JOURNAL OF NANO- AND ELECTRONIC PHYSICS
Vol. 9 No 4, 04002(4pp) (2017)
ЖУРНАЛ НАНО- ТА ЕЛЕКТРОННОЇ ФІЗИКИ
Том 9 № 4, 04002(4cc) (2017)

The Performance Optimization of Thin-Film Solar Converters Based on *n*-ZnMgO / *p*-CuO Heterojunctions

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(Received 15 April 2017; revised manuscript received 25 July 2017; published online 27 July 2017)

In this paper, we present the results of the calculations of optical losses in the solar cells layers based on heterojunction *n*-ZnMgO / *p*-CuO with ZnO and ITO frontal contacts. The calculations were carried out taking into account a light absorption in the auxiliary layers of the device. As a result, the spectral dependencies of transmittance $T(\lambda)$ in the absorber layer of solar cell were defined. It is made possible to optimize the design of the solar cells based on such heterojunctions.

Keywords: Zinc magnesium oxide, Copper oxide, Optical losses, Recombination losses, Efficiency, Thickness, Heterojunction.

DOI: 10.21272/jnep.9(4).04002 PACS numbers: 88.40.hj, 42.25.Bs

1. INTRODUCTION

Solar power is one of the most promising areas of renewable energy. Today, solar cells based on silicon dominate in photovoltaics. However, the need to reduce the cost of obtaining solar energy leads to the necessity of finding the new materials for photovoltaic cells.

Copper oxides such as CuO and Cu_2O are promising photovoltaic materials. They are p-type semiconductors and have band gap ~1.3 eV (CuO) and ~2.3 eV (Cu_2O), respectively [1-6]. Because of Cu is abundant in nature, cheap and nontoxic, the first oxide could be used as an absorbing layer, and the second as a window layer of thin-film solar cells for large-scale solar energy conversion [3, 7, 8]. Theoretical studies indicate that the maximum efficiency of thin-film solar cells based on CuO absorbing layer is (32-34) % while using Cu_2O the solar cells can be obtained with an efficiency exceeding 20 % [9].

The modern thin-film solar cell is usually constructed using heterojunctions [1, 2, 5, 6]. Generally, a transparent conductive layer (ITO), are used as the conductive and the window layer of such devices, although in recent years solar cells with a layer of aluminum-doped zinc oxide (ZnO: Al) become increasingly popular [10, 11]. However, a number of studies [12], [13] have found that *n*-ZnO / *p*-CuO heterojunctions have good rectifying properties despite the fact that the contacting materials have a different crystal structure. This is due to the good agreement of lattice parameters of materials for facets formed by vectors *b* and *c* [12]. Unfortunately, the efficiency of solar cells based on *n*-ZnO / *p*-CuO heterojunction in our time does not exceed 2.88 % [14]. Increasing the efficiency of real solar cells is possible by minimizing energy loss due to optimization of their design and to improve the properties of layers.

One way to improve the performance of solar cells is the adding impurities of isovalent Mg in zinc oxide. This allows controllably change a band gap, lattice parameters and work function of a material and thus optimize heterojunction characteristics. This led to the goal and objectives of the study. The main purpose of this work is to calculate the optical losses in solar cells based on *n*-ZnMgO / *p*-CuO heterojunction with frontal ZnO and ITO contacts to optimize their designs.

2. RESULTS AND DISCUSSION

2.1 The Losses of Light Reflection from Layers in Solar Cell

Usually, thin film solar cell consist of a window and absorbing layers, front and back contacts. In this paper, we discuss the thin film solar cells on the basis of heterojunctions which have the «superstrate» type. Their design is schematically shown in Fig 1.

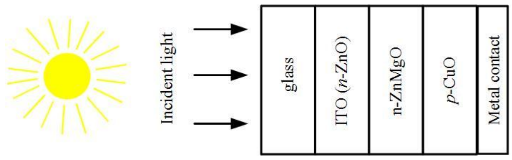

Fig. 1 – The schematic design of solar cell based on *n*-ZnMgO / *p*-CuO heterojunction

The thickness of the ZnMgO window layer was chosen in the range of d = 30 nm up to 400 nm to modeling the process of reflection and absorption of the light in auxiliary layers of photovoltaic devices. The thickness of the ZnO (ITO) layers was taken as d = 100 and 200 nm. These values of thicknesses have layers of the real solar cells [11]. The ZnMgO solid solution containing 30 percent of magnesium. Recently, ZnMgO solid solution also being used for creating a solar cell containing a copper oxide layer, based on ZnMgO / CuO_2

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heterojunction [15].

The sunlight flows before getting into the absorbing layer CuO, where the photogeneration of electron-hole pairs occurs under his influence, passes through a number of auxiliary layers of solar cell: glass, ITO (ZnO) and ZnMgO. With this occurs a reflection of the radiation from boundaries of different materials (air-glass, glass-ITO (ZnO), ITO (ZnO)-ZnMgO and ZnMgO-CuO) and absorption of light in the window and buffer layers of the solar converter and in the glass. These losses lead to reduced effectiveness of solar converter.

We have used Fresnel equation for calculating the reflection coefficient at the interface between two contacting materials [16, 17]:

$$R = \left(\frac{n_1 - n_2}{n_1 + n_2}\right)^2, \tag{1}$$

where n_1 and n_2 – refractive indexes of the contacting materials.

For the electrically conductive materials, reflection coefficient was determined using the following expression [17]:

$$R = \frac{\left|n_1^* - n_2^*\right|}{\left|n_1^* + n_2^*\right|} = \frac{(n_1 - n_2)^2 + (k_1 - k_2)^2}{(n_1 + n_2)^2 + (k_1 + k_2)^2}, \tag{2}$$

where n_1^*, n_2^* – complex refractive index; k_1, k_2 – is the extinction coefficient.

To obtain the spectral dependences of n and k were used refractive index and extinction coefficient of ITO, ZnO, ZnMgO and CuO given in [18]. The values of refractive index and extinction coefficient for air were taken $n_1 = 1$, and $k_1 = 0$, respectively.

Fig. 2a shows the calculated spectral dependencies of reflection coefficient from layers of a solar cell at their direct contact with air. As shown in the figure, the lowest reflection coefficient on the interface air - glass, and the largest observed at the interface air - CuO.

The calculated spectral dependencies of reflection coefficient from the interfaces between layers, that located one after another in a solar cell are presented in Fig. 2b. As expected, because of the low refractive index of light in the material we observe the lowest value of reflection coefficients at the interfaces ZnMgO-ZnO ($R = 1\text{-}2 \cdot 10^{-3}$) та ZnMgO-ITO ($R = 1\text{-}10 \cdot 10^{-3}$), and the biggest values at the interface ZnMgO-CuO ($R = 0.22\text{-}0.28$). The value of R for interfaces air-ZnMgO and air-glass taking values (0.10-0.15) and (0.03-0.04), respectively.

Apart from the absorption processes in solar cell layers, the transmittance of the light in CuO absorbing layer can be defined by the formula $T = 1 - R$. So transmittance of the photovoltaic converter with a multilayer structure can be found by the formula [16, 19]:

$$T(\lambda) = (1 - R_{12})(1 - R_{23})(1 - R_{34})(1 - R_{45}), \tag{3}$$

where R_{12}, R_{23}, R_{34}, R_{45} – reflection from the following interfaces: air-glass, glass-ZnO(ITO), ZnO(ITO)-ZnMgO, ZnMgO-CuO.

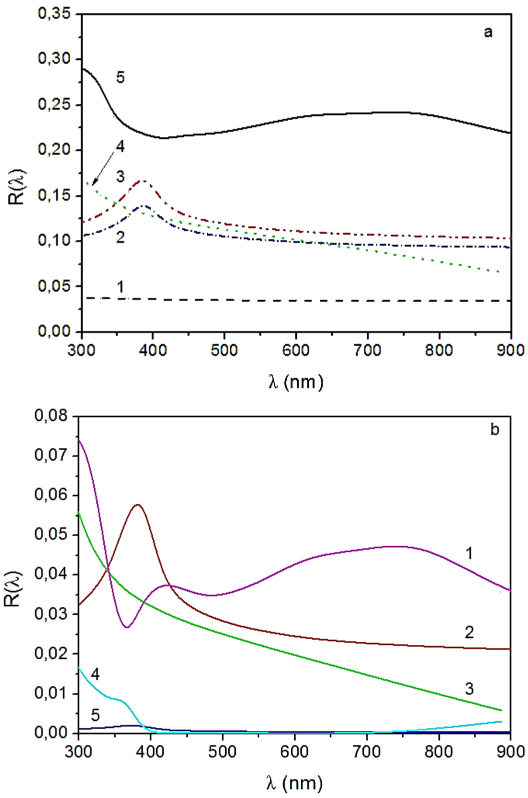

Fig. 2 – The spectral dependences of the reflection coefficient (R) for interfaces: air-glass (1), air-ZnMgO (2), air-ZnO (3) air-ITO (4) air-CuO (5) (a) and ZnMgO-CuO (1) glass-ZnO (2) glass-ITO (3), ITO-ZnMgO (4), ZnO-ZnMgO (5) (b)

It should be noted that this equation does not account for multiple reflections in the glass plate, ZnO (ITO) and CuO layers, which is quite acceptable because of the small difference of reflection coefficients at the interfaces (Fig. 2b). It also allows us to ignore interference effects.

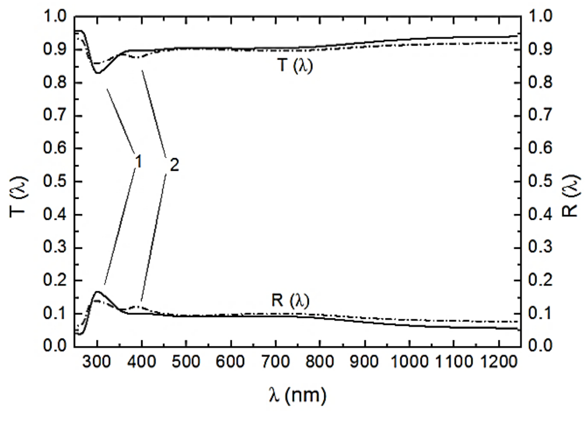

Fig. 3 – Spectral dependence transmittance T(λ) and reflectance R(λ) of a solar cell with ITO / ZnMgO / CuO (1) and ZnO / ZnMgO / CuO (2) structures. The reflection of light from the interphase interfaces was taking into account

Fig. 3 shows the dependence of the transmission T and reflection R of the wavelength λ considered for the solar converter. Solar cells based on n-ZnMgO / p-CuO heterojunction as with the ZnO as well as with ITO layer have very high-value of light transmission coefficient (> 90 %), which affects their efficiency of converting solar energy into electricity. As shown in Fig. 4, the transmittance of ZnO layer is very close to the values obtained for the device containing ITO.

To determine the optimal material of conductive layer solar cell was calculated a so-called coefficient of optical power loss of the device. It was determined by the formula:

$$\eta = \frac{T_{\max}(\lambda) - \frac{1}{n}\sum_{i=1}^{n} T_i(\lambda)}{T_{\max}(\lambda)}, \qquad (4)$$

Knowing that $T_{\max}(\lambda) = 1$, then expression (4) is simplified to the form:

$$\eta = 1 - \frac{1}{n}\sum_{i=1}^{n} T_i(\lambda), \qquad (5)$$

The results of calculation of the coefficient of optical power loss in the solar cells with various structure are presented in Table 1.

Table 1 – Coefficients of optical power loss in the solar cells

Structure of solar cell	Optical power loss coefficient, %	The coefficient of light passing, %
ITO/ZnMgO/CuO	8.45	91.55
ZnO/ZnMgO/CuO	9.52	90.48

As the table shows, the optical loss in the structures ITO / ZnMgO / CuO and ZnO / ZnMgO / CuO differ by only 1.07 %. But the best value of passage of light to the absorber layer has a structure with ITO (91.55 %).

2.2 The Losses of Light Absorption in Solar Cell Layers

In addition to losses on light reflection from layers should take into account the optical losses on light absorption in the auxiliary layers for solar converters. The transmittance coefficient of a multilayer structure in view of losses of reflection and absorption at all layers of the solar cell can be calculated using the expression [20]:

$$T(\lambda) = (1 - R_{12})(1 - R_{23})(1 - R_{34})(1 - R_{45})(e^{-\alpha_1 d_1})(e^{-\alpha_2 d_2}) \qquad (6)$$

where α_1, α_2 – are absorption coefficients of the materials of the window and the conductive layer; d_1, d_2 – the thicknesses of these layers.

The absorption coefficient of solar radiation $\alpha(\lambda)$ in view it's extinction coefficient as a function of wavelength $k(\lambda)$ is calculated by the following equation:

$$\alpha(\lambda) = \frac{4\pi}{\lambda} k. \qquad (7)$$

Fig. 4 shows the dependence of T on the wavelength λ for solar cell based on n-ZnO / p-CuO heterojunction including losses on light absorption in the auxiliary layers with different thickness values. Analysis of the dependencies indicates that changing the thickness of 30 to 400 nm of ZnMgO layer somewhat reduces the value of transmittance solar converter. It is established that an increase the thickness of the layer from d = 30 nm to d = 400 nm the optical losses increase for the device with a layer of ITO by 2.16 % при d_{ITO} = 100 nm and 0.92 % at d_{ITO} = 200 nm. For the solar cell with a layer of ZnO, the loss value increased to 2.14 % at d_{ZnO} = 100 nm and to 0.9 % at d_{ZnO} = 200 nm. At the same time transmittance values of the device with ITO

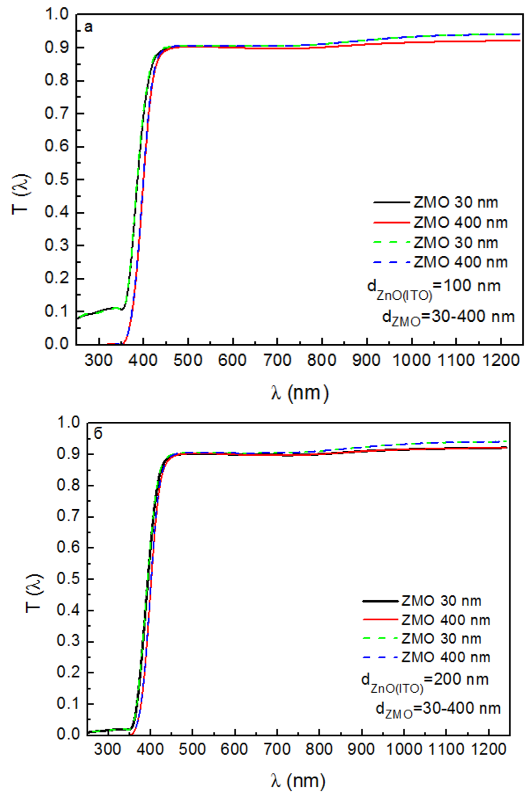

Fig. 4 – Spectral transmittance coefficients of multilayer structures glass / ITO / ZnMgO / CuO and glass / ZnO / ZnMgO / CuO at ZnMgO thickness: 30-400 nm and ITO (ZnO): 100 nm (a) and 200 nm (b)

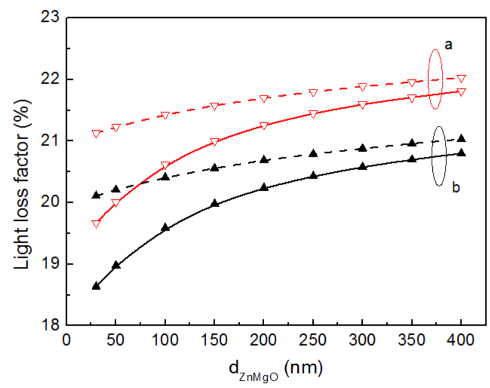

Fig. 5 – Dependence of losses of light for structures glass / ITO / ZnMgO / CuO (solid lines) and glass / ZnO / ZnMgO / CuO (dotted lines) at thickness of ITO (ZnO): 100 nm (a) and 200 nm (b)

layer is somewhat greater than the corresponding value for the structure with ZnO layer.

Thus, calculations show that a layer of ITO is more attractive compared with ZnO for use in solar cells because improves the volume of a passage of light to the CuO absorber layer.

3. CONCLUSIONS

In the paper, the optical losses were defined in thin film solar converters based on n-ZnMgO / p-CuO heterojunction with frontal contacts ZnO and ITO. Such solar cells have a very high value of light transmittance (> 90 %) as in the case of the conductive layer of ZnO as well as ITO.

It is established that the value of transmittance device with a layer of ITO by 1.07 % higher than the corresponding values obtained for the structure with ZnO layer.

The summary (optical and recombination) losses of the solar converter with different structures at $d_{ZnMgO} = 30$ nm is equaled 14.26 % and 18.70 % for ZnO and ITO respectively.

On the basis of calculations, it is possible to optimize the structure of photovoltaic converter minimizing these losses.

AKNOWLEDGEMENTS

This research was supported by the Ministry of Education and Science of Ukraine (Grant No. 0116U002619, No. 0115U000665c, No. 0116U006813).

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