NAP-2017, 2017 IEEE 7th International Conference on Nanomaterials: Applications and Properties (NAP)

The Optimization of Functional Layers of Solar Cells Based on *n*-ZnMgO / *p*-CuO and *n*-ZnMgO / *p*-Cu_2O Heterojunctions

O.V. Diachenko, A.S. Opanasyuk, D.I. Kurbatov, O.A. Dobrozhan, V.V. Grynenko
Department of Electronics and Computer Technology,
Sumy State University,
Sumy, Ukraine
alexey.dyachenko@ukr.net, opanasyuk_sumdu@ukr.net

***Abstract*—In this paper, we present the results of the calculations of optical losses in the solar cell layers based on *n*-ZnMgO / *p*-CuO(*p*-Cu_2O) heterojunctions with AZO and ITO front contacts. The calculations were carried out considering of light absorption in the auxiliary layers of the device. Thus, the spectral dependencies of transmittance 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, transmittance, heterojunction

I. INTRODUCTION

Photovoltaics is one of the most promising areas of renewable energy. It allows to generate electricity from a free, inexhaustible source of energy, namely sunlight. Today, silicon-based solar panels dominate in solar energy. But the need to reduce the cost of solar energy needs to find new cheap and non-toxic materials for energy-efficient applications.

Copper oxides such as CuO and Cu_2O are promising photovoltaic materials. They are semiconductor oxides with *p*-type conductivity with the band gap energy lying in the near infrared and visible regions of the spectrum ~ 1.3 eV (CuO) and ~ 2.3 eV (Cu_2O) [1 – 3]. These oxides attract attention due to such properties as high optical absorption, band gap energy that correlates well with the solar spectrum, a presence of cheap, abundant and non-toxic components in the compound [4]. Theoretical studies have shown that solar cells on the basis of copper oxides absorbing layers can be created with the efficiency of conversion of solar energy of 28% (CuO) and 15% (Cu_2O) in light conditions AM1.5 [4].

Modern thin film solar cells usually are created on the basis of heterojunctions [2, 3]. As a rule, a transparent ITO layer is used as the conductive layer of such devices, although in the last time is becoming increasingly popular with a layer of zinc oxide doped with aluminum (AZO) [5, 14]. Several studies have found [6] that the *n*-ZnO / *p*-CuO heterojunctions, despite the fact that the contact materials belong to different crystal system, have good rectifier properties. This is due to the good agreement of the crystalline lattice parameters of materials for the faces formed by the vectors *b* and *c* [6]. Unfortunately, nowadays the efficiency of the solar cells based on the *n*-ZnO / *p*-CuO heterojunction does not exceed 2.88% [7].

Despite the fact that the band gap energy of Cu_2O is significantly greater than the Shockley-Queisser optimum (Eg=1.5 eV) [8], the thin-film solar cells based on the heterojunction of this material (for example, n-ZnO / p-Cu_2O) attract more attention of researchers due to the possibility of creating transparent devices in the visible region, which can be applied to the window glass, almost not worsening its transparency [8]. However, the efficiency of such solar cells in our time does not exceed 4%. Increasing the efficiency of real devices is possible by minimizing energy losses as a result of optimizing their design and improving the properties of the layers.

One way to improve performance solar cells based on heterojunctions *n*-ZnO / *p*-CuO (*p*-Cu_2O) is the introduction of an isovalent element Mg into zinc oxide that allows controllably to change the lattice parameters, the band gap energy and the work function of the material, with the aim to optimizing the characteristics of the heterojunction. This set 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 and *n*-ZnMgO/*p*-Cu_2O heterojunction with transparent frontal ZnO and ITO contacts and to study their effect on the efficiency of devices.

II. THE LOSSES OF LIGHT REFLECTION FROM LAYERS IN SOLAR CELL

Thin film solar cells consist of several layers and typically include window, buffer, absorbing layers, as well as front and rear contacts. The photovoltaic converter with a structure glass / *n*-ITO (AZO) / *n*-ZnMgO / *p*-CuO (Cu_2O) / rear contact, was investigated in the work.

The thickness of the ZnMgO window layer was chosen in the range of d = 30 nm up to 400 nm in order to modelling the process of reflection and absorption of the light in auxiliary layers of photovoltaic devices. The thickness of the AZO (ITO) layers was taken as d = 100 and 200 nm. These values have layers of the real solar cells [9]. The simulation was conducted in the range of wavelengths from 300 nm (the radiation of the

Sun of less length to the Earth's surface is practically non-existent) to 1250 nm (~ 1 eV).

During the operation of the device, the flow of sunlight passes through the multilayered structure of thin film solar cell, where part of the light reflected from the boundaries of interfaces of various materials (air-glass, glass-ITO (AZO), ITO (AZO) -ZnMgO and ZnMgO-CuO (Cu_2O)), as well exist the absorption of light in the window and buffer layers and substrate (glass) of the photovoltaic cell. These losses lead to a decrease in the efficiency of photo converters.

To calculate the optical losses in the auxiliary layers of the solar cell, we used the technique described in [10].

Figure 1 shows the spectral dependence of the refraction index and extinction coefficient of each layer of the multilayer structure of the device. Since the solar cells used the special glass with a very small value of the absorption coefficient, the extinction coefficient of glass was taken as zero $k = 0$. To determine the refractive index of glass, the Sellmeier formula was used [11]. For air, the following values were used for modeling: n_1=1 and k_1=0.

The reference values of the refractive index and extinction coefficient of the solar cell layers (ITO, ZnO, MgO, CuO, and Cu_2O) were used by us to construct the spectral dependences n and k [12]. For the ZnMgO layer, the values of these coefficients were calculated based on the values of zinc oxide and magnesium oxide, using the Vegard law for solid solutions.

The calculated spectral dependencies of reflection coefficient from layers of a solar cell at their direct contact with air are presented in Fig. 2a. As shown in the figure, the lowest reflection coefficient at the interface air - glass, and the largest observed at the interface air – CuO and air – Cu_2O.

Fig. 2 (b, c, d) shows the calculated spectral dependencies of reflection coefficient from the interfaces between layers, that located one after another in a solar cell. As expected, because of the low refractive index in the material we observe the lowest value of reflection coefficients at the interfaces ZnMgO-ZnO та ZnMgO-ITO (fig. 2c). As can be seen from the fig. 2d the biggest values at the interface ZnMgO – Cu_2O. It is established that the reflection coefficient from the glass / ZnO interface is smaller than the glass / ITO only in the UV region of the spectrum ($\lambda < 350$ nm) (fig. 2b). In all another area of the spectrum, the best features have a pair of glass / ZnO. The value of the reflection coefficient from the ZnMgO / absorption layer is the lowest for a ZnMgO / CuO pair (R = 0.07-0.15), and only at the wavelength $\lambda = (650\text{-}920)$ nm the ZnMgO / Cu_2O pair have best characteristics (fig. 2c).

Fig. 3 shows the dependence of the transmission T and reflection R of the wavelength λ in the solar cells on the basis of the n-ZnMgO / p-CuO (Cu_2O) heterojunctions with the frontal contacts of ITO and AZO.

Solar cells based on the considered heterojunctions, namely AZO and ITO layers have fairly high values of light transmission coefficient (~90%), which positively affects their efficiency of converting solar energy into electricity.

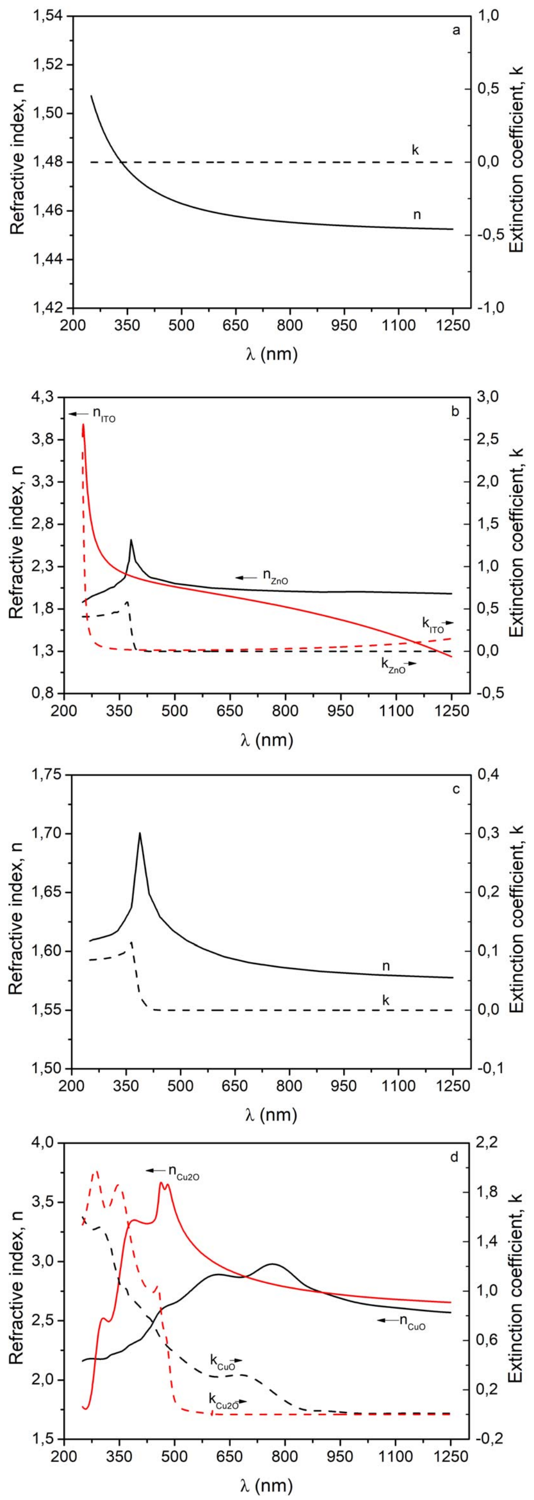

Fig. 1. The spectral dependences of the refractive index and extinction coefficient for glass (a), ITO / AZO (b), ZnMgO (c), CuO / Cu_2O (d).

As can be seen from Fig. 3, the transmission coefficient of the solar cell with the AZO layer is very close to that of ITO.

To determine the optimal material of conductive layer solar cell was calculated coefficient of optical power loss of the device [13]. These results of calculation of the coefficient of

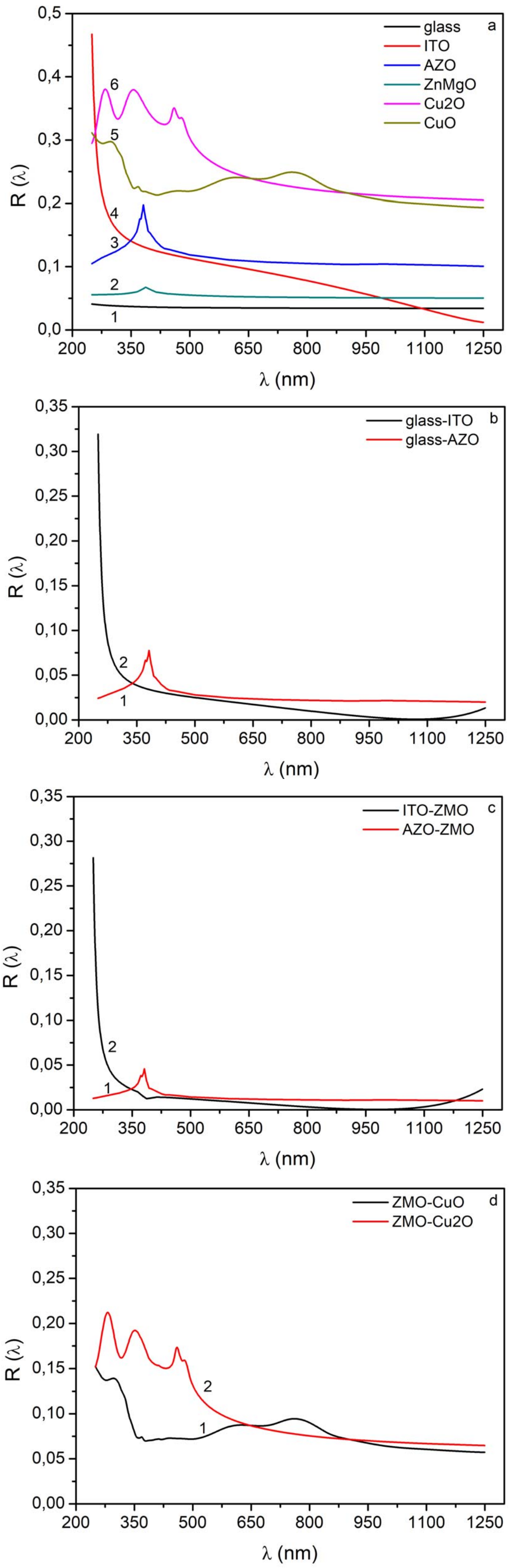

Fig. 2. The spectral dependences of the reflection coefficient (R) for interfaces: air - glass (1), air-ZnMgO (2), air-ZnO (3), air-ITO (4), air-CuO (5), air-Cu_2O (6) (a) and glass-ITO, glass-ZnO (b), ITO-ZnMgO, ZnO-ZnMgO (c), CuO-ZnMgO, Cu_2O-ZnMgO (d).

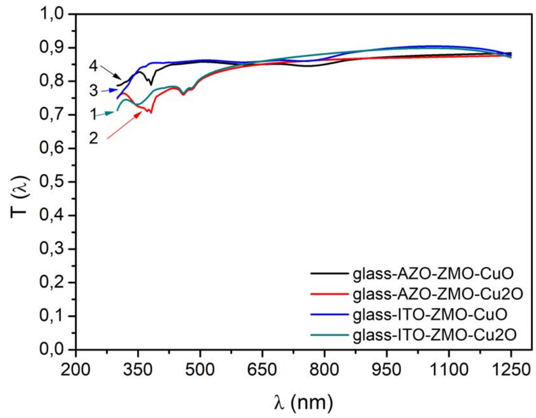

Fig. 3. Spectral dependence transmittance T(λ) of a solar cell with ITO / ZnMgO / Cu_2O (1), AZO / ZnMgO / Cu_2O (2), ITO / ZnMgO / CuO (3) and AZO / ZnMgO / CuO (4) structures.

optical loss in the solar cells with various structures are presented in Table 1.

TABLE I. THE COEFFICIENTS OF OPTICAL POWER LOSS IN THE SOLAR CELLS

Structure of solar cell	Optical loss coefficient, %	The coefficient of light passing, %
glass/AZO/ZMO/CuO	14.29	85.71
glass/AZO/ZMO/Cu_2O	16.12	83.88
glass/ITO/ZMO/CuO	12.83	87.13
glass/ITO/ZMO/Cu_2O	14.68	85.32

As can be seen from the table, the optical losses in a solar cell of different construction (with ITO and AZO layers) differ by 1.46% and 1.44% for devices with CuO and Cu_2O absorbing layers respectively. In turn, the change in the absorbing layer results in 1.83% and 1.85% loss coefficient difference for the AZO and ITO front contact, respectively. The best light transmission coefficient still has a solar cell with a glass/ITO/ZnMgO/CuO construction.

III. The Losses of Light Absorption in Solar Cell Layers

In addition to losses on light reflection from layers should consider 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 [9, 10].

Fig. 4 shows the dependence of T on the wavelength λ for solar cell based on ZnMgO/CuO and ZnMgO/Cu_2O heterojunction including losses on light absorption in the auxiliary layers with different thickness values.

Analysis of the dependencies indicates that changing the thickness of 25 to 200 nm of ZnMgO layer somewhat reduces the value of transmittance of solar cells. The transmittance values of the device with ITO layer is somewhat greater than the corresponding value for the structure with AZO layer in the wavelength range λ = (650-920) nm.

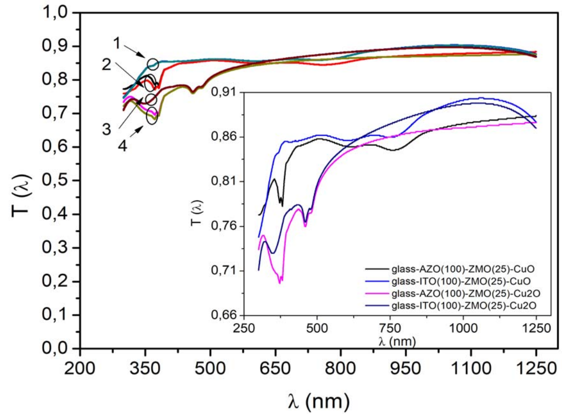

Fig. 4. Spectral dependence of transmission coefficients of solar cells with structure glass/ITO/ZnMgO/CuO (1), glass/AZO/ZnMgO/CuO (2), glass/ITO/ZnMgO/Cu_2O (3), glass/AZO/ZnMgO/Cu_2O (4) at $d_{ZnO(ITO)}$ = 100-200 nm, d_{ZnMgO} = 25 nm; and the spectral dependence at $d_{ZnO(ITO)}$ = 100 nm, d_{ZnMgO} = 25 nm (on the insert).

As calculations show, the ITO layer is more attractive compared to AZO in a copper oxide solar cell, because it allows improving the rate of passage of light to the absorbing layer. Analysis of the dependencies shown in Fig. 4 and Table 2 indicate that with increasing the thickness of the ZnMgO layer from d = 25 nm to d = 200 nm, the loss of light increases by 0.04% at d_{ITO} = 100 nm and 0.05% at d_{ITO} = 200 nm for structures with a layer of ITO. For a structure with an AZO layer, the loss factor increases by 0.04% as with d_{ZnO} = 100 nm as well as d_{ZnO} = 200 nm.

TABLE II. THE COEFFICIENTS OF OPTICAL LOSS IN THE SOLAR CELLS WITH DIFFERENT STRUCTURE INCLUDING LOSSES ON LIGHT ABSORPTION WITH DIFFERENT THICKNESS VALUES (GLASS/AZO/ZMO/CUO (1), GLASS/AZO/ZMO/CU_2O (2), GLASS/ITO/ZMO/CUO (3), C GLASS/ITO/ZMO/CU_2O (4))

№	Optical loss coefficient, %					
	$d_{ITO\ (ZnO)}$ = 100 nm					
d_{ZnMgO} nm	25	50	75	100	150	200
1	14.42	14.42	14.43	14.44	14.45	14.46
2	16.24	16.24	16.25	16.26	16.27	16.28
3	12.89	12.90	12.90	12.91	12.92	12.94
4	14.75	14.75	14.76	14.76	14.78	14.79
	$d_{ITO\ (ZnO)}$ = 200 nm					
1	14.54	14.54	14.55	14.56	14.57	14.58
2	16.35	16.35	16.36	16.37	16.38	16.39
3	12.95	12.96	12.96	12.97	12.98	13.00
4	14.80	14.81	14.82	14.82	14.83	14.85

As expected, the transmission coefficient of solar cell worsens when the thickness of the frontal contact layer is increased. The same effect causes an increase in the thickness of the window layer of the device. Consequently, in order to increase the efficiency of the solar cells, their layers should have a minimum technologically achievable thickness.

IV. CONCLUSIONS

In the paper, the optical losses were defined in thin film solar cells based on n-ZnMgO / p-CuO (p-Cu_2O) heterojunctions with frontal contacts AZO and ITO. Such solar cells have a very high value of light transmittance (~90%) as in the case of the conductive layer of AZO as well as ITO.

It was found that the transmittance coefficient with the ITO layer is slightly larger than the corresponding value for the structure with AZO.

The overall optical losses at d_{ZnMgO} = 25 nm and $d_{ZnO(ITO)}$ = 100 nm in solar cells with different structure are: 14.42 %, 16.24 %, 12.89 % and 14.75 % for glass/AZO/ZMO/CuO, glass/AZO/ZMO/Cu_2O, glasso/ITO/ZMO/CuO and glass/ITO/ZMO/Cu_2O respectively.

Thus, it is possible to optimize the design of the solar cells based on such heterojunctions.

ACKNOWLEDGMENT

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

REFERENCES

[1] A. Bhaumik, A. Haque, P. Karnati, M. Taufique, R. Patel, and K. Ghosh, “Copper oxide-based nanostructures for improved solar cell efficiency,” Thin Solid Films, vol. 572, pp. 126–133, 2014.

[2] V. Kumar, S. Masudi-Panah, C. C. Tan, T. K. S. Wong, D. Z. Chi, “Copper Oxide Based Low-Cost Thin Film Solar Cells,” Nanoelectronics Conference (INEC), IEEE, pp. 443–445, 2013.

[3] R. Wick, S. D. Tilley, “Photovoltaic and Photoelectrochemical Solar Energy Conversion with Cu_2O,” J. Phys. Chem. C, vol. 119, pp. 26243-26257, 2015.

[4] T. Oku, R. Motoyoshi, K. Fujimoto, T. Akiyama, B. Jeyadevan, J. Cuya, “Structures and photovoltaic properties of copper oxides/fullerene solar cells,” J. Phys. Chem. Solids, vol. 72, no. 11, pp. 1206–1211, 2011.

[5] Li, D., Leung, Y. H., Djurišić, A. B., Liu, Z. T., Xie, M. H., Gao, J., “CuO nanostructures prepared by a chemical method,” J. Cryst. Growth, vol. 282, no. 1, pp. 105–111, 2005.

[6] A. S. Ethiraj and D. J. Kang, “Synthesis and characterization of CuO nanowires by a simple wet chemical method.,” Nanoscale Res. Lett., vol. 7, no. 1, p. 70, 2012.

[7] A. Rios-Flores, O. Arés, J. Camacho, V. Rejon, and J. Peña, “Procedure to obtain higher than 14% efficient thin-film CdS/CdTe solar cells activated with HCF 2 Cl gas,” Sol. Energy, vol. 86, pp. 780–785, 2012.

[8] A. Luque, Handbook of photovoltaic science and engineering, Chichester, UK: John Wiley & Sons Ltd, 2011

[9] O.V. Diachenko, A.S. Opanasyuk, D.I. Kurbatov, P.B. Patel, et. al. “The performance optimization of thin-film solar converters based on n-ZnMgO/p-CuO heterojunctions,” J. Nano- Electron. Phys., in press.

[10] O. A. Dobrozhan, A. S. Opanasyuk, V. V. Grynenko, “Optical and Recombination Losses in Thin Film Solar Cells Based on Heterojunctions n-ZnS (n-CdS)/p-CdTe with Current Collecting Contacts ITO and ZnO.” J. Nano- Electron. Phys., vol. 6, p. 4035, 2014.

[11] S. O. Kasap, Optoelectronics and Photonics : principles and practices. New Jersey: Prentice-Hall, 2001.

[12] S. Adachi, Handbook of Physical Properties of Semiconductors. Boston: Kluwer Academic Publishers, 2004.

[13] K. Ito, “An Overview of CZTS-Based Thin-Film Solar Cells,” in Copper Zinc Tin Sulfide-Based Thin-Film Solar Cells, Chichester, UK: John Wiley & Sons Ltd, 2015.

[14] O. Dobrozhan, A. Opanasyuk, M. Kolesnyk, M. Demydenko, and H. Cheong “Substructural investigations, Raman, and FTIR spectroscopies of nanocrystalline ZnO films deposited by pulsed spray pyrolysis,” phys. status solidi a, vol. 212, pp. 2915-2921, September 2015.