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Design of Al:ZnO/*p*-Si Heterojunction Solar Cell Using SCAPS Simulation Program

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ZnO thin film is a prominent candidate to be used as a buffer layer in silicon solar cells. In this paper, the effect of Al concentrations (1, 5, 10 wt. %) on the conversion efficiency of Al:ZnO/Si thin film solar cells has been investigated through simulation by SCAPS program. It has been found that the main photovoltaic parameters such as open-circuit voltage, short-circuit current density, fill factor, conversion efficiency, quantum efficiency and ideality factor increased as Al enrichment occurred. At 10 wt. % of Al the optimum conversion efficiency was approximately 7 %, the maximum value of the ideality factor was 17.51, and the bandgap value was 3.56 eV. Additionally, the resistivity, carrier concentration and mobility were determined for all measurements. It has been found that a decrease in the Hall coefficient led to an increase in the carrier concentration with increasing Al content, while an increase in the mobility occurred due to a decrease in the electrical resistivity. The quantum efficiency of the solar cell measured at a wavelength in the range of 400-1000 nm was between 0.4-0.5.

Keywords: Al:ZnO thin films, Heterojunction solar cell, SCAPS.

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1. INTRODUCTION

Solar cell capacitance simulator SCAPS-3200 is a graphic program for the solar cell simulation developed with LabWindows/CVI of National Instruments at the University of Gent [1]. It is organized in the form of a number of panels and is successfully used for complex modeling the optical and photoelectric properties of solar cells, for instance, ZnO/CdS/CdTe/CuO, Si-CdS-ZnO, CdS/CdTe etc. [2-4]. Additionally, it realistically simulates the electrical characteristics of heterojunction solar cells [5]. For example, polycrystalline semiconductor CdTe film and Cu(In,Ga)Se solar cell have been modeled by SCAPS to establish the current-voltage, capacitance-voltage and capacitance-frequency characteristics [6].

A heterojunction solar cell is necessary for the large-scale applications in photodetectors and other semiconductors such as silicon, which have a band gap between 1.1 and 1.6 eV. It has the potential for higher efficiency, reliability and low cost. A transparent conducting oxide semiconductor is one of the most interesting heterojunction solar cells that includes oxide semiconductors, such as tin oxide (SnO_2), indium oxide (In_2O_3) and zinc oxide. Compared to other oxides, it is used more frequently because of its lower cost, good physical, optical and electrical properties, and a large band gap of 3.3 eV [7-9]. Moreover, it is among the most demanded materials for application in TCO because of its abundance in nature, the absence of toxicity, and the ability of the deposited films at low temperatures [8].

2. EXPERIMENTAL DETAILS

The schematic structure of the investigated Al:ZnO/Si solar cell is given in Fig. 1. The *n*-type ZnO thin film is an intermediate (buffer) layer between *p*-Si absorber layer and Al metal *p*-type window layer with the main objective to make a good *p*-*n* junction.

For the system presented in Fig. 1, we performed five independent SCAPS simulations to study the effect of Si and Al layers on Al:ZnO/Si solar cell parameters such as short-circuit current density (J_{sc}), open-circuit voltage (V_{oc}), fill factor (FF), conversion (η), quantum efficiency (QE), and ideality factor (n). The concentration of aluminium was changed (1, 5 and 10 wt. %) in order to determine advances of Al window layer in the investigated solar cell.

From all measurements, the carrier concentration, resistivity and mobility were additionally found. The determination of optimal conditions will lead to the production of transparent, highly conductive and well-crystallized ZnO/Al films.

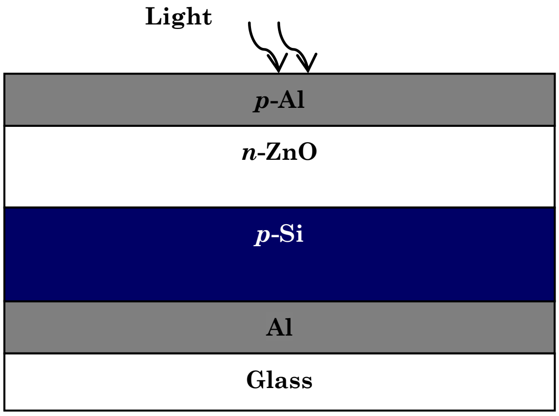

Fig. 1 – Schematic structure of Al/ZnO/Si thin film solar cell

3. RESULTS AND DISCUSSION

Fig. 2 presents the dependences of the carrier concentration and band gap on the Al content in Al:ZnO/Si solar cell. It is obvious that when Al concentration in-

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creases, the carrier concentration also linearly increases due to the decrease in the Hall coefficient. A similar tendency occurs for the band gap. The maximum value of the band gap of 3.56 eV is obtained for 10 wt. % Al, which is 2 % higher than for 5 wt. % Al and 5 % higher than for 1 wt. % Al. The obtained values of the band gap are in good agreement with the already established value of 3.35 eV reported in [10, 11].

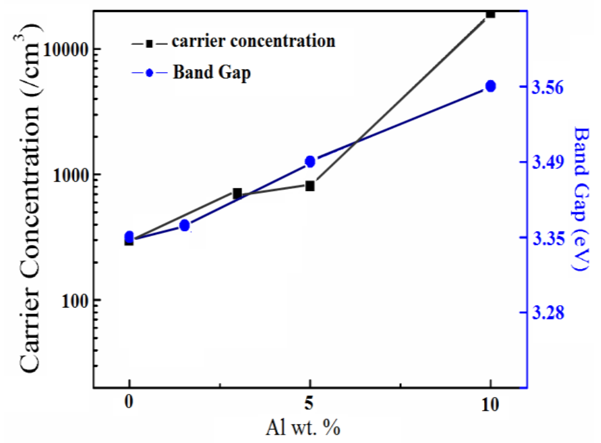

Fig. 2 – Variation of the carrier concentration and band gap with Al content

The electrical resistivity was calculated using a standard four-point probe method at a distance of $s = 2$ mm according to the following equation [12]:

$$\rho_m = 2\pi s(V/I)\,. \tag{1}$$

Fig. 3 shows the dependences of the electrical resistivity and mobility on the Al content in Al:ZnO/Si solar cell. It is defined that the electrical resistivity decreases to 4.8×10^{-3} Ω.cm as Al concentration increases to 10 wt. %. This is due to the replacement of Al at zinc sites in the hexagonal lattice or isolation of Al into a homogeneous region at the grain boundary. When doped with Al, the formation of AlZn can be attributed to the influence of the free-carrier concentration in the film; therefore, it has an effect on the resistivity, but not on the Al boundary.

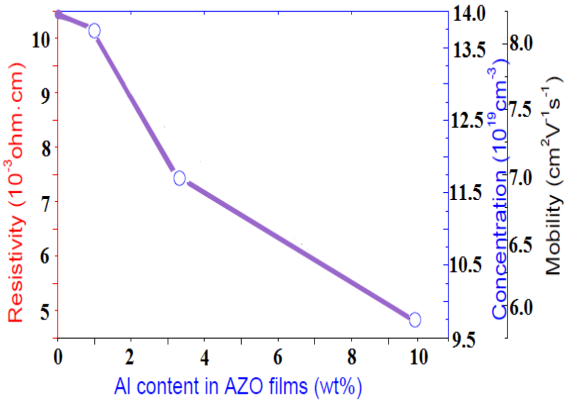

Fig. 3 – Variation of the resistivity and mobility with Al content

The mobility μ of the film is determined as

$$\mu = RH/\rho\,, \tag{2}$$

where RH is the Hall coefficient and ρ is the resistivity.

The mobility of Al/ZnO films increases with increasing Al content due to a decrease in the resistivity and an increase in the grain boundary scattering (Fig. 3).

Fig. 4 shows the *J-V* characteristics of the solar cell modeled using SCAPS.

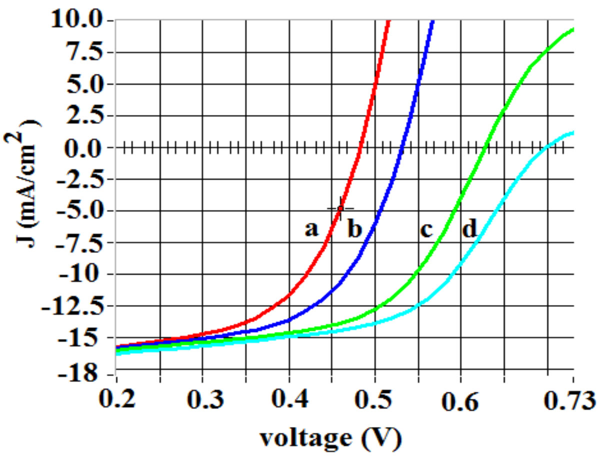

Fig. 4 – *J-V* spectra at different Al content (1, 5, 10 wt. %) in the solar cell

The fill factor (FF) and efficiency (η) of Al:ZnO/Si solar cell are calculated from relations (3) and (4), respectively [13, 14]:

$$FF = \left[\frac{I_m V_m}{I_{sc} V_{oc}}\right] \times 100\%\,, \tag{3}$$

where I_m and V_m are the current and voltage obtained at maximum power, respectively.

$$\eta = \left[\frac{I_{sc} V_{oc} FF}{P_{h\nu}}\right] \times 100\%\,, \tag{4}$$

where I_{sc} is the short-circuit current, V_{oc} is the open-circuit voltage, $P_{h\nu}$ is the power density of the incident radiation.

The ideality factor (n) depending on the voltage is calculated from equation (5) [15]

$$n(V) = \frac{qV}{kT\ln(I/I_0)}\,, \tag{5}$$

where q is the electron charge (Coulomb), k is the Boltzmann constant (J/K), T is the room temperature, I_0 is the reverse saturation current calculated from the linear region of the plot between V and ln$I$.

The solar cell parameters obtained during modeling are presented in Table 1. It is obvious that the values of the solar cell parameters (V_{oc} and J_{sc}) increase as Al content increases.

It is observed that the fill factor and efficiency increase with increasing Al content. The optimum conversion efficiency is about 7.02 % at 10 wt. % of Al (Fig. 5). In addition, the applied illumination caused an increase in the current amount of the solar cell [16].

In Fig. 6, we can observe that the ideality factor increases in the solar cell from 12.22 with pure ZnO/Si to 17.51 with 10 wt. % of Al, which means that it has a maximum value with increasing Al content. In this study, the obtained high ideality factor is due to the homogeneous distribution of carriers at the interfaces [17] and tunnelling processes [18] because of the interfacial Al-doped ZnO films.

Table 1 – Solar cell parameters obtained at Al content of 1, 5 and 10 wt. % by SCAPS modeling

Sample	V_{oc} (Volt)	J_{sc} (mA/cm^2)	FF (%)	η (%)	n
ZnO	0.482	16.985	59.43	4.87	12.22
1 wt. % Al:ZnO	0.531	16.998	60.46	5.45	13.46
5 wt. % Al:ZnO	0.627	17.070	60.99	6.45	15.84
10 wt. % Al:ZnO	0.698	17.266	61.17	7.02	17.51

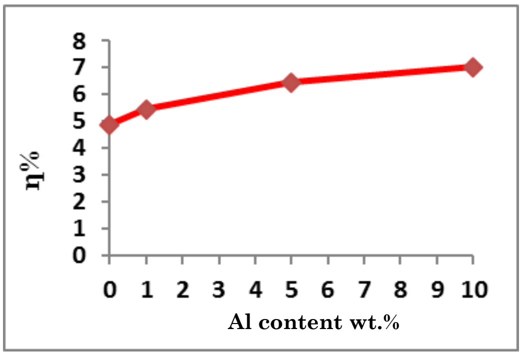

Fig. 5 – Variation of the efficiency as a function of Al content

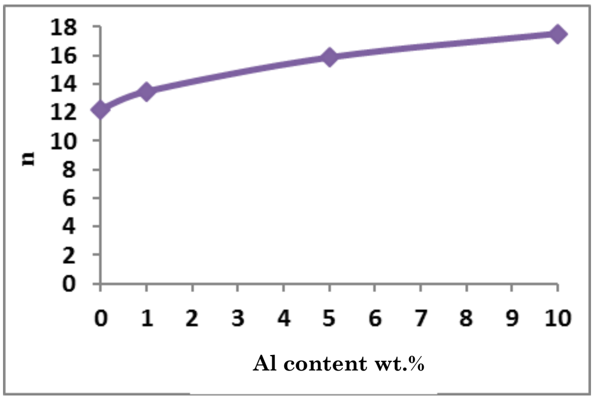

Fig. 6 – Variation of the ideality factor as a function of Al content

The quantum efficiency spectra as a function of the wavelength for different Al concentrations are shown in Fig. 7. We observe the maximum peak at a wavelength of 640 nm. The plot shows nearly overlap between samples (b) 1 wt. % Al:ZnO and (c) 5 wt. % Al:ZnO at a wavelength of 800-900 nm. At a higher Al concentration (10 wt. %) (d), the sample absorbs more photons, which increases the overall efficiency of the solar cell.

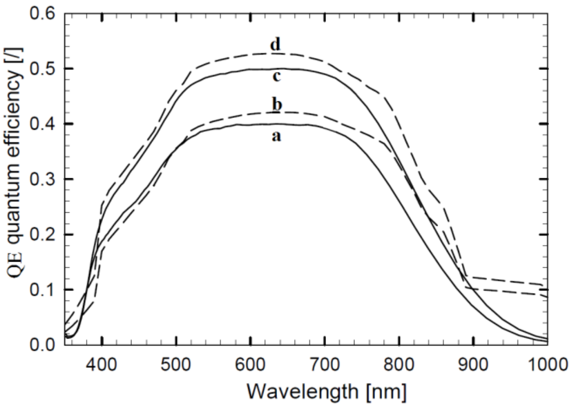

Fig. 7 – Quantum efficiency spectra as a function of wavelength (a – 0 wt. % Al, b – 1 wt. % Al, c – 5 wt. % Al, d – 10 wt. % Al)

4. CONCLUSIONS

In summary, we have investigated the effect of Al content (1, 5, 10 wt. %) on the electrical properties of Al:ZnO/Si solar cell using SCAPS program. It has been established that the band gap increases and reaches 3.56 eV at 10 wt. % of Al. For the sample with 10 wt. % of Al, a minimum resistivity of 4.8×10^{-3} Ω.cm has been obtained. The carrier concentration and Hall mobility of all samples increase with increasing Al content, but the resistivity decreases. From all measurements, as the Al content increases to 10 wt. %, the efficiency and ideality factor increase to 7.02 % and 17.51, respectively. The maximum peak for the quantum efficiency for all samples is 640 nm.

REFERENCES

1. M. Burgelman, J. Verschraegen, S. Degrave, P. Nollet, *Prog. Photovoltaics Res. Appl.* **2** No 2-3, 143 (2004).
2. Z. Zapukhlyak, L. Nykyruy, G. Wisz, V. Rubish, V. Prokopiv, M. Halushchak, I. Lishchynskyy, L. Katanova, R. Yavorskyi, *Phys. Chem. Solid State* **21**, 660 (2020).
3. N. Jamil, S. Abdulla, A. Muhammed, A. Pogrebnjak, M. Ivashchenko, *Proceedings of the International Conference Nanomaterials: Applications and Properties (NAP-2012)*, **1**, 04NMEEE09 (2012).
4. N.Y. Jamil, *Raf. J. Sci.* **26**, 133 (2017).
5. J. Verschraegen, M. Burgelman, *Thin Solid Films* **515**, 6276 (2007).
6. M. Bugelman, M. Bugelman, P. Nollet, S. Degrave, *Thin Solid Films* **361-362**, 527 (2000).
7. B. Asenjo, A.M. Chaparro, M.T. Guyerrez, J. Herrero, J. Klaer, *Sol. Energy Mater. Sol. C.* **87**, 647 (2005).
8. X. Zi-qiang, D. Hong, L. Yan, C. Hang, *Mat. Sci. Semicon. Proc.* **9**, 132 (2006).
9. S.W. Xue, X.T. Zu, W.G. Zheng, M.Y. Chen, X. Xiang, *Physics B* **382**, 201 (2006).
10. S.A. Najim, N.Y. Jamil, K.M. Muhammed, *J. Nano- Electron. Phys.* **11**, 02003 (2019).
11. S.A. Najim, K. M. Muhammed, A.D. Pogrebnjak, *IEEE International Conference on "Nanomaterials: Applications & Properties" (NAP-2020)*, 01NP04 (2020).
12. F.M. Smits, *Bell. Syst. Tech. J.* **37**, 711 (1958).
13. V.D. Das, L. Damodare, *J. Appl. Phys.* **81**, 1522 (1997).
14. T.J. Coutts, *Sol. Energy Mater.* **50**, 99 (1978).
15. H.C. Card, E.H. Rhoderick., *J. Phys D.* **4**, 1589 (1971).
16. S.A. Najim, *J. Basic Education College* **15**, 3167 (2019).
17. Y.X. Luo, C.H. Shih, *Semicond. Sci. Technol.* **29**, 115006 (2014).
18. J. Lee, T. Uhrmann, T. Dimopoulos, H. Bruckl, J. Fidler, *IEEE Trans. Magn.* **46**, 2067 (2010).

Конструювання Al:ZnO/*p*-Si сонячного елемента з гетеропереходом за допомогою програми для моделювання SCAPS

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Тонка плівка ZnO є потенційним кандидатом для використання в якості буферного шару в силіконовій сонячній батареї. У роботі досліджено вплив концентрації Al (1, 5, 10 мас. %) на ефективність перетворення сонячних елементів з тонких плівок Al:ZnO/Si за допомогою програми для моделювання SCAPS. Було виявлено, що основні фотоелектричні параметри, такі як напруга розімкнутого ланцюга, щільність струму короткого замикання, коефіцієнт заповнення, ефективність перетворення, квантова ефективність та коефіцієнт ідеальності зростали в міру збагачення плівки Al. При 10 мас. % Al оптимальна ефективність перетворення становила приблизно 7 %, максимальне значення коефіцієнта ідеальності складало 17,51, а значення ширини смуги – 3,56 еВ. Крім того, для всіх вимірювань визначали питомий опір, концентрацію носія та рухливість. Встановлено, що зменшення коефіцієнта Холла призвело до збільшення концентрації носія із збільшенням вмісту Al, тоді як збільшення рухливості відбувалося через зменшення електричного опору. Квантова ефективність сонячного елемента, виміряна на довжині хвилі в діапазоні 400-1000 нм, знаходилася в межах 0,4-0,5.

Ключові слова: Тонкі плівки Al:ZnO, Сонячний елемент з гетеропереходом, SCAPS.