_x Thin Films in Solar Cell Applications. Coatings, 9 (8), 520. https://doi.org/10.3390/coatings9080520
- 11. Paudel, N. R., Yan, Y. (2014). Enhancing the photo-currents of CdTe thin-film solar cells in both short and long wavelength regions. Applied Physics Letters, 105 (18). https://doi.org/10.1063/1.4901532
- 12. Fiducia, T. A. M., Mendis, B. G., Li, K., Grovenor, C. R. M., Munshi, A. H., Barth, K. et al. (2019). Understanding the role of selenium in defect passivation for highly efficient selenium-alloyed cadmium telluride solar cells. Nature Energy, 4 (6), 504–511. https://doi.org/10.1038/s41560-019-0389-z
- Poplawsky, J. D., Guo, W., Paudel, N., Ng, A., More, K., Leonard, D., Yan, Y. (2016). Structural and compositional dependence of the CdTe_xSe_{1-x} alloy layer photoactivity in CdTe-based solar cells. Nature Communications, 7 (1). https://doi.org/10.1038/ ncomms12537
- 14. Burgelman, M., Nollet, P., Degrave, S. (2000). Modelling polycrystalline semiconductor solar cells. Thin Solid Films, 361–362, 527–532. https://doi.org/10.1016/s0040-6090(99)00825-1
- Zheng, X., Kuciauskas, D., Moseley, J., Colegrove, E., Albin, D. S., Moutinho, H. et al. (2019). Recombination and bandgap engineering in CdSeTe/CdTe solar cells. APL Materials, 7 (7). https://doi.org/10.1063/1.5098459
- Doroody, C., Sajedur Rahman, K., Chelvanathan, P., Adib Ibrahim, M., Sopian, K., Amin, N. et al. (2023). Incorporation of Magnesium-doped Zinc Oxide (MZO) HRT Layer in Cadmium Telluride (CdTe) Solar Cells. Results in Physics, 47, 106337. https://doi.org/10.1016/j.rinp.2023.106337
- 17. Nykyruy, L. I., Yavorskyi, R. S., Zapukhlyak, Z. R., Wisz, G., Potera, P. (2019). Evaluation of CdS/CdTe thin film solar cells: SCAPS thickness simulation and analysis of optical properties. Optical Materials, 92, 319–329. https://doi.org/10.1016/j.optmat.2019.04.029
- 18. Bhari, B. Z., Rahman, K. S., Chelvanathan, P., Ibrahim, M. A. (2023). Plausibility of ultrathin CdTe solar cells: probing the beneficial role of MgZnO (MZO) high resistivity transparent (HRT) layer. Journal of Materials Science, 58 (40), 15748–15761. https://doi.org/10.1007/s10853-023-09001-5
- 19. Filipe, D. I., Chenene, M. L. (2023). Front interface defect signature and benefits of CdSeTe thickness and band gap in CdSeTe/CdTe graded solar cell. https://doi.org/10.21203/rs.3.rs-3462048/v2
- 20. Zyoud, S. H., Zyoud, A. H., Ahmed, N. M., Abdelkader, A. F. I. (2021). Numerical Modelling Analysis for Carrier Concentration Level Optimization of CdTe Heterojunction Thin Film-Based Solar Cell with Different Non-Toxic Metal Chalcogenide Buffer Layers Replacements: Using SCAPS-1D Software. Crystals, 11 (12), 1454. https://doi.org/10.3390/cryst11121454
- Liu, X., Abbas, A., Togay, M., Kornienko, V., Greenhalgh, R., Curson, K. et al. (2024). The effect of remnant CdSe layers on the performance of CdSeTe/CdTe photovoltaic devices. Solar Energy Materials and Solar Cells, 267, 112717. https://doi.org/10.1016/ j.solmat.2024.112717
- 22. Munshi, A. H., Kephart, J., Abbas, A., Raguse, J., Beaudry, J.-N., Barth, K. et al. (2018). Polycrystalline CdSeTe/CdTe Absorber Cells With 28 mA/cm² Short-Circuit Current. IEEE Journal of Photovoltaics, 8 (1), 310–314. https://doi.org/10.1109/jphotov.2017.2775139