

## Efficiency Modeling of Solar Cells Based on the $n\text{-Zn}_{1-x}\text{Mg}_x\text{O} / p\text{-SnS}$ Heterojunction

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The recombination and optical losses were determined in auxiliary and absorbing layers of solar cells (SCs) based on the  $n\text{-Mg}_x\text{Zn}_{1-x}\text{O} / p\text{-SnS}$  heterojunction (where  $x = 0; 0.3; 1$ ) with transparent front contacts (ZnO:Al and ITO). The spectral dependences of the transmittance of light by SCs have been calculated, taking into account the reflection of light from the boundaries of the contacting materials, as well as its absorption in the auxiliary layers of the devices. The quantum yield of the investigated structures of photoconductors were determined. The effect of recombination and optical losses in such SCs on the short-circuit current and the efficiency were determined with different thickness of window layer  $\text{Mg}_x\text{Zn}_{1-x}\text{O}$  (25-400 nm) and constant thickness of Al:ZnO and ITO layers (100-200 nm). The efficiency of the structures was calculated for the case of the open circuit voltage  $U_{oc}$  determined from the energy diagrams and taken from the literature. It was found that in the first case, the SCs can have an efficiency that increases from 4.91 % (ZnO / SnS) to 10.8 % (MgO / SnS) with an increase in the Mg content in the solid solution. In the second case, SCs based on the ZnO/SnS heterojunction with a conductive contact Al:ZnO have the highest efficiency values ( $\eta = 11.62$  %). Devices based on  $\text{Mg}_{0.3}\text{Zn}_{0.7}\text{O} / \text{SnS}$  and  $\text{MgO} / \text{SnS}$  heterojunction show an efficiency value of 5.97 % and 5.84 %, respectively. The material of the front conductive contact has little effect on the efficiency of the SCs. The obtained results allow to determine the maximum value of the efficiency of considered SCs taking into account recombination and optical losses in device layers and to optimize the parameters of real devices in order to achieve these values of efficiency.

**Keywords:** Efficiency, Losses, Heterojunction, Solar cells, Window layer, SnS, ZnO.

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### 1. INTRODUCTION

The problem of energy supply is one of the most pressing problems that mankind solves in our time. One of the solutions to this is the widespread using of renewable energy sources (RES). It should be noted that today the renewable energy, in particular, solar energy, is rapidly developing, and including in Ukraine. First of all, this was made possible by a number of factors, in particular, the state policy of support for renewable energy [1].

Today the most common are Solar Cells (SCs) based on silicon technologies (the first generation of SCs), but recently thin-film SCs with absorbing layers of CdTe and  $\text{CuIn}_{1-y}\text{Ga}_y\text{Se}_2$  (CIGS) with different window layers (mostly CdS) and front current spreading layers (most often ITO ( $\text{In}_2\text{O}_3$  (90 %) +  $\text{SnO}_2$  (10 %) or Al-doped ZnO (AZnO)) that belong to the second generation of devices [2]. Today's efficiency for these SCs reaches 22.9 % [3]. However, such disadvantages as the high cost of In, Ga, and Te, and the toxicity of Cd give impetus to the search for alternative materials of the functional layers and structures of the SCs for large-scale use. Nowadays, such materials as  $\text{Cu}_2\text{ZnSnSe}_4$  (CZTSe) and SnS are considered as absorbing layers of the third-generation SCs [4]. This is due to the close band gap to optimum for the conversion of the sunlight energy (the Shockley Queisser limit), the high light absorption coefficient ( $\sim 10^5 \text{ cm}^{-1}$ ), the  $p$ -type electrical conductivity, the high charge carriers lifetime, and also their fairly high mobility [4, 5]. Unlike other semiconductors that are used today as absorbing layers of thin-film SCs, these compounds do

not contain rare and environmentally hazardous metals, the elements that are part of them are widespread in the Earth's crust, and the cost of their extraction is relatively low. However, the obtaining of films of a four-component compound CZTSe is associated with certain difficulties, since its components have significantly different values of vapor pressure, and the domain of homogeneity is rather narrow [6]. As a result, the resulting layers often contain several phases with different bandgap widths, and the efficiency of the devices on their basis is low [3]. This has led to the growing interest of researchers to the two-component SnS compound [4, 5], monophasic films of which can be easily synthesized by various methods, for example [7].

Traditionally, as a window material to different absorption layers of SCs, a binary CdS compound having  $n$ -type conductivity and a band gap equal to  $E_g = 2.42 \text{ eV}$  has been used for a long time [2, 3]. This compound was used in [8] to obtain thin-film SCs with a SnS absorbing layer. However, the efficiency of such devices is small, and nowadays it does not exceed 4.36 % [9]. Several studies have shown that such a low efficiency of the SCs may be due to poor coordination of the electrical characteristics of the materials of heterojunction [4, 5]. Measurements by photoelectron spectroscopy of gap zones on band diagrams between  $p$ -type SnS and  $n$ -type conductivity CdS,  $\text{SnS}_2$ ,  $\text{In}_2\text{S}_3$ ,  $\text{ZnIn}_2\text{Se}_4$ , ZnO and  $\text{Mg}_x\text{Zn}_{1-x}\text{O}$  showed that among the considered compounds, the  $\text{Mg}_x\text{Zn}_{1-x}\text{O}$  solid solution most meets the requirements for materials to create effective solar converters. The  $n\text{-Mg}_x\text{Zn}_{1-x}\text{O}/p\text{-SnS}$  heterojunction refers to structures of

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I type and can have high efficiency of converting solar energy into electrical energy [10, 11].

It is known [12] that the electrical characteristics of  $Mg_xZn_{1-x}O$  are easy to control by varying the concentration of Mg in the solid solution. In this case, the optimal for use as a window material to SnS is a semiconductor with a magnesium concentration, which lies in the range  $0 < x < 0.3$ . However, in our time for thin-film SCs based on the  $n-Mg_xZn_{1-x}O/p-SnS$  heterojunctions, an efficiency of 2.1% has been achieved [11], while theoretical calculations show that it can reach more than 20% [13]. The difference between the theoretical predictions and the actual values of the efficiency of devices is explained by electrical, recombination and optical losses during the transformation of solar radiation into electrical energy.

The key energy losses in the photoelectric transformation of solar energy are related to: the light reflection from the heterojunction interface and device surface, the passage of the radiation part through the SCs without absorption, the scattering of photon energy by the heat fluctuations of the lattice, the recombination of the electron-hole pairs that arose under the action of light, both in volume and on the surface of the device, as well as its internal resistance and other physical processes. Increase in the efficiency of SCs is possible by reducing such losses by optimizing their design and improving the structural, optical and electrical properties of the composite layers.

The main purpose of the work is to determine the recombination and optical losses in the SCs on the basis of  $n-Mg_xZn_{1-x}O/p-SnS$  heterojunction ( $x = 0; 0.3; 1$ ) with transparent front contacts of AZnO or ITO and to determine the effect of these losses on the efficiency of devices.

## 2. THE LOSSES OF LIGHT REFLECTION

"Substrate" and "superstrate" are two well-known basic designs of thin film SCs [2]. The last one has several advantages associated with the simplicity of sealing the device, its higher efficiency, etc. [2, 3]. That is why modeling was carried out by us for the SCs of this design.

Thin-film SCs with superstrate type consist of several layers and include a substrate (glass), a front conductive transparent contact (ITO, AZnO), a window (ZnO,  $Mg_{0.3}Zn_{0.7}O$ , MgO) and an absorbing (SnS) layers and a metallic rear contact. The structure of such a solar cell is shown in Fig. 1.

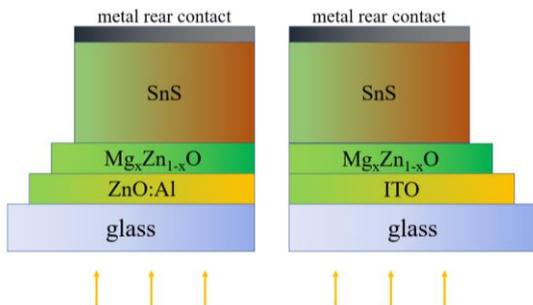


Fig. 1 – Solar cell design based on SnS absorbing layer and  $Mg_xZn_{1-x}O$  ( $x = 0; 0.3; 1$ ) window layer

The processes of light reflection from the SCs layers

were modeled at a variable thickness of the window layer  $d = (25-400)$  nm and at a constant thickness  $d = 100$  and  $200$  nm of the transparent front layer AZnO (ITO). Such values are usually used in real SCs [2, 14].

On the way to the SnS absorbing layer, where the electron-hole pairs are generated under the action of light, the solar radiation flux passes through the auxiliary layers of the SCs glass, ITO (AZnO) and  $Mg_xZn_{1-x}O$  (ZnO, MgO). At the same time, on the boundaries between the air - glass, glass - ITO (AZnO), ITO(AZnO) -  $Mg_{0.3}Zn_{0.7}O$  (ZnO, MgO) and  $Mg_{0.3}Zn_{0.7}O$  (ZnO, MgO) - SnS, due to a light reflection, there are optical losses of solar energy. It is also necessary to take into account the absorption of the sunlight in the auxiliary layers of the SCs: glass, ITO (AZnO) and  $Mg_xZn_{1-x}O$ .

The method of calculating optical losses in the device and the main expressions used in this case are given in [15].

The spectral dependences of the refractive index and extinction coefficient of SnS absorbing layer used in the modeling are shown in Fig. 2. The spectral dependences of  $n$  and  $k$  of other layers of SCs are given in [16].

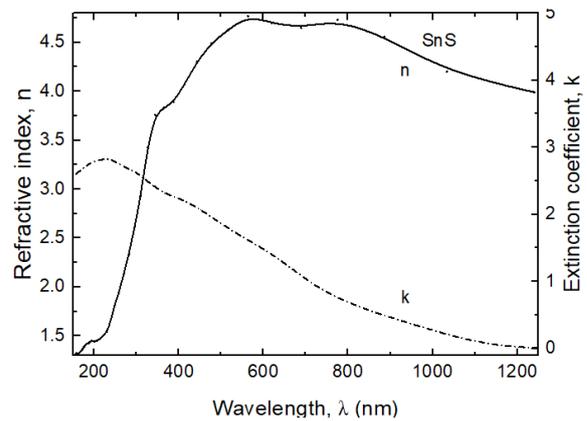


Fig. 2 – Spectral dependencies of the refractive index and the extinction coefficient of SnS absorbing layer

For  $Mg_{0.3}Zn_{0.7}O$  solid solution layer, these values were calculated from the known values of  $n$  and  $k$  of zinc oxide and magnesium oxide using the Vegard's law. At modeling, for air, the coefficients were equal to  $n = 1, k = 0$ .

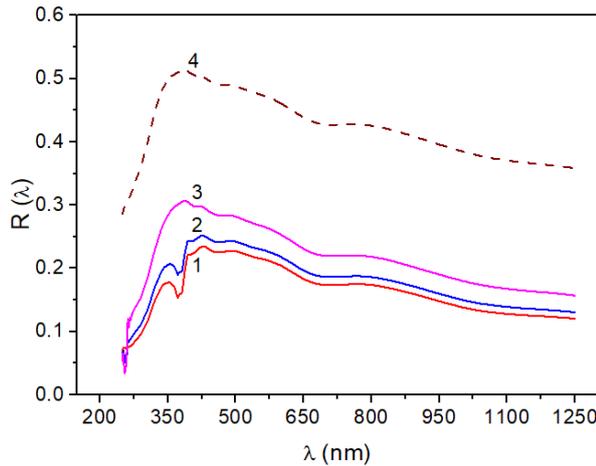
The received spectral dependences of the reflection coefficient from the boundaries of the window layer – the absorption layer of SCs and the layer  $Mg_xZn_{1-x}O$  in direct contact with air are shown in Fig. 3.

Therefore, the formula for determining the light transmittance coefficient for a multilayer structure of the SCs has the form [15, 16]:

$$T(\lambda) = (1 - R_{12})(1 - R_{23})(1 - R_{34})(1 - R_{45}),$$

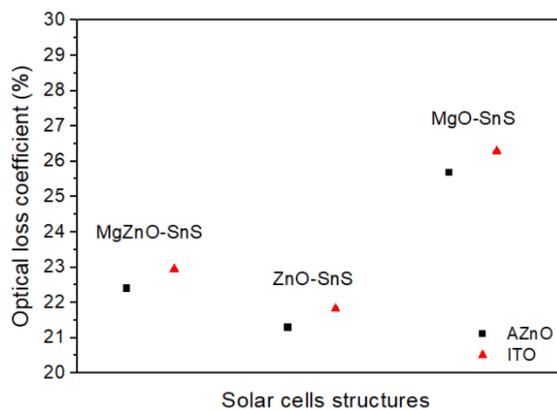
where  $R_{12}, R_{23}, R_{34}, R_{45}$  are the reflection coefficients at the interfaces: air - glass, glass - ITO (AZnO), ITO (ZnO) -  $Mg_xZn_{1-x}O, Mg_xZn_{1-x}O$  - SnS.

It is worth noting that this ratio does not take into account the multiple reflections of sunlight in device layers: glass, ITO (AZnO),  $Mg_xZn_{1-x}O$ , which can be neglected at low values of reflection coefficients at the boundaries of the section of different materials. Small reflection coefficients also allow ignoring interference effects in thin films.



**Fig. 3** – Spectral dependences of reflection coefficients ( $R$ ) from the boundaries: ZnO/SnS (1),  $Mg_{0.3}Zn_{0.7}O/SnS$  (2), MgO/SnS (3) and air/SnS (4)

It was found that the transmittance coefficient of the SCs with a AZnO layer is almost the same as that with the ITO layer, but it is still somewhat smaller in the wavelength range  $\lambda = (300-900)$  nm. Therefore, in order to determine the optimal combination of auxiliary layers of the SCs, the optical loss coefficient of energy was calculated [15]. The results of calculations of the optical loss coefficient in SCs on the basis of considered heterojunctions with AZnO and ITO layers are presented in Fig. 4 and in Table 1. As can be seen from the figure, such SCs have a rather high reflection coefficient (21.3-26.3 %), which negatively influences the efficiency of the sun energy conversion.



**Fig. 4** – Optical loss coefficient in SCs taking into account the light reflection from the boundaries of the various materials

**Table 1** – The value of the optical loss coefficient in the SCs with different constructions

No	Solar cell constructions	Optical loss coefficient, %	Light passing coefficient, %
1	AZnO/ZnO/SnS	21.31	78.69
2	ITO/ZnO/SnS	21.82	78.18
3	AZnO/ $Mg_{0.3}Zn_{0.7}O/SnS$	22.41	77.59
4	ITO/ $Mg_{0.3}Zn_{0.7}O/SnS$	22.95	77.05
5	AZnO/MgO/SnS	25.70	74.30
6	ITO/MgO/SnS	26.29	73.71

It is seen from Table 1 that the optical losses of the SCs with the constructions of ITO/ $Mg_xZn_{1-x}O/SnS$  and ZnO/ $Mg_xZn_{1-x}O/SnS$  differ by (0.51-0.59) %. But the best light transmission coefficient still belongs to SCs with a conductive transparent contact AZnO - 78.69 %.

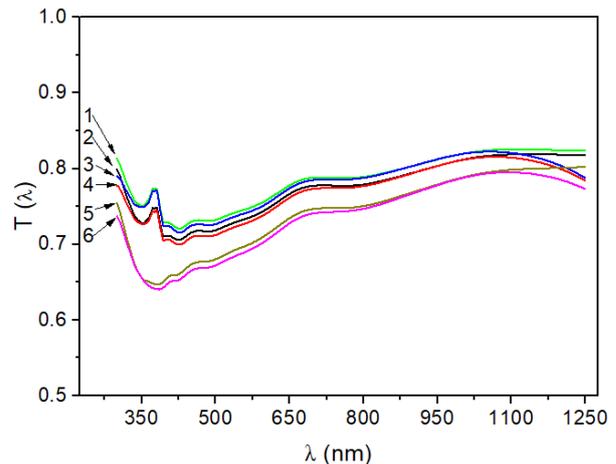
### 3. THE LOSSES OF LIGHT ABSORPTION

In order to objectively analyze the optical losses in addition to light reflection, it is important to take into account the loss of light absorption in the auxiliary layers of the SCs. The light transmittance of a multilayered structure, taking into account absorption and reflection losses in the conductive and window layers of the SCs was calculated using the expressions given in [16].

Spectral dependences of the transmittance coefficient on the wavelength for SCs containing layers of AZnO or ITO on the basis  $Mg_xZn_{1-x}O/SnS$  heterojunction taking into account the absorption effects in auxiliary layers at different thickness values are shown in Fig. 5.

The analysis of dependences (Fig. 5) shows that the transmittance coefficient of the SCs with the ITO layer at a wavelength  $\lambda < 800$  nm is slightly lower than the corresponding coefficient for the structure with AZnO. The value of the light loss coefficient, taking into account the absorption of light in the auxiliary layers for the considered SCs of various structures, is given in Table 2.

As calculations show, AZnO, as a transparent front layer of the solar cell, is more attractive than ITO, because it allows to slightly reduce the loss of light entering the absorbing layer SnS. Dependency analysis presented in Fig. 5 and in Table 2 shows that the increase in the thickness of the window layer from  $d = 25$  nm to  $d = 200$  nm leads to an increase in energy losses by (0.13-0.14) % at the thickness of the transparent front layer AZnO (ITO)  $d = 100$  nm and 200 nm.



**Fig. 5** – Spectral dependence of the transmittance coefficients of the considered structures: glass/AZnO/ZnO/SnS (1), glass/AZnO/ $Mg_{0.3}Zn_{0.7}O/SnS$  (2), glass/AZnO/MgO/SnS (5), glass/ITO/ZnO/SnS (3), glass/ITO/ $Mg_{0.3}Zn_{0.7}O/SnS$  (4), glass/ITO/MgO/SnS (6) at the thickness of the window layer of 25 nm and ITO (AZnO) of 100 nm

### 4. QUANTUM YIELD OF SOLAR CELL

An important parameter that influences the efficiency of sunlight conversion into electrical energy and is used for the analysis of recombinant losses in the SCs

**Table 2** – The value of the loss coefficient in the SCs with different constructions (taking into account the absorption of light)

Solar cell constructions	Loss coefficient, %					
$d_{\text{ITO (ZnO)}} = 100 \text{ nm}$						
$d_{\text{MgxZn1-xO}}$ , nm	25	50	75	100	150	200
AZnO/ZnO/SnS	21.37	21.39	21.41	21.43	21.47	21.51
ITO/ZnO/SnS	21.90	21.92	21.94	21.96	22.00	22.04
AZnO/Mg <sub>0.3</sub> Zn <sub>0.7</sub> O/SnS	22.47	22.49	22.51	22.53	22.57	22.61
ITO/Mg <sub>0.3</sub> Zn <sub>0.7</sub> O/SnS	23.02	23.04	23.06	23.08	23.12	23.16
AZnO/MgO/SnS	25.75	25.77	25.79	25.81	25.84	25.88
ITO/MgO/SnS	26.36	26.38	26.39	26.41	26.45	26.48
$d_{\text{ITO (ZnO)}} = 200 \text{ nm}$						
AZnO/ZnO/SnS	21.41	21.43	21.45	21.47	21.51	21.55
ITO/ZnO/SnS	21.95	21.97	21.99	22.01	22.05	22.09
AZnO/Mg <sub>0.3</sub> Zn <sub>0.7</sub> O/SnS	22.50	22.52	22.54	22.56	22.60	22.64
ITO/Mg <sub>0.3</sub> Zn <sub>0.7</sub> O/SnS	23.07	23.09	23.11	23.13	23.17	23.21
AZnO/MgO/SnS	25.79	25.80	25.82	25.84	25.88	25.91
ITO/MgO/SnS	26.41	26.43	26.44	26.46	26.50	26.53

is the internal quantum yield [15, 16]. It is calculated as the ratio of the number of electron-hole pairs generated by the light radiation to the total number of photons that have reached the absorption layer, which create the drift and diffusion components of the photocurrent in the SCs and the short circuit current.

The internal quantum yield of the SCs depends on the recombination losses of the carriers at the boundary of the  $n$ -Mg<sub>x</sub>Zn<sub>1-x</sub>O/ $p$ -SnS heterojunction and in the volume of materials, as well as on the back side of the absorption and window layers. Since effects of light losses when reflected and absorbed in the auxiliary layers of the device occur in the SCs, it is also important to determine the external quantum yield of the device, which takes into account these losses [16].

The value of the space charge region, occurring on the material contact, is necessary for the analysis of recombination losses in the device. This value depends on the concentration of uncompensated acceptors  $N_a - N_d$  found in the material [11, 17] and on the potential difference in the heterojunction. The last value was found from the band zone diagram, as described in [16].

Due to the high level of doping of the absorbing layer material, the space charge region is in the window and absorbing layers of the SCs and its width is determined by the ratios given in [18]. For the calculation, we used the values presented in Table 3.

**Table 3** – The main parameters of the values that were used for calculations of  $d$  and  $Q$ 

Parameters	Values
$\epsilon$	16
$\varphi_0 - qU$ , eV	(0.22) ZnO, (0.15) Mg <sub>0.3</sub> Zn <sub>0.7</sub> O, (0.50) MgO
$S, S_b$ , cm/s	$10^6 - 10^8$
$\tau_n$ , ns	2.58
$D_n$ , cm <sup>2</sup> /s	0.25
$D_p$ , cm <sup>2</sup> /s	2
$T$ , K	300

The drift component of the internal quantum yield of a solar cell, which takes into account the recombination at the boundary of the heterojunction and in the space charge region, was determined by the relations

given in [19].

The diffusion component of the quantum yield, taking into account the recombination losses in the quasi-neutral region of the window and absorber materials, and on the back of the layers, was calculated using the expressions presented in the works [16, 19].

The total internal quantum yield of SCs is defined as the sum of all quantum yields, taking into account the directions of diffusion and drift currents in the device.

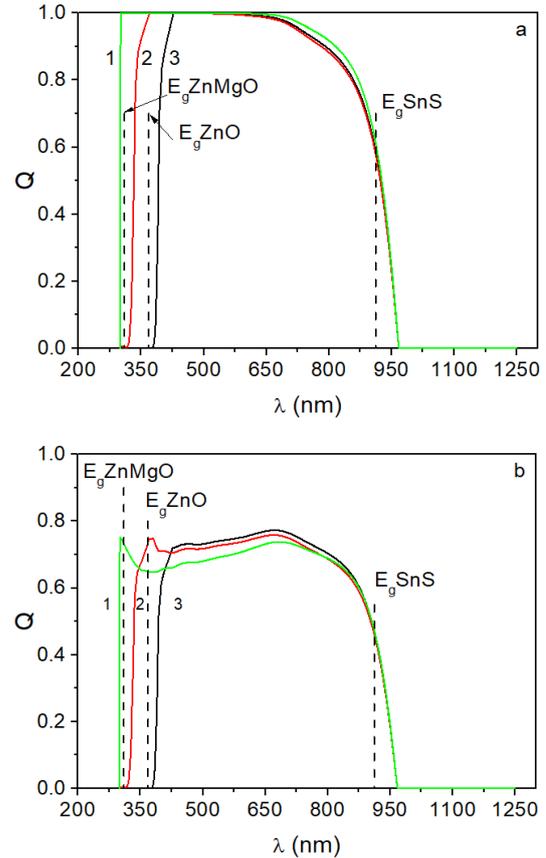
**Fig. 6** – Spectral dependences of internal quantum yield (a) and external quantum yield (b). The window layer MgO (1), Mg<sub>0.3</sub>Zn<sub>0.7</sub>O (2) and ZnO (3)

Fig. 6a presents the spectral dependence graphs of the internal quantum yield of SCs with the values  $N_a = 10^{18} \text{ cm}^{-3}$ ,  $N_d = 10^{17} \text{ cm}^{-3}$ .

The calculations were carried out for SCs with a thickness of the absorber layer of  $1 \mu\text{m}$  ( $A_{hv} = \sim 97\%$ ) and the window layer of  $25 \text{ nm}$  (the minimal technologically achievable thickness of the window layer [14]).

As expected, with photon energy, which is lower than the band gap  $E_g$  of the material, the quantum yield of the devices is close to zero. As calculations have shown, the change in the recombination rate  $S$  in the range from  $10^6$  to  $10^8$  has a weak effect on the value of the quantum yield.

Subsequently, we investigated the effect of optical losses, which were calculated in the previous section on the quantum yield of devices. With their consideration, we have constructed the spectral dependence of the external quantum yield for the considered SCs (Fig. 6b). In this case, the thickness of all functional layers was taken close to the values used in the real SCs [14].

The analysis of the obtained dependences (Fig. 6b) shows that the devices with window layers, which have a larger band gap, show larger values of quantum yield.

## 5. SOLAR CELL EFFICIENCY

The short-circuit current density of the investigated SCs was calculated by the expression given in [15, 16].

Table 4 presents the calculated values of  $J_{sc}$  for SCs ITO(AZnO)/Mg<sub>x</sub>Zn<sub>1-x</sub>O/SnS, taking into account the losses of absorption and reflection light in the auxiliary layers of SCs. At this time, the thickness of the conductive ITO (AZnO) layer was  $100 \text{ nm}$ .

**Table 4** – The values of short-circuit current density for structures ITO/Mg<sub>x</sub>Zn<sub>1-x</sub>O/SnS and AZnO/Mg<sub>x</sub>Zn<sub>1-x</sub>O/SnS

	Short-circuit current $J_{sc}$ , mA/cm <sup>2</sup>		Percentage of losses, %	
	ITO	AZnO	ITO	ZnO
$d_{\text{Mg}_x\text{Zn}_{1-x}\text{O}}$ , nm				
$d_{\text{ITO (ZnO)}} = 100 \text{ nm}$				
ZnO/SnS	25.00	25.10	28.20	27.91
Mg <sub>0.3</sub> Zn <sub>0.7</sub> O/SnS	24.70	24.83	29.06	28.69
MgO/SnS	24.10	24.29	30.79	30.24
Max short-circuit current	34.82			

Thus, taking into account light losses on absorption and reflection in auxiliary layers of SCs with the structure AZnO/Mg<sub>x</sub>Zn<sub>1-x</sub>O/SnS, the value of the short-circuit current density is slightly higher (0.10-0.19) mA/cm<sup>2</sup> than the corresponding values for ITO/Mg<sub>x</sub>Zn<sub>1-x</sub>O/SnS SCs. The general (recombination and optical) losses at the window layer thickness  $d = 25 \text{ nm}$  and ITO(AZnO) =  $100 \text{ nm}$  in these structures are 27.91%-30.79%.

In the future, using the ratios given in [16] we calculated the efficiency of the SCs  $\eta$  (%).

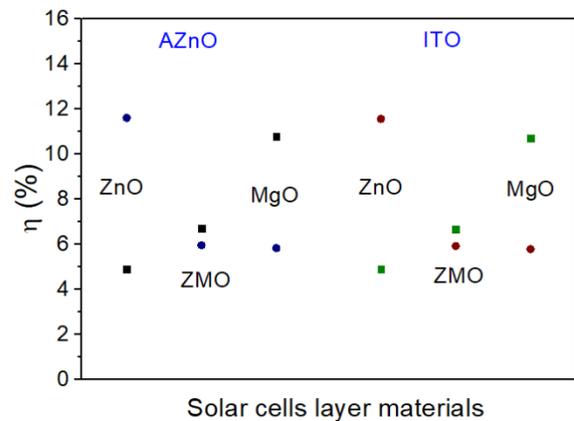
Table 5 shows the open-circuit voltage values calculated from the energy diagrams of the heterojunction, and the value of  $U_{oc}$  for the pair of contacting layers Mg<sub>0.3</sub>Zn<sub>0.7</sub>O/SnS was found by the Vegard's law. Also,

Table 5 shows the maximum values of the fill factor and the open-circuit voltage of real SCs taken from literary sources. These values were used by us to further calculate the efficiency of photovoltaic converters.

In Fig. 7, the indicated efficiency values are obtained for devices with different conductive transparent, window, and absorbing layers.

**Table 5** – The values of the basic parameters of the real SCs and values from the literature for determining the efficiency

SCs structure	$U_{oc}$ , mV	FF, %	$P_{in}$ , mW/cm <sup>2</sup>	From literature $U_{oc}$ , mV
ZnO/SnS	220	89	100	520 [20]
Mg <sub>0.3</sub> Zn <sub>0.7</sub> O/SnS	300			270 [7]
MgO/SnS	500			270



**Fig. 7** – Effect of recombination and optical losses on the efficiency of SCs with different structure in the case with  $d_{\text{AZnO(ITO)}} = 100 \text{ nm}$ ,  $d_{\text{Mg}_x\text{Zn}_{1-x}\text{O}} = 25 \text{ nm}$ . The results obtained on the basis of literary data are indicated in the form of circles, the squares represent the results obtained on the basis of the values of  $U_{oc}$  found from the energy diagrams of the heterojunction

From Fig. 7 it is evident that in the case of the use of the  $U_{oc}$  values found from the energy diagram of the transition, the efficiency of the SCs increases with an increase in the content of magnesium in the solid solution from 4.91% (ZnO/SnS,  $U_{oc} = 220 \text{ mV}$ ) to 10.8% (MgO/SnS,  $U_{oc} = 500 \text{ mV}$ ). The material of the transparent front contact weakly affects the efficiency of the SCs, but when using the AZnO layer, the efficiency of the devices is still slightly higher than with the ITO layer, by 0.01% in the case of ZnO/SnS and 0.07% in the case of ZnO/SnS.

In the case for the calculation of the efficiency of the devices, the values  $U_{oc}$  are taken from literary sources, then it turns out that the SCs based on the ZnO/SnS heterojunction ( $U_{oc} = 520 \text{ mV}$  [20]) with the front conductive contact AZnO have the highest values of efficiency. These values reach 11.62% at the thickness of the front conductive contact  $d_{\text{AZnO}} = 100 \text{ nm}$  and the thickness of the window layer  $d_{\text{ZnO}} = 25 \text{ nm}$ . Somewhat lower is the value of the efficiency of the SCs with the ITO layer (11.57%). Devices based on heterojunctions Mg<sub>0.3</sub>Zn<sub>0.7</sub>O/SnS and MgO/SnS ( $U_{oc} = 270 \text{ mV}$  [7], AZnO layer) show the values of the efficiency of 5.97% and 5.84%, respectively. It should be noted that for the SCs

based on the  $\text{Mg}_{0.3}\text{Zn}_{0.7}\text{O}/\text{SnS}$ , heterojunction, the values of the open-circuit voltage which were found theoretically ( $U_{oc} = 300$  mV) are well correlated with those indicated in the literature ( $U_{oc} = 270$  mV [7]).

However, such correlation is not observed for SCs with  $\text{ZnO}/\text{SnS}$  heterojunction, for which experimental values ( $U_{oc} = 520$  mV) are significantly higher than those found from the band zone diagram ( $U_{oc} = 220$  mV). Such a significant difference needs to be explained. In our opinion, this is due to the fact that the authors of the work [20] used the devices not with the usual "superstrate" design, but with the flexible SCs based on an array of nanowires with a shell oriented in the direction of the hexagonal zinc oxide axis  $C$  with an ITO window, which may observe piezoelectric effect.

## 6. CONCLUSIONS

The recombination and optical losses in the auxiliary and absorption layers of the SCs based on the heterojunction  $n\text{-Mg}_x\text{Zn}_{1-x}\text{O}/p\text{-SnS}$  with the transparent front contacts of AZnO and ITO are calculated.

It is established that SCs based on heterojunctions  $n\text{-Mg}_x\text{Zn}_{1-x}\text{O}/p\text{-SnS}$  with AZnO and ITO layers have a rather high reflection value (20-30 %), which adversely affects the efficiency of solar energy conversion. It was found that the transmission coefficient of the considered SCs with the AZnO layer is almost the same as that for a structure with an ITO layer.

The total (recombination and optical) energy losses

in SCs of different design reach 27.91-30.79 % with  $d_{\text{Mg}_x\text{Zn}_{1-x}\text{O}} = 25$  nm and  $d_{\text{ITO(AZnO)}} = 100$  nm.

As a result of these losses, it was found that for SCs based on the  $\text{Mg}_x\text{Zn}_{1-x}\text{O}/\text{SnS}$  heterojunction in the case of using  $U_{oc}$  values found from the energy band zone diagram, the efficiency increases with an increase in magnesium content in the solid solution from 4.91 % ( $\text{ZnO}/\text{SnS}$ ) to 10.8 % ( $\text{MgO}/\text{SnS}$ ). In the case of calculating the efficiency of devices to use the  $U_{oc}$  values taken from literary data, SCs based on the  $\text{ZnO}/\text{SnS}$  heterojunction with the transparent front contact AZnO have the highest efficiency values  $\eta = 11.62$  %. The devices based on the  $\text{Mg}_{0.3}\text{Zn}_{0.7}\text{O}/\text{SnS}$  and  $\text{MgO}/\text{SnS}$  heterojunctions show efficiency 5.97 % and 5.84 %, respectively. It has been shown that the transparent front contact material has little effect on the efficiency of SCs, but when using the AZnO layer, the efficiency of the devices is still somewhat higher than with the use of the ITO layer.

The obtained results allow to determine the maximum value of the efficiency of considered SCs taking into account recombination and optical losses in device layers and to optimize the parameters of real devices in order to achieve these values of efficiency.

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## REFERENCES

1. T. Kurbatova, H. Khlyap, *Renew. Sust. Energy Rev.* **52**, 217 (2015).
2. J. Poortmans, V. Arkhipov, *Thin Film Solar Cells: Fabrication, Characterization, and Application* (Chichester: John Wiley&Sons: 2006).
3. M.A. Green, Y. Hishikawa, E.D. Dunlop, D.H. Levi, J. Hohl-Ebinger, A.W. Ho-Baillie, *Prog. Phot.* **26**, 427 (2018).
4. S. Di Mare, D. Menossi, A. Salavei, E. Artegiani, F. Piccinelli, A. Kumar, A. Romeo, *Coatings* **7**, 34 (2017).
5. J.A. Andrade-Arvizu, M. Courel-Piedrahita, O. Vigil-Galán, *J. Mater. Sci.: Mater. Electron.* **26**, 4541 (2015).
6. D. Nam, A.S. Opanasyuk, P.V. Koval, A.G. Ponomarev, A.R. Jeong, G.Y. Kim, W. Jo, H. Cheong, *Thin Solid Films* **562**, 109 (2014).
7. S.H. Chaki, M.D. Chaudhary, M.P. Deshpande, *J. Semicond.* **37**, 053001 (2016).
8. A.M.S. Arulanantham, S. Valanarasu, K. Jeyadheepan, V. Ganesh, M. Shkir, *J. Mol. Struct.* **1152**, 137 (2018).
9. P. Sinsersuksakul, L. Sun, S.W. Lee, H. Park, S. Kim, C. Yang, R.G. Gordon, *Adv. Energy Mater.* **4**, 1400496 (2014).
10. K.T.R. Reddy, K. Ramya, G. Sreedevi, T. Shimizu, Y. Murata, M. Sugiyama, *Energy Procedia* **10**, 172 (2011).
11. T. Ikuno, R. Suzuki, K. Kitazumi, N. Takahashi, *Appl. Phys. Lett.* **102**, 193901 (2013).
12. J.-S. Shiao, S. Brahma, C.-P. Liu, J.-L. Huang, *Thin Solid Films* **620**, 170 (2016).
13. R.K. Herzenberg, *Rev. Miner.* **4**, 33 (1932).
14. R. Scheer, H. Schock, *Chalcogenide Photovoltaics*, (Weinheim: Wiley-VCH Verlag GmbH & Co: 2011).
15. O.V. Diachenko, A.S. Opanasyuk, D.I. Kurbatov, P.B. Patel, C.J. Panchal, P. Suryavanshi, V. Kheraj, *J. Nano-Electron. Phys.* **9**, 04002 (2017).
16. O.V. Diachenko, O.A. Dobrozhan, A.S. Opanasyuk, M.M. Ivashchenko, T.O. Protasova, D.I. Kurbatov, A. Čerškus, *Superlatt. Microstr.* **122**, 476 (2018).
17. K. Narinder Kumar, *Comprehensive Physics for Class XII*, (New Delhi: Laxmi Publications: 2004).
18. M. Balkanski, R.F. Wallis, F. Richard, *Semiconductor Physics and Applications*, (New York: Oxford University Press: 2000).
19. L. Kosyachenko, T. Toyama, *Sol. Energy Mater. Sol. Cells* **120**, 512 (2014).
20. L. Zhu, L. Wang, F. Xue, L. Chen, J. Fu, X. Feng, *Adv. Sci.* **4**, 1600185 (2017).

## Моделювання ефективності сонячних елементів на основі гетеропереходу $n\text{-Mg}_x\text{Zn}_{1-x}\text{O}/p\text{-SnS}$ із контактами $\text{ZnO:Al}$ та $\text{ITO}$

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Визначено рекомбінаційні та оптичні втрати в допоміжних і поглинаючому шарах фотоелектричних перетворювачів сонячної енергії на основі гетеропереходу (ГП)  $n\text{-Mg}_x\text{Zn}_{1-x}\text{O}/p\text{-SnS}$  ( $x = 0; 0.3; 1$ ) із струмознімальними прозорими фронтальними контактами  $\text{AZnO}$  та  $\text{ITO}$ . Отримані спектральні залежності коефіцієнту пропускання світла сонячними елементами (СЕ), враховуючи відбиття світла від меж поділу контактуючих шарів матеріалів, а також його поглинання в допоміжних шарах приладів. Визначено квантовий вихід досліджуваних структур фотоперетворювачів. Досліджено вплив рекомбінаційних і оптичних втрат в СЕ з конструкцією  $\text{ITO}(\text{AZnO})/\text{Mg}_x\text{Zn}_{1-x}\text{O}/\text{SnS}$  на струм короткого замикання за різної товщини віконного шару  $\text{Mg}_x\text{Zn}_{1-x}\text{O}$  (25-400 нм) та сталій товщині струмознімальних шарів  $\text{AZnO}$  і  $\text{ITO}$  (100-200 нм). Розраховано ККД структур для випадку напруги холостого ходу  $U_{\text{ох}}$  знайденої з енергетичних діаграм переходів та взятої з літературних даних. Встановлено, що в першому випадку СЕ можуть мати ефективність, яка зростає при збільшенні вмісту Mg в твердому розчині від 4.91 % (ГП  $\text{ZnO}/\text{SnS}$ ) до 10.8 % (ГП  $\text{MgO}/\text{SnS}$ ). У другому випадку найбільші значення ефективності ( $\eta = 11.62\%$ ) мають СЕ на основі ГП  $\text{ZnO}/\text{SnS}$  зі струмопровідним контактом  $\text{AZnO}$ . Прилади на основі ГП  $\text{Mg}_{0.3}\text{Zn}_{0.7}\text{O}/\text{SnS}$  та  $\text{MgO}/\text{SnS}$ , показують значення ККД 5.97 % та 5.84 % відповідно. Матеріал верхнього струмопровідного контакту слабо впливає на ефективність СЕ. Одержані результати дають змогу визначити максимальне значення ефективності розглянутих СЕ з урахуванням рекомбінаційних та оптичних втрат в шарах фотоперетворювачів та провести оптимізацію параметрів реальних приладів з метою досягнення цих значень ККД.

**Ключові слова:** Ефективність, Втрати, Гетероперехід, Сонячні елементи, Віконний шар,  $\text{SnS}$ ,  $\text{ZnO}$ .