

Design of ZnO/Si heterojunction solar cell using solar cell capacitance simulator

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Received 17 March 2025; accepted 11 July 2025

This study explores the optimization of ZnO/Si heterojunction solar cells to enhance device performance using a Solar Cell Capacitance Simulator. Solar cells have a lot of potential for converting solar energy into electricity efficiently & affordably. With the help of computational modeling, we study zinc oxide (ZnO) and Si Heterojunction (HJ) in order to enhance the device performance. By employing numerical methods such as, including drift-diffusion modeling and optical simulations, the charge transport within the heterojunction solar cells have been investigated. The effects of parameter variations on the device efficiency have been systematically explored and design approaches are identified to enhance the power conversion efficiency. This study investigates the performance of a ZnO-based solar cell, focusing on its electrical characteristics. The results show a short circuit voltage of 0.52 V, a current density of 19.64 mA/cm², and a fill factor of 0.78%. The power conversion efficiency of the ZnO-based solar cell is found to be 7.83% indicating its promising potential for application in solar energy conversion.

Keywords: Numerical methods, Power conversion efficiency, Simulation design, ZnO/Si heterojunction solar cell

Introduction

Solar energy is one of the forms of clean and renewable energy that may be used to generate both power and clean fuels. Solar cells are able to harvest the limitless energy of the sun and transform it into electricity through a process known as the photovoltaic (PV) effect, which has received a lot of attention from researchers as of late¹. In recent years, the heterojunction solar cells (HJSCs) have attracted research and industrial interest due to their promise of high efficiency at an affordable price². These HJSCs are comprised of two or more distinct materials, each having bandgap energy. The interface between these materials produces a voltage by separating the photo-generated electron-hole pairs. ZnO-based Si HJSCs are a desirable alternative due to their high electron affinity & large bandgap of ZnO, which allow for an increase in the cell's power conversion efficiency^{3,4}. Optimization and design of HJSCs involves of a variety of materials and configurations have been the subject of many research groups⁵⁻⁹. Mohr *et al.* showed that a Si/nanocrystalline-Si PV system has a life cycle of 2.3 years to 3.4 years with an efficiency 14.4%¹⁰. Kim *et al.* have investigated that Nc-Si/a-Si

module have efficiency 6.3%- 8% and life cycle 0.7 – 0.8 years^{11,12}. The optimization of layer thickness ZnO based perovskite solar cell allowed for the increased charge transport, efficiency, fill factor, low resistance leading to design novel charge transport materials and high performance optoelectronics devices^{13,14}. Numerical simulations have also been utilized to design & improve the performance of ZnO-based Si HJSCs. One study discovered that the n-ZnO/p-Si single HJSC's performance may be enhanced by tuning ZnO's electron affinity & bandgap¹⁵. This is done by modifying electron affinity and bandgap of the ZnO layer could enhance the simulation performance of the solar cell¹⁶. Computer models have also been employed to examine the impact of the ZnO layer's thickness on the output of the solar cell. According to modeling research, the optimal ZnO layer thickness is dependent on the Si layer's doping level¹⁷. Various materials & architectures such as ZnO/CdS/CuInSe₂ and SiC/Si HJSCs explored for HJSCs to increase their efficiency & general design¹⁸. A simulation study established that solar cell efficiency could be improved by varying thickness of the CdS layer in this design of a HJSC¹⁹. ZnO is more

efficient than cSi because it functions as a window for light transmission. The open circuit voltage (V_{oc}), acquiescence of surface & grain boundaries play the important role to reduce the dark current of the present material²⁰. In contrast to many other transparent conductive defect oxide (TCO) materials, ZnO films offer the desired electrical and optical qualities at a reasonable cost. Because of their double-band electronic structure, ZnO/Si HJSCs can efficiently absorb solar light. High-energy ultraviolet and visible photons are captured in the p-Si depletion zone after passing through the ZnO layer and are then absorbed by the material^{21,22}.

In the present study, ZnO-based Si HJSCs have been developed and optimized by using solar cell capacitance simulations method. The simulation results cast light on how ZnO-based Si HJ can be used to construct solar cells with high efficiency. The present research focuses on the simulation-based study aimed at enhancing the efficiency of heterojunction solar cells (HSCs), which combine crystalline and amorphous silicon layers to improve photovoltaic performance. The model was designed to analyze the impact of various parameters on key performance metrics²³⁻²⁶.

Experimental Section

In the present study "SILVACO Atlas" simulation software is used for modeling heterojunction solar cells.

Simulation tools

SCAPS-1D (Solar Cell Capacitance Simulator) tool is used to analyzed & designs n-ZnO/p-cSi and p-ZnO/ncSi-based HJSCs.

Basic Principle of Solar Cell Capacitance Simulator (SCAPS) 1D SCAP

1-D SCAP discretized device with length L into N intervals and N + 1 major grid points, which may or may not be uniform. It solves numerically using Poisson's equation and continuity equations at each grid point with the correct boundary conditions. After solving for the three variables E_{Fn} , and E_{Fp} at each specific grid point from 1 to N+1, which are depicted by solid lines under the light, voltage and temp conditions and defining additional variables including the electric field, carrier concentration, or trapped charges, it is possible to determine the recombination profiles, electron and hole current densities and other transport data. Using the formula $J(x) = J_n(x) + J_p$, we can determine the total JV characteristic (x) This includes not only the I-V characteristics, but also the

spectral response $Q(h)$ as well as the C-V and C-F capacitance measurements. In the present study, the charge transport mechanism of ZnO-based Si HJSCs is analyzed. In order to optimize the device design, various parameters such as ZnO layer thickness, doping concentration, and interface properties are studied. Optical simulations are utilized to evaluate the light absorption characteristics of the HJSC. Finally, the device design approaches and strategies are identified to enhance the power conversion efficiency of ZnO-based Si HJSCs. The layer designs of the n-ZnO/p-cSi and p-ZnO/ncSi-based HJSCs employed in the theoretical design investigation. A 200 nm thick layers of cSi and n/p doped ZnO were designed. Aluminum (Al) metal that was 100 nm thick was used as a conductive electrode. The details of the ZnO/cSi modeling parameters are shown in Table 1¹⁹.

Results and Discussion

The energy band diagrams of the single HJ of n-ZnO/p-cSi and p-ZnO/n-cSi are shown in Fig. 1. The majority of the energy offset for both structural types happen in the valence band. The Anderson model, often known as the "electron affinity model," is employed in this study because it ignores lattice mismatch & instead links the conduction band discontinuities with the different electron affinities of the two semiconductor materials. The valence band calculated in this work has a substantial discontinuity as well. It is possible that the analyzed structures have bottlenecks that prohibit photogenerated holes from reaching & being collected at their appropriate device contact. The relationship between the current density & external quantum efficiency for various n-ZnO/pcSi HJ layer thicknesses is shown in Fig. 2. Despite thicker layers having lower open circuit voltages, the thickness of the ZnO had no impact on current density. Note that the ZnO devices exhibit higher external quantum efficiencies at short wavelengths than the reference Si devices due to higher absorption^{9,27}.

Table 1 — Modeling Parameters used in the simulation

Parameters	ZnO	cSi
E_g (eV)	3.3	1.08
n/p doping (cm^{-3})	1×10^{19}	1×10^{15}
χ (eV) variable	3.8-5.0	4.18
τ_e, τ_h (sec)	1×10^{-9}	1×10^{-3}
μ_n ($cm^2/V.s$)	60	1000
μ_h ($cm^2/V.s$)	10	500
DOS (N_c) (cm^{-3})	2.2×10^{18}	2.8×10^{19}
DOS (N_v) (cm^{-3})	1.8×10^{19}	1.04×10^{19}

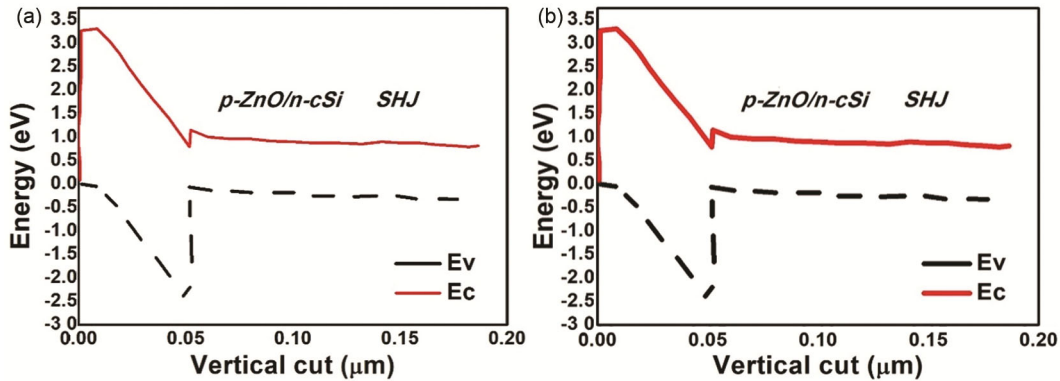
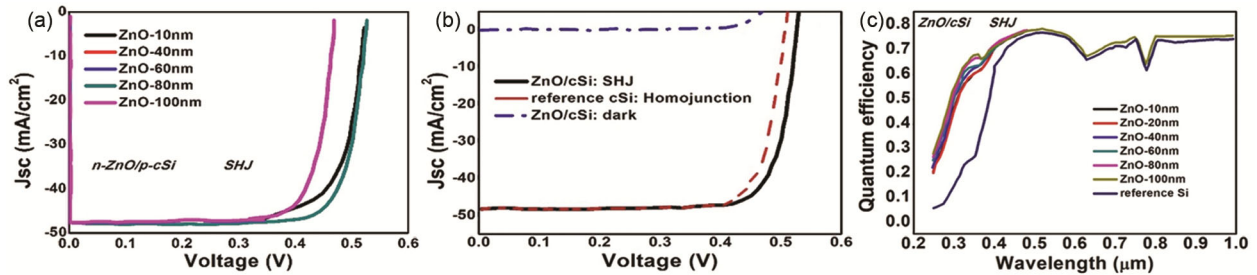


Fig. 1 — Energy band diagram of n-ZnO/p-cSi & pZnO/n-cSi SHJ

Fig. 2 — (a) Variation of Current density with voltage of the n-ZnO/p-cSi SHJ for different thickness, (b) comparing the dark characteristics with homojunction cSi reference device and (c) The variation of quantum efficiency with increasing wavelength (in μm)

The electrical property of the interface between ZnO and c-Si are critical to the performance of HJSCs. The interface lies within the space charge zone, making its qualities critical to the solar cell's overall efficiency. Before the deposition or development of the thin ZnO films, microscopically smooth crystalline silicon (cSi) surface must be provided in order to lower the defect density D_{it} to a safe level (typically below 10^{11} cm^{-2}). Research into effective surface cleaning technologies is essential to reduce the micro-roughness & density of states of cSi. The presence of stretched bonds & broken/dangling bonds at the cSi surface causes the band gap to have several electronic states, similar to the interface between two distinct materials (like ZnO and Si). Additional electronic states are induced in the band gap of a native oxide when it is exposed to hydrogen and oxygen in the atmosphere. The existence of surface states & traps at the interface of the HJ as a result of the lattice mismatch of Si and ZnO & the difference in thermal expansion coefficients among the two materials at ambient temperature have been studied in previous publications on n-ZnO/p-cSi HJ. These interface states, sometimes termed interface traps, which act as effective recombination hotspots, diminish potential current density & solar cell

efficiency. The performance of solar cells can be greatly improved by using high-quality float zone Si wafers, but surface recombination at the metal- or semiconductor-semiconductor interface still presents a substantial challenge⁸.

The simulation involves the application of fixed positive charges at the hetero-interface to represent recombination at the n-ZnO/p-cSi interface. The current density basically remains the same but the open circuit voltage lowers when additional fixed charges are added to the crystalline surface. Given a range of interface charges, Fig. 3 shows how short circuit voltage (V_{oc}), efficiency and Fill factor drop as recombination velocity increases. The fill factor, V_{oc} and efficiency are essentially unaffected by the interface charge up to $5.0 \times 10^3 \text{ cm}^2/\text{sec}$. Starting at relatively low recombination velocities, increasing the interface charge results in a progressive decrease in open circuit voltage, fill factor & efficiency²⁸.

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-cSi hetero-interface. Remember that the conduction and valence bands exchange charge with the trap centers via electron emission & capture; the associated energy of the trap centers resides in a forbidden gap. The trap

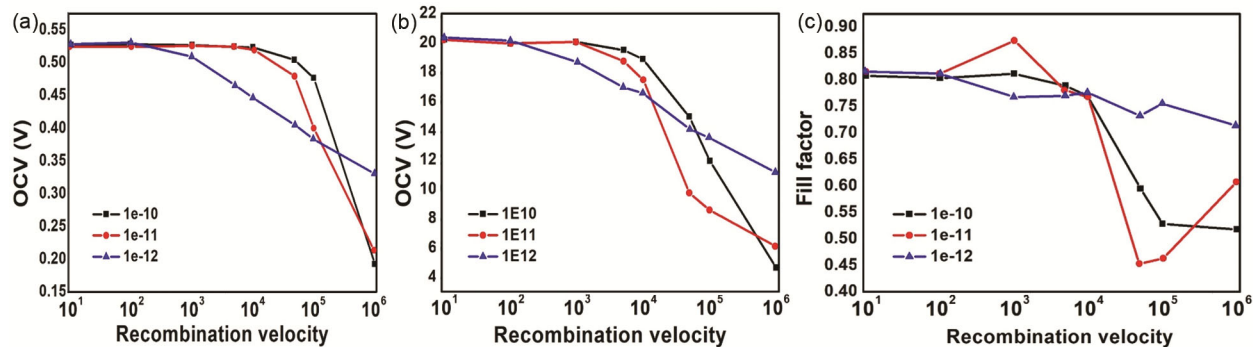


Fig. 3 — a) V_{OC} , (b) efficiency and (c) fill factor by varying interface recombination velocity for various fixed interface charge densities at the heterojunction of n-ZnO/p-cSi solar cell

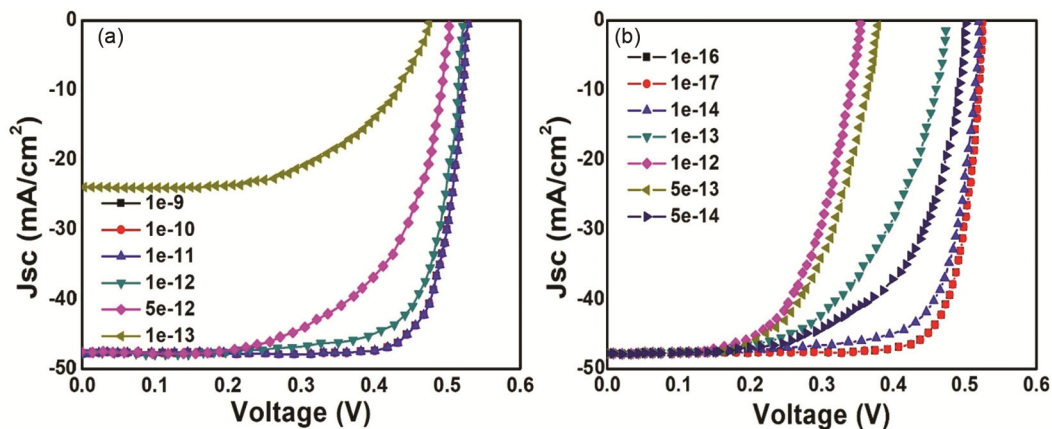


Fig. 4 — Current density-Voltage ($J-V$) curve for different (a) acceptor interface trap density and (b) trap cross-section of n-ZnO/p-cSi HJSC

centers have different effects on the space charge density in the semiconductor bulk, at the interface, & 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 Fig. 4. Trap density and electron cross-section are two examples of inefficiencies that lower the fill factor².

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} & 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 (Fig. 5). Because the valence band offset for the p-ZnO/n-cSi heterojunction is greater than the conduction band offset, the photogenerated holes cannot cross the huge potential barrier & are lost. The extremely low current density values (1-2% efficiency) obtained by the p-ZnO/n-cSi HJ system are shown in Fig. 5. 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 & physical characteristics as the

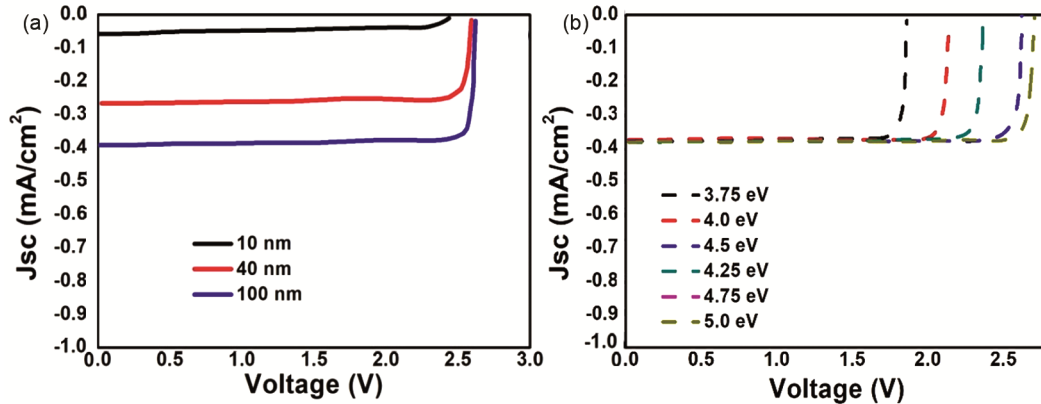


Fig. 5 — Current density- Voltage (J-V) curve for different thicknesses of the (a) ZnO layer and (b) ZnO affinities of p-ZnO/n-cSi HJSC

experimental device ($\eta=7.83\%$, $J_{sc}=19.64 \text{ mA}/\text{cm}^2$, $V_{oc}=0.51 \text{ V}$, $FF=0.78\%$) has been found³.

Conclusion

In conclusion, Si wafer-based n-ZnO/p-cSi and p-ZnO/ncSi-based HJSCs have been designed and were simulated using solar cell capacitance simulation method with experimental data taken from literature. Solar cell structures have been optimized in terms of ETL, ZnO thickness, doping concentration, and interface properties. The optimized solar cell achieved a $V_{oc} = 0.51 \text{ V}$, $J_{sc} = 19.64 \text{ mA}/\text{cm}^2$, $FF = 0.78\%$ and $PCE = 7.83\%$, which is promising for photovoltaic device application. Notably, the highest efficiency of solar cells is attained with ZnO at affinities between 4.0 to 4.5, consistent with experimental and numerical data reported in the literature. The findings in the present work highlight the importance of energy band alignment and interface engineering to achieve stable and high performance ZnO-based Si HJSCs. These results suggest a viable route to efficiently and cost-effectively develop ZnO-based Si HJ solar cells, which is a step toward the ultimate goal of producing silicon-based photovoltaic technology for sustainable & clean energy generation.

Acknowledgements

The data analysis of the present materials/device (heterojunction solar cell) was done at Prerna Society of Technical Education and Research, New Delhi and Research lab, Department of Physics, School of Physical Sciences, Starex University, Gurugram. The authors greatly acknowledge the facilities extended by them for the present work.

Conflict of interest

The authors declare no conflict of interest.

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