

Modeling of Fabricated NiO/TiO₂ P-N Heterojunction Solar Cells

Ukoba, O.K; and Inambao, F.L

Discipline of Mechanical Engineering, University of KwaZulu-Natal, Durban, South Africa.

Email :ukobaking@yahoo.com

Abstract

This paper reports modelling and theoretical validation of a fabricated NiO/TiO₂ P-N heterojunction solar cell. The solar cell equations were modelled and thereafter theoretical validation of the fabricated solar cells was performed. Modelling tools were used to validate the influence of NiO material features such as deposition temperature, voltage and defect densities on the performances of an ITO/TiO₂/NiO heterojunction solar cell structure. The working points used included a temperature of 350 °C, illumination of 1000 W/m² using an AM1.5 lamp, with voltage range of 0 to 1.5 volts. The output gave V_{oc} of 0.1445 V, J_{sc} of 247.959195E-6 mA/cm² and FF of 37.87 % and Voc 0.7056 and J_{sc} 28.366911 mA/cm² when both contacts were added. This opens a new frontier for modelling of metal oxide based thin film solar cells especially NiO thin film solar cells. These findings enhance the quest to develop affordable and sustainable energy and encourage further research in solar cell technologies in low-income countries.

Keyword: NiO; solar cells; modelling; simulation

INTRODUCTION

Despite the potential that solar energy holds for being an environmentally benign and sustainable energy source [1], large-scale production and costs still hinder the usage, especially in low-income countries [2]. This may be attributed to the difficulty in scaling up existing methods or the expense and complexities associated with vacuum environment fabrication [3]. The way forward is to develop materials and techniques that will encourage low cost or focus on a few experimental techniques [4]. The latter can be achieved with more success when combined with modelling. The modelling of result improves the planning and implementation of the experiment.

Solar cells produce about 0.5 volts to 0.6 volts of open circuit voltage and 1 to 8 amps DC current depending on a range of factors but mainly related to the semiconductor used [5]. About 36 to 72 solar cells are stacked together in series to form a module which can produce meaningful output. A solar panel is an arrangement of solar modules either in series or parallel. When the solar modules are connected in parallel the currents are added while the voltage is the same, while for series the voltages are added and the current produced remains the same [6].

Solar cells can be grouped into monocrystalline, polycrystalline, and thin film technology [7]. Both monocrystalline and polycrystalline are referred to as traditional technologies of solar cells and collectively grouped as crystalline silicon. Solar cells can also be grouped by

generations of the solar cells [8, 9]. The traditional technologies of solar cell manufacture use microelectronic manufacturing with an efficiency ranging from 10 % to 15 % and 9 % to 12 % for monocrystalline and polycrystalline respectively. Thin films' efficiency varies depending on the fabrication techniques and materials used. The monocrystalline solar cells tend to have the highest efficiency and are also very expensive.

Metal oxide heterojunction solar cells are currently attracting attention due to their potential [10]. Metal oxides offer great promise for being a solution to affordable, environmentally friendly, sustainable and viable energy, so ending the world energy problem, especially in developing and low-income countries [11, 12]. Metal oxides, especially NiO thin film, are the most promising materials to be used as solar cell absorber layers due to their excellent optical properties They have good band gaps, low cost and great absorption coefficients as well as constituents that are nontoxic and abundant naturally [13].

However, most of them still exhibit weak conversion efficiencies resulting in several experiments in the laboratory in an attempt to obtain the optimum power conversion efficiency with current levels being about 8.4 % [14] compared to those of other technological paths in the photovoltaic field like CIGS-based solar cells which reach record efficiencies of over 20 % [10]. However, despite the development of several physical and chemical fabrication techniques for PV [15-17], several reasons could explain this situation, such as various loss mechanisms due to absorber features.

Modelling has been used in other fields to reduce the amount of person-hours and resources spent performing experiments [18]. Modelling of solar energy spans many decades, with most models focusing on photovoltaic panels and modules. The few studies on solar cells are mainly on silicon and related solar cells [19-21]. There is, therefore, a need to explore ways of modelling metal oxide cells due to the increasing interest in them.

This study attempts to model metal oxides heterojunctions (NiO/TiO₂) using modelling tools (including SCAPS) which were successfully deployed in previous generations of solar cell research. SCAPS stands for Solar Cell Capacitance Simulator and is used for one or two-dimensional solar cell simulation. Therefore, a detailed analysis of the effect of deposition temperature, thickness, and defects densities of a NiO layer is necessary and has been presented in this work using the numerical simulation package SCAPS [22]. The results proposed in this study are a useful guideline for design of high performances NiO based solar cells.

METHODOLOGY

The Mathematical Model

A solar cell is basically a P-N heterojunction. Photovoltaic systems exhibit nonlinear I-V characteristics that vary with the temperature of the solar cell and the radiant intensity. Under ideal conditions, a solar cell can be theoretically modelled as a current source under a diode. A direct current is produced when the solar cell is exposed to light and this current varies linearly with the solar radiation. This is represented in Figure 1.

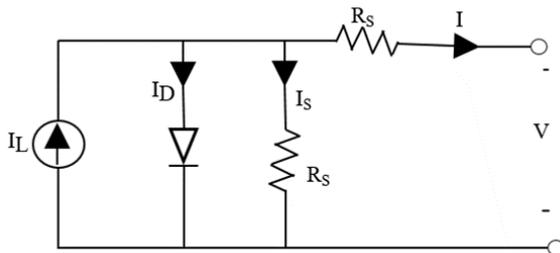


Figure 1. Solar cell model equivalent circuit

From the aforementioned, the characteristic equations are given as:

$$I_{ph} = \frac{I_T \times I_{sc}}{I_{r0}} \quad (1)$$

Equation (1) shows that the photocurrent depends on the temperature of the solar cell and solar insolation.

$$V_t = \frac{kT}{q} \quad (2)$$

$$I_s = I_{sc} \times \left(e^{\left(\frac{V_{oc}}{n \cdot V_t} \right)} - 1 \right) \quad (3)$$

It can be seen from Equation (3) that the cell's saturation current varies with the cell temperature,

$$I_d = I_s \times \left(e^{\left(\frac{V + I \cdot R_s}{n \cdot V_t \cdot N_s} \right)} - 1 \right) \quad (4)$$

Equation (4) gives the Shockley equation.

$$I = I_{ph} - I_d - I_{sh} \quad (5)$$

The output current of the solar cell is represented in Equation (5).

Equations (1) to (5) give the electrical behaviour and relationship between the current supplied and voltage, where; I_{ph} is photocurrent, I_{sc} is reverse saturation current, R_s and R_{sh} are inherent resistances in series and parallel associated with the cell, N_s is number of cells in series, q is the electron charge, K is Boltzmann's constant and A , the modified ideality factor. Table 1 shows the ideality factor of some of the solar cells.

Table 1. Ideality factor of some solar cells

S/N	Technology	Ideality factor (A)
1.	Monocrystalline silicon (Si Mono)	1.2
2.	Polycrystalline silicon (Si Poly)	1.3
3.	AsGa	1.3
4.	CIS	1.5
5.	CdTe	1.5
6.	a-Si:H	1.8
7.	a-Si: H tandem	3.3
8.	a-Si: H triple	5

The solar cell is not an active device in darkness but behaves as a diode in such an environment i.e. as a P-N junction. During this phase it does not produce current and voltage. Conversely, a current is generated when an external load is connected to the solar cells. This current is called diode current or dark current and the diode defines the I-V characteristics of the cell.

Therefore, from Figure 1 and from equation (5), the I-V characteristic equation of a solar cell can be expressed in Equation (6):

$$I = I_{ph} - I_s \left[e^{\left(\frac{q(V + R_s I_{pv})}{AKTc} \right)} - 1 \right] - \frac{V + R_s I_{pv}}{R_{sh}} \quad (6)$$

Theoretical validation

SCAPS is a one-dimensional solar cell simulation program used for Opto-electrical simulation of the 1-D or 2-D structures of semiconductor layers [23-26]. SCAPS was originally developed for cell structures of the CuInSe₂ and the CdTe family. However, there have been improvements since then making room for other types of solar cells. SCAPS uses finite difference methods to solve the differential equations which, along with several relations from the physics of semiconductors, describe mathematically the performance of a solar cell. SCAPS performs a complete simultaneous numerical solution of the two continuity equations and Poisson's equation, conditional on the boundary conditions appropriate to one and two-dimensional cells [27]. The equations are expressed as shown in Equations (7-9).

$$\nabla^2 v = - \frac{q}{\epsilon} (p - n + N_D - N_A) \quad (7)$$

$$\nabla \cdot J_p = q(G - R) \quad (8)$$

$$\nabla \cdot J_n = q(R - G) \quad (9)$$

The general terms of Equations (8) and (9) can be represented as:

$$G(x) = \int_0^\infty \phi a e^{-ax} d\lambda \quad (10)$$

The hole and electron current densities which appear in Equations (8) and (9) are given by:

$$J_p = -q\mu_p p \nabla V_p - kT\mu_p \nabla p \quad (11)$$

$$J_n = -q\mu_n n \nabla V_n + kT\mu_n \nabla n \quad (12)$$

$$V_p = V - (1 - \gamma) \frac{\Delta G}{q} \quad (13)$$

$$V_n = V + \gamma \frac{\Delta G}{q} \quad (14)$$

where v_p and v_n represent the effective potentials expressed in Equations (13) and (14), and ΔG and γ account for variations in the band structure, such as density of states and band gap, and account for Fermi-Dirac statistics.

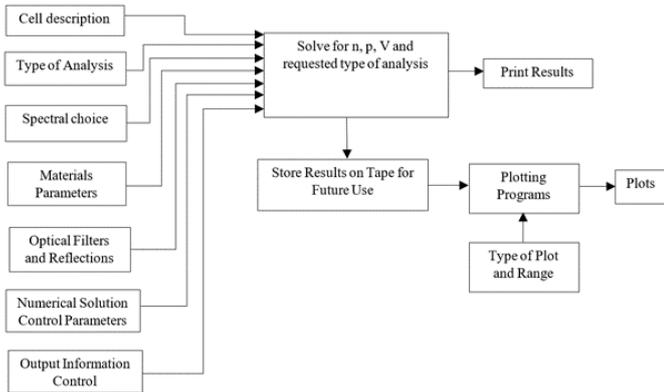


Figure 2. Block Diagram of the structure of SCAP1D and SCAP2D

Figure 2 depicts the structure of the SCAPS programme, and summarizes the working of the programme. The operator inputs the information related to the materials' parameters, a description of the device to be analyzed, the type of analysis to be performed and the spectrum (optional). The results are printed in summary form and the detailed results of the calculation are stored. A separate plotting routine is used to access the information and to display the appropriate parameters. The plotting capability is one of the most valuable features of the code because it allows one to effectively have a microscopic view of most of the parameters of interest in the interior of the cell under operating conditions.

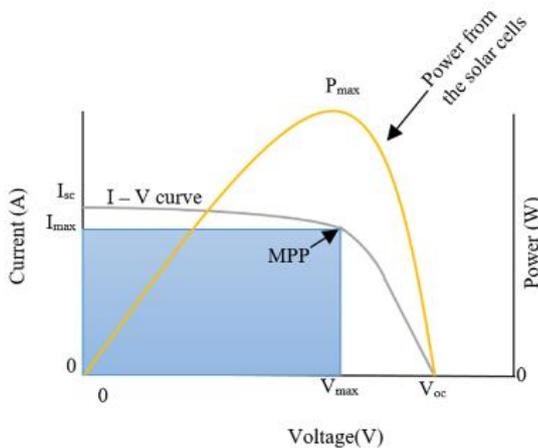


Figure 3. Typical characteristics of a solar cells

Figure 3 shows typical characteristics of solar cells. It shows the behaviour of the voltage and current with irradiation and the temperature of solar cells. The maximum power is obtained by computing the V_{max} and I_{max} . The maximum power point (MPP) technique is mainly used in computing the maximum power of solar module. The fundamental parameters related to the solar cell are short circuit current (I_{sc}), open circuit voltage (V_{oc}), and MPP [28, 29].

In this study, a temperature of 350 °C (623.15 K) was used as the working temperature. This was the temperature at which the experimental NiO/TiO₂ P-N heterojunction was spray pyrolysis deposited, while the illumination was done with AM1.5 using a lamp of 1000 W/m² with a voltage range of 0 volts to 1.5 volts as shown in Figure 4.



Figure 4. Defined parameters used for the modelling the solar cells

Figures 5 and 6 give the output of the I-V characteristics using SCAP-1D. Figure 5 varies the voltage from 0 volts to 1 volt while Figure 6 varies it from 0 volts to 1.5 volts. The generated plot of current density versus voltage corresponds to the typical I-V characteristic curve. The fill factor (FF) obtained was 37.87 % while the output voltage (V_{oc}) was 0.1445 volts. These parameters agree with the fabricated NiO/TiO₂ solar cells with FF of 39 % [4].

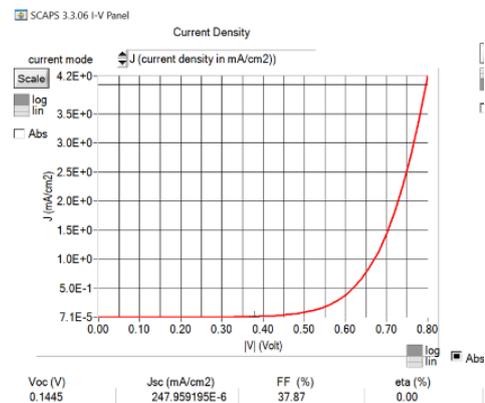
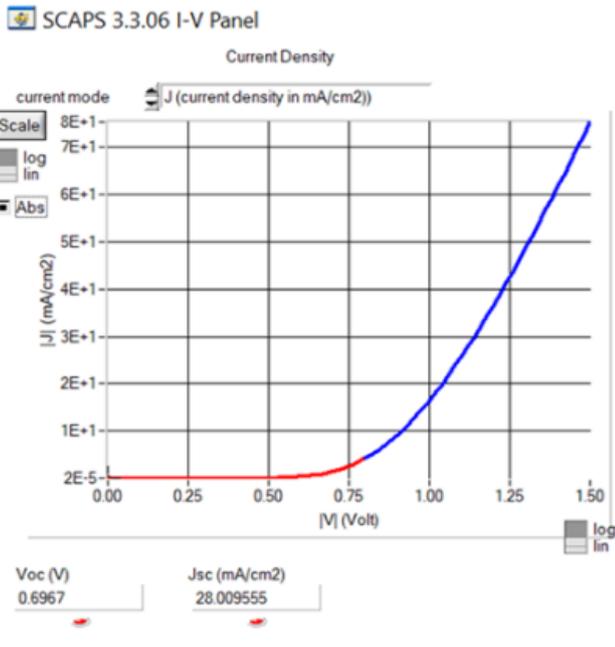


Figure 5. SCAP-1D generated I-V characteristic curve for the solar cells



/ui

Figure 6. SCAP-1D generated I-V characteristic curve for the solar cells 0 to 1.5 v

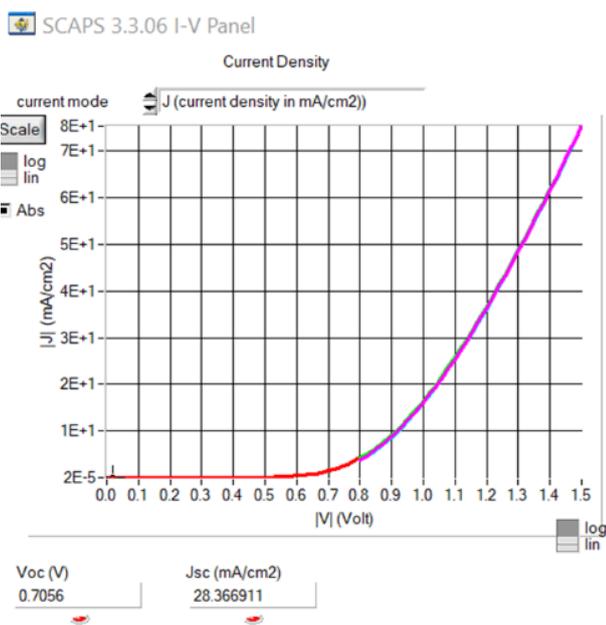


Figure 7. SCAP-1D generated I-V characteristic curve for the solar cells with gold and ITO added to 0 to 1.5V

Figure 7 shows the SCAP-1D generated I-V characteristic curve for the solar cells with gold and ITO added to 0 V to 1.5 V.

CONCLUSION

This paper was able to give the mathematical model and theoretical validation of a sprayed deposited NiO/TiO₂

heterojunction solar cell at 350 °C. The model used the deposition parameters of the fabricated solar cell and generated the I-V characteristics of the solar cell. The results show excellent correspondence to reported experimental fabrication. The experimental fill factor obtained was 39 % while this study reported 37.87 %. This shows that this can be used to model another metal oxides especially NiO related solar cells. This will help to reduce several person-hours and resources spent on trying different optimization parameters in the laboratory. These findings enhance the quest to develop affordable and sustainable energy and encourages further research in solar cells technologies in low-income countries.

ACKNOWLEDGEMENT

The financial assistance of the National Research Foundation (NRF/TWAS) of South Africa towards this research under grant number 105492 is hereby acknowledged. Authors appreciate the SCAPS team for allowing us the usage of the program.

REFERENCE

- [1] Kabir, E., Kumar, P., Kumar, S., Adelodun, A.A., and Kim, K.-H., 2018, "Solar Energy: Potential and Future Prospects," *Renewable Sustainable Energy Rev.*, 82, pp. 894-900.
- [2] Ukoba, O., Inambao, F., and Eloka-Eboka, A., 2017, "Influence of Annealing on Properties of Spray Deposited Nickel Oxide Films for Solar Cells," *Energy Procedia*, 142, pp. 244-252
- [3] Ukoba, O.K., Eloka-Eboka, A.C., and Inambao, F.L., 2018, "Review of Nanostructured NiO Thin Film Deposition Using the Spray Pyrolysis Technique," *Renewable and Sustainable Energy Rev.*, 82, pp. 2900-915.
- [4] Ukoba, K., Inambao, F., and Eloka-Eboka, A., 2018, "Fabrication of Affordable and Sustainable Solar Cells Using NiO/TiO₂ P-N Heterojunction," *Int. J. Photoenergy*, Hindawi, 2018
- [5] Cutter, A., 2012, *The Electricians Green Handbook*, Delmar, New York.
- [6] Singla, V., and Garg, V.K., 2013, "Modeling of Solar Photovoltaic Module & Effect of Insolation Variation Using Matlab/Simulink," *Int. J. Adv. Eng. Tech.*, 4(3) pp.5-9.
- [7] Xiao, W., Dunford, W.G., and Capel, A., 2004, "A Novel Modeling Method for Photovoltaic Cells," *Proc. 35th Annual IEEE Power Electronics Specialists Conference*, Aachen, Germany, 20-25 June 2004; pp. 1950-1956.
- [8] Bagher, A.M., Vahid, M.M.A., and Mohsen, M., 2015, "Types of Solar Cells and Application," *Am. J. Optics Photonics*, 3(5), pp. 94-113.
- [9] Liu, M., Johnston, M.B., and Snaith, H.J., 2013,

- “Efficient Planar Heterojunction Perovskite Solar Cells by Vapour Deposition,” *Nature*, 501(7467), pp. 395.
- [10] Liu, H., Avrutin, V., Izyumskaya, N., Özgür, Ü., and Morkoç, H., 2010, “Transparent Conducting Oxides for Electrode Applications in Light Emitting and Absorbing Devices,” *Superlattices and Microstructures*, 48, (5), pp. 458-484
- [11] Omer, A.M., 2008, “Energy, Environment and Sustainable Development,” *Renewable Sustainable Energy Rev.*, 12(9), pp. 2265-2300.
- [12] Özgür, Ü., Alivov, Y.I., Liu, C., Teke, A., Reshchikov, M., Doğan, S., Avrutin, V., Cho, S.-J., and Morkoc, H. 2005, “A Comprehensive Review of ZnO Materials and Devices,” *J. Appl. Phys.*, 98(4), p 11.
- [13] Djinkwi Wanda, M., Ouédraogo, S., Tchoffo, F., Zougmore, F., and Ndjaka, J., 2016, “Numerical Investigations and Analysis of Cu₂ZnSnS₄ Based Solar Cells by SCAPS-1D,” *Int. J. Photoenergy*, 2016.
- [14] Shin, B., Gunawan, O., Zhu, Y., Bojarczuk, N.A., Chey, S.J., and Guha, S., 2013, “Thin Film Solar Cell with 8.4% Power Conversion Efficiency Using an Earth-Abundant Cu₂ZnSnS₄ Absorber,” *Prog. Photovoltaics Res. Appl.*, 21(1) pp. 72-76.
- [15] Katagiri, H., Jimbo, K., Yamada, S., Kamimura, T., Maw, W.S., Fukano, T., Ito, T., and Motohiro, T., 2008, “Enhanced Conversion Efficiencies of Cu₂ZnSnS₄-Based Thin Film Solar Cells by Using Preferential Etching Technique,” *Appl. Phys. Express*, 1(4), p. 041201.
- [16] Ahmed, S., Reuter, K.B., Gunawan, O., Guo, L., Romankiw, L.T., and Deligianni, H., 2012, “A High Efficiency Electrodeposited Cu₂ZnSnS₄ Solar Cell,” *Adv. Energy Mater.*, 2(2), pp. 253-259.
- [17] Maeda, K., Tanaka, K., Fukui, Y., and Uchiki, H. 2011, “Influence of H₂S Concentration on the Properties of Cu₂ZnSnS₄ Thin Films and Solar Cells Prepared by Sol-Gel Sulfurization,” *Sol. Energy Mater. Sol. Cells*, 95(10), pp. 2855-2860.
- [18] Arashpour, M., Wakefield, R., Blismas, N., and Minas, J., 2015, “Optimization of Process Integration and Multi-Skilled Resource Utilization in Off-Site Construction,” *Autom. Constr.*, 50, pp. 72-80.
- [19] Altermatt, P.P., 2011, “Models for Numerical Device Simulations of Crystalline Silicon Solar Cells—A Review,” *J. Comput. Electron.*, 10(3), pp. 314-330.
- [20] Fossum, J.G., 1976, “Computer-Aided Numerical Analysis of Silicon Solar Cells,” *Solid-State Electron.*, 19(4), pp. 269-277.
- [21] Ingenito, A., Zeman, M., and Isabella, O., 2016, “Opto-Electrical Surface Engineering of Wafer-Based C-Si Solar Cells,” Master’s dissertation, Delft University of Technology, Delft, Netherlands.
- [22] Degraeve, S., Burgelman, M., & Nollet, P. 2003. “Modelling of Polycrystalline Thin Film Solar Cells: New Features in SCAPS Version 2.3,” *Proc. 3rd World Conference on Photovoltaic Energy Conversion*, Osaka (Japan), May 2003.
- [23] Burgelman, M., and Marlein, J., 2008, “Analysis of Graded Band Gap Solar Cells with SCAPS,” *Proc. 23rd European Photovoltaic Conference*, Valencia, Spain, 2008.
- [24] Burgelman, M., Nollet, P., and Degraeve, S., 2000, “Modelling Polycrystalline Semiconductor Solar Cells,” *Thin Solid Films*, 361, pp. 527-532.
- [25] Decock, K., Khelifi, S., and Burgelman, M., 2011, “Modelling Multivalent Defects in Thin Film Solar Cells,” *Thin Solid Films*, 519, pp. 7481-7484.
- [26] Verschraegen, J., and Burgelman, M., 2007, “Numerical Modeling of Intra-Band Tunneling for Heterojunction Solar Cells in SCAPS,” *Thin Solid Films* 515, pp. 6276-6279.
- [27] Schwartz, R., Gray, J., and Lundstrom, M., 1985, “Current Status of One-And Two-Dimensional Numerical Models: Successes and Limitations,” *Proc. of the Flat-plate Solar Array Project Research Forum on High-efficiency Crystalline Silicon Solar Cells*, JPL Publication 85-38.
- [28] Mohammed, S.S., 2011, “Modeling and Simulation of Photovoltaic Module Using MATLAB/Simulink,” *Int. J. Chem. Environ. Eng.*, 2(5).
- [29] Sahu, R., Sen, S.K., Kaushal, A., and Yadav, S., 2017, “Modelling of Photovoltaic Cell using Incremental Conductance MPPT Method,” *Int. J. Eng. Sci. Comp.*, 7(6), 13271-13275