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Original Research Article

Optimization of electrical properties of ZnO/Si heterojunction solar cell using simulation method

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ABSTRACT

Today thin film technology has dominated over the market of optoelectronic devices based on heterojunction solar cell. In the present work, ZnO/Si heterojunction solar cell has been designed by using simulation method. To investigate the electrical properties of ZnO/Si heterojunction, computational modeling and structural engineering has been used. We explore charge transport characteristics of such a using computational modelling. To enhance the power efficiency of ZnO based solar cell, structured parameter discrepancy has been used to optimize device efficiency and identify suitable design approaches. The present simulation results indicate towards optimization of ZnO-based Si heterojunction solar cells, enabling the development of efficient and reliable solar energy conversion technologies. The present results should be useful for simple, robust and economical optoelectronic devices.

1. Introduction

In the recent time, the pre-requisite of various electronic device application is growing rapidly and many more efforts have been employed more to implement successfully. The development of high quality electronic devices is the key requirement of each country in the era of modern science and technology of 21st century [1-3]. To accelerate the application of thin films for emerging device applications, thin films fabrication must be cost effective, eco friendly, robust more efficient and highly utilized at nanoscale. Thus, the thin film technology has been widely studied and attracting everyone's attention because of its easy fabrication, long durability, highly efficient and stable performance [4]. One of the expected results of these efforts is a thin-film based nanotechnology which is employed in the numerous industries at very high scale of the manufacturing [5, 6]. Now days, a lot of research have focused their attention in developing alternative materials towards enhancing device performance. To promote the use of thin films for emerging device applications, thin film must be cost effective, highly efficient, eco-friendly, robust and social utility at nanoscale [7-9].

Zinc oxide (ZnO) is a most preferred material among other solid state materials. ZnO have few excellent properties which makes it most desirable material for various practical application such as it is wide band gap semiconductor, piezoelectric properties etc [10, 11]. Moreover, zinc oxide is a very encouraging material due to its excellent physical and chemical properties such as good resistivity (1.3×10^{-4} SI units) [12].

1.1 Heterojunction solar cell

Heterojunction solar cells incorporate two distinct technologies: crystalline silicon sandwiched between two layers of amorphous "thin film" silicon. By combining these technologies, more energy can be harvested than if they were used separately. Literature reveals that crystalline silicon, either mono-crystalline or poly-crystalline, is the material most commonly used to fabricate solar panels. To make individual cells, silicon crystals are grown into blocks and then sliced into thin sheets, frequently using a diamond wire saw [13].

Thin-film photovoltaic cells, which are manufactured with a range of materials, including amorphous silicon, are a less prevalent type of solar cell. Amorphous silicon, unlike crystalline silicon, lacks a regular crystalline structure. Instead, the silicon atoms are organized at random. This allows amorphous silicon to be deposited onto a surface for manufacture, which is a simpler and less expensive method than growing and cutting silicon crystals [14].

Alone, amorphous silicon converts sunlight into electricity less efficiently. However, it has the benefit of less expensive production. On a variety of materials, amorphous silicon can be deposited at a cheaper cost and with a greater degree of versatility.

In heterojunction solar cells, the front and back surfaces of a standard crystalline silicon wafer are coated with amorphous silicon shown in Figure 1. This results in a couple layers of thin film solar that absorb additional photons that would not have been collected by the crystalline silicon wafer in the middle [15].



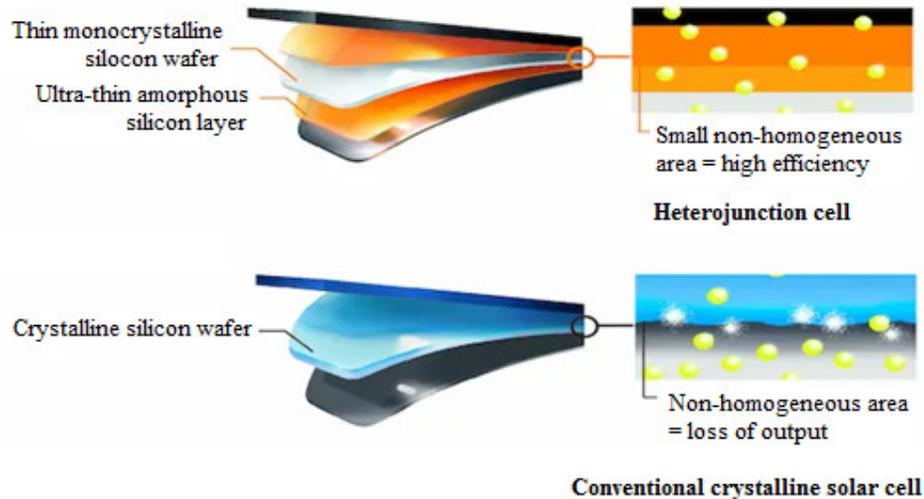


Figure 1: Wafer structure of heterojunction formation [16].

Roy et al. in 2023 studied p-Si/ZnO solar cells with the aid of experimental research and SCAPS 1-D simulation. Spray pyrolysis was used to create thin ZnO layer on the Si substrate. Bandgap of ZnO was estimated from Tauc plot to be approximately 3.29 eV [17]. Similarly, Islam et al. [18] proposed the use of PCBM, C60, CeOX, and ZnO to optimize the efficiency of the different electron transport layers (ETLs) in a SnS-based solar cell. To predict execution of the tin monosulfide situated solar cell, they utilized a solar cell capacitance simulator (SCAPS). With PCBM, C60, and CeOX as ETLs, the devices attained efficiencies of approximately 26.44, 26.33, and 26.44 %, respectively. By integrating ZnO ETL into the design, the PCE of the SnS-based solar cell was increased to 28.15 %. They also evaluated how tin mono-sulfide situated ZnO ETL absorber layer affected by varying the thickness, charge concentration and bulk. Furthermore, the role of defect of the NiOX/SnS and SnS/ZnO interfaces, the work function of the back metal contact, and the operating temperature on the performance of the SnS-based solar cell with ZnO ETL were also examined. It was revealed that changes to any of the device's numerous settings substantially affected its performance. In particular, the SnS-based solar cell's properties such as V_{OC} , I_{SC} , FF and PCE were drastically enhanced [18]. In another work, Naim et al. [19] found the ideal numerical value of the essential photovoltaic parameters for HJ -based c-Si solar cells. The ZnO/Si HJ-based c-Si presented an average reflectance of 7.65% in the 400–1000 nm range. The highest efficiency ($\eta = 24.8\%$) of the ZnO/Si HJ-based c-Si solar was achieved with a base thickness of 400 m, emitter thickness of 20 m, base doping concentration of $1.1 \times 10^{17} \text{ cm}^{-3}$, and emitter doping concentration of $5.1 \times 10^{16} \text{ cm}^{-3}$. The high-efficiency ZnO/Si HJ-based device mentioned is one of the most promising alternatives to the typical single homo-junction c-Si solar cell [19].

2. Experimental techniques

The set of tools and reusable models that Silvaco had previously developed was selected after an in-depth assessment of the available modelling and analytical tools and relevant publications. In present research work "SILVACO Atlas" software is used to modeling and analyses of data. This modelling is used to enhance the efficiency of heterojunction

solar cell and finding different properties of ZnO based solar cell. For a variety of computational analyses, ATLAS can be carried out. It is a framework that can be extended and is modular, and it has the ability to mimic semiconductor devices in one, two, and three dimensions. It is developed with up-to-date practices in software engineering that improve the system's stability, maintainability, and extensibility, and it is implemented [20-23].

2.1 Simulation tools

SCAPS-1D (Solar Cell Capacitance Simulator)
AMPS-1D (Analysis of Microelectronic and Photonic Structures)

2.2 Data collection

The data for present study was collected by "SILVACO Atlas" and "MATLAB" simulation software. We modelled the construction of a solar cell by changing the default parameters to manual and simulating a variety of different layers with varying thicknesses. With the use of this, we are able to gather a collection of data that assists us in calculating the output of a modelled heterojunction solar cell [24-26].

3. Results and discussion

To examine the interface properties further, acceptor traps (a single energy level 0.3 eV below the conduction band) were created at the nZnO/p-c Si hetero-interface. Remember that the conduction and valence bands exchange charge with the trap centers via electron emission and capture; the associated energy of the trap centers resides in a forbidden gap. The trap centers have different effects on the space charge density in the semiconductor bulk, at the interface, and on the recombination statistics depending on where they are located. Simulations have leveraged adjustments in acceptor trap density and electron trap capture cross-section to evaluate the influence on carrier capture and generation rate. For a range of acceptor interface trap densities (with capture cross-sections held stable at 10^{-15} cm^2) and electron capture cross-sections (with acceptor trap density held constant at 10^{11} cm^{-2}), the properties of current by varying voltage are shown in Figure 2. Trap density and electron cross-section are two examples of inefficiencies that lower the fill factor [27].

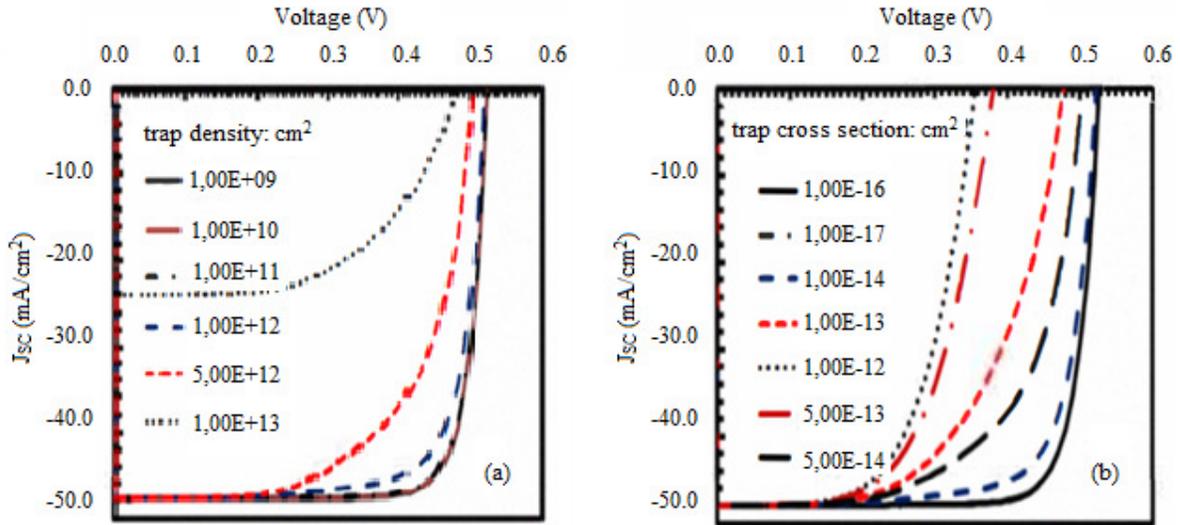


Figure 2: Current density-Voltage (J-V) curve for different: (a) acceptor interface trap density, (b) trap cross-section of n-ZnO/p-cSi HJSC.

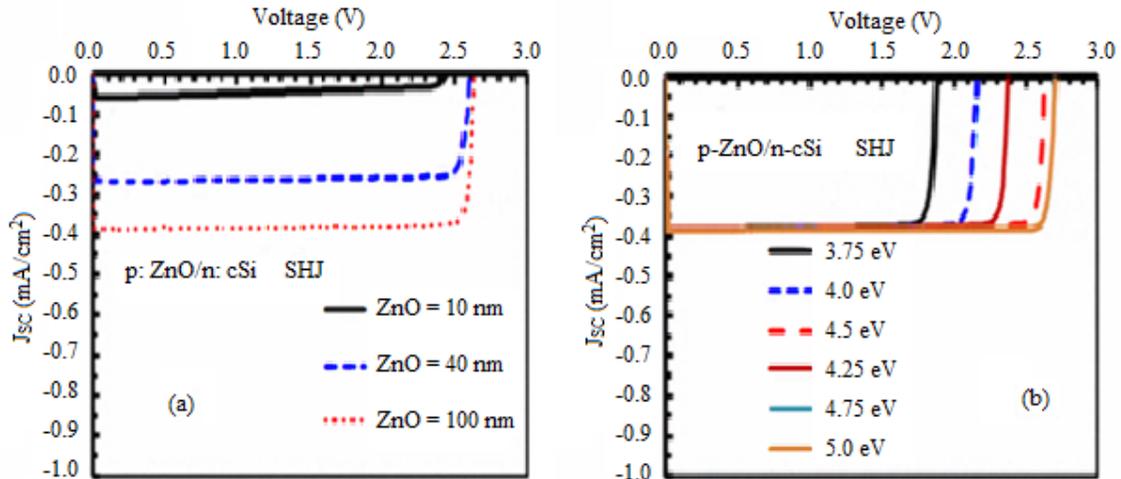


Figure 3: Current density - Voltage (J-V) curve for different thicknesses of the (a) ZnO layer (b) ZnO affinities of p-ZnO/n-cSi HJSC.

Most of the variation in open-circuit voltage and current density can be attributed to differences in trap density. If there are not many traps at the interface, the open circuit voltage will be high. A significant decrease in V_{OC} and J_{SC} is observed for interface trap densities greater than $1 \times 10^{11} \text{ cm}^{-2}$. Significant effects of capture cross-section on V_{OC} and fill factor are seen at large capture cross-sections ($< 1 \times 10^{-14} \text{ cm}^2$) for a constant trap density. We found that trap capture cross-sections for electrons of 10^{-16} , 10^{-10} , 10^{-14} , and 10^{-12} cm^2 resulted in efficiencies of 20.3, 20.0, 18.8, 12.9 and 10.

Simulated photovoltaic performance for a variety of i-ZnO thicknesses & affinity values in a p-ZnO/n-cSi HJ structure is underwhelming (Figure 3). Because the valence band offset for the p-ZnO/n-cSi heterojunction is greater than the conduction band offset, the photo-generated holes cannot cross the huge potential barrier and are lost. The extremely low current density values (1-2% efficiency) obtained by the p-ZnO/n-cSi HJ system are shown in Figure 3. As a result, nZnO/p-cSi has much greater efficiency than p-ZnO/n-cSi. Despite the challenge of producing a high-quality p-doped ZnO layer in actual systems, the current simulation demonstrates that the p-ZnO/n-cSi HJ is applicable to design for optoelectronics

devices. Lastly, a good agreement between the two sets of data after modeling an n-ZnO/p-cSi heterojunction with the same geometrical and physical characteristics as the experimental device ($\eta = 7.83\%$, $J_{SC} = 19.64 \text{ mA/cm}^2$, $V_{OC} = 0.51 \text{ V}$, $FF=0.78\%$) has been found [28].

4. Conclusions

In conclusion of this research study, researchers have been attracted towards the simulation technique to design and analyse the data. Based on this study, it has been accomplished that Si wafer-based n-ZnO/p-cSi and p-ZnO/n-cSi thin film have been design shows that by using simulation method. The composition, geometry, structure, electrical and opto-electrical properties have been optimized. The efficiency, fill factor and J_{SC} of ZnO based solar cell was found to be 7.83%, 0.78% and 19.64. These findings give the opportunity to tune the microstructure for developing the suitable material for several device applications. By using different simulation techniques and precisely optimizing the various process parameters, it is exploring other dopant to achieve higher efficiency. This study will be utilized to demonstrate the comparison and provide

insight into the topic of encouraging environmentally responsible industrial methods. In addition, it is anticipated that this study would represent the beginning of an ongoing body of study in the field of power generation using solar energy. This belief is based on the fact that there is widespread consensus that this initiative will take place.

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Authors' contributions

The author read and approved the final manuscript.

Conflicts of interest

The author declares no conflict of interest.

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Data availability

No new data were created.

References

- [1] C. Wang, L. Yin, L. Zhang, D. Xiang, R. Gao, Metal oxide gas sensors: Sensitivity and influencing factors, *Sensors* **10** (2010) 2088-2106.
- [2] G. F. Fine, L.M. Cavanagh, A. Afonja, R. Binions, Metal oxide semi-conductor gas sensors in environmental monitoring, *Sensors* **10** (2010) 5469-5502.
- [3] A. Dey, Semiconductor metal oxide gas sensors: A review, *Mater. Sci. Eng.: B* **229** (2018) 206-217.
- [4] K. Wetchakun, T. Samerjai, N. Tamaekong, C. Liewhiran, C. Siri Wong, V. Kruefu, A. Wisitsoraat, A. Tuantranont, S. Phanichphant, Semiconducting metal oxides as sensors for environmentally hazardous gases, *Sensors Act. B: Chem.* **60** (2011) 580-591.
- [5] X.S K. Wetchakun, T. Samerjai, N. Tamaekong, C. Liewhiran, C. Siri Wong, V. Kruefu, A. Wisitsoraat, A. Tuantranont, S. Phanichphant K. Wetchakun, T. Samerjai, N. Tamaekong, C. Liewhiran, C. Siri Wong, V. Kruefu, A. Wisitsoraat, A. Tuantranont, S. Phanichphant. Wang, Z.C. Wu, J.K. Webb, Z.G Liu, Ferroelectric and dielectric properties of Li-doped ZnO thin films prepared by pulsed laser deposition, *Appl. Phys. A* **77** (2003) 561-565.
- [6] N. Shakti, P.S. Gupta, Structural and optical properties of sol-gel prepared ZnO thin film, *Appl. Phys. Res.* **2** (2010) 19-28.
- [7] J.S. Bhat, A.S. Patil, N. Swami, B.G. Mulimani, B.R. Gayathri, N.G. Deshpande, G. H. Kim, M.S. Seo, Y.P. Lee, Electron irradiation effects on electrical and optical properties of sol-gel prepared ZnO films, *J. Apply. Phys.* **108** (2010) 0453513.
- [8] E. Abd El-Wahabb, A.E. Bekheet, Effect of annealing on optical properties of Ag₃₃Sb₃₁Se₃₆ thin films, *Appl. Surf. Sci.* **173** (2001) 103-114.
- [9] B. Hussain, A. Ebong and I. Ferguson, Zinc oxide and silicon based heterojunction solar cell model, *2015 IEEE 42nd Photovoltaic Specialist Conference (PVSC)*, New Orleans, LA, USA (2015), pp. 1-4.
- [10] L.W. Zhong, Zinc oxide nanostructures: growth, properties and applications, *Cond. Matter* **16** (2004) R829-R858.
- [11] A. Remhof, D. Labbergerie, G. Song, C. Shutter, K. Theis-Brohl, H. Zabel, et al., Hydrogen in thin epitaxial metal films and superlattices: Structure, magnetism, and transport, *J. Magnet. Magnetic Mater.* **198** (1999) 264-266.
- [12] V. Bhosla, A. Tiwari, J. Narayan, Electrical properties of transparent and conducting Ga doped ZnO, *J. Appl. Phys.* **100** (2006) 33713.
- [13] B.K. Mondal, M.A. Newaz, M.A. Rashid, K.M. Hossain, S.K. Mostaque, M.F. Rahman, M.H.K. Rubel, J. Hossain, Electronic structure of In_{3-x}Se₄ electron transport layer for chalcogenide/p-Si heterojunction solar cells, *ACS Omega* **4** (2019) 17762-17772.
- [14] K. Yoshikawa, H. Kawasaki, W. Yoshida, T. Irie, K. Konishi, K. Nakano, T. Uto, D. Adachi, M. Kanematsu, H. Uzu, K. Yamamoto, Silicon heterojunction solar cell with interdigitated back contacts for a photo conversion efficiency over 26%, *Nat. Energy* **2** (2017) 17032.
- [15] J. Tersoff, Theory of semiconductor heterojunctions: The role of quantum dipoles, *Phys. Rev. B* **30** (1984) 4874.
- [16] <https://industry.panasonic.eu/panasonic-industry-news/heterojunction-technology-increased-solar-yield>
- [17] A. Roy, M. Benhaliliba, Investigation of ZnO/p-Si heterojunction solar cell: Showcasing experimental and simulation study, *Optik* **274** (2023) 170557.
- [18] M.E. Islam, M.R. Islam, S. Ahmmed, M.K. Hossain, M.F. Rahman, Highly efficient SnS-based inverted planar heterojunction solar cell with ZnO ETL, *Physica Scripta* **98** (2023) 065501.
- [19] H. Naim, D.K. Shah, A. Bouadi, M.R. Siddiqui, M.S. Akhtar, C.Y. Kim, An in-depth optimization of thickness of base and emitter of ZnO/Si heterojunction-based crystalline silicon solar cell: A simulation method, *J. Electron. Mater.* **51** (2022) 586-593.
- [20] K. Zeghdar, L. Dehimi, F. Pezzimenti, S. Rao, F.G. Della Corte, Simulation and analysis of the current-voltage-temperature characteristics of Al/Ti/4H-SiC Schottky barrier diodes, *Jpn. J. Appl. Phys.* **58** (2019) 014002.
- [21] H. Bencherif, L. Dehimi, F. Pezzimenti, G. De Martino, F.G. Della Corte, Multiobjective optimization of design of 4H-SiC power MOSFETs for specific applications, *J. Electron. Mater.* **48** (2019) 3871-3880.
- [22] S. Selberherr, *Analysis and Simulation of Semiconductor Devices*, Springer, Vienna, Austria (1984).
- [23] M.L. Megherbi, F. Pezzimenti, L. Dehimi, A. Saadoun, F.G. Della Corte, Analysis of the forward I-V characteristics of Al-implanted 4H-SiC p-n diodes with modeling of recombination and trapping effects due to intrinsic and doping-induced defect states, *J. Electron. Mater.* **47** (2018) 1414-1420.
- [24] F. Bouzid, F. Pezzimenti, L. Dehimi, M.L. Megherbi, F.G. Della Corte, Numerical simulations of the electrical transport characteristics of a Pt/n-GaN Schottky diode, *Jpn. J. Appl. Phys.* **56** (2017) 094301.
- [25] D. Guo, D. Vasileska, 1D fast transient simulator for modeling CdS/CdTe solar cells, *Proc. IEEE, 39th Photovoltaic Specialists Conference, PVSC* (2013) 1961-1965.
- [26] D.B.M. Klaassen, A unified mobility model for device simulation-II: Temperature dependence of carrier mobility and lifetime, *Solid-State Electron.* **35** (1992) 961-967.
- [27] N. Johrin, F.P. Chee, S. Nasir, P.Y. Moh, Numerical study and optimization of GO/ZnO based perovskite solar cell using SCAPS, *AIMS Energy*, **11** (2023) 683-693.
- [28] J. Gulomov, O. Accouche, Z. Al Barakeh, R. Aliev, I. Gulomova, B. Neji, Atom-to-device simulation of MoO₃/Si heterojunction solar cell, *Nanomaterials* **12** (2022) 4240.