TCAD Based Assessment and Performance Optimization of ZnO/Si Heterojunction Based Thin-film Solar Cell

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Abstract: In this paper 2D numerical simulation of n-ZnO/i-ZnO/p-Si p-i-n heterojunction solar cell using TCAD has been presented. In this work the design and performance optimization of p-i-n heterojunction solar cell using two-dimensional computer aided design (TCAD) tool has been presented. The device has been simulated and analyzed with respect to the I-V characteristics of the device in dark and illuminated condition. Further figure of merits like short circuit current (I_{sc}), Open circuit Voltage (V_{oc}), fill factor (FF), internal and external quantum efficiency (IQE &EQE), maximum power generated (P_{max}) and conversion efficiency of the designed solar cell has been extracted. The I-V characteristics of the device and performance in terms of power conversion efficiency has been optimized for the proposed structure of solar cell with respect to doping concentration in n-ZnO and i-region thickness of the device. The simulation results indicate that the n-ZnO/i-ZnO/p-Si p-i-n heterojunction solar cell could be a good candidate for solar cells.

Keywords: TCAD, Heterojunction, Solar cell, ZnO, Numerical simulation.

1. INTRODUCTION

Recently research interest of the researchers in the area of renewable energy is increasing. Thin film based solar cell is one of the important area of interest of the researchers and zinc oxide (ZnO) semiconductor materials are of great interest for solar cell applications [1-33]. Interest in ZnO is due to its promise in optoelectronic applications because of its direct wide bandgap (Eg ~ 3.3 eV at 300K) [1]. ZnO is a very interesting material due to its high transmittance in the visible region and its high chemical, thermal and mechanical stability. The use of ZnO in optoelectronic devices has the advantage that high quality ZnO thin films and polycrystalline zinc oxide thin films can be grown at room temperature [2]. In addition to the intense UV light response, the ability to operate at high temperatures and harsh environments makes ZnO particularly interesting for many applications. Since zinc oxide has a wide band gap, low resistivity and high transparency it can be used as a window layer in ZnO/Si heterojunction solar cell. Above properties of ZnO material provide advantages such as excellent response to blue light, easy processing steps, low temperature treatment and non-toxicity [3]. The ZnO has many advantages, due to which it is currently used in the short wavelength optoelectronics. A binding energy of about 60 meV, a higher radiation hardness, a step for simplified processing, the ability to adapt to the chemical wet etching, non-toxic and relatively low deposition temperature is a part of these benefits. Since systematic experimental investigation of the microelectronic devices demands huge cost and large amount of time, technology computer aided design (TCAD) becomes very important for investigation of these devices [6-36]. In this paper effect of thickness of i-ZnO on efficiency of ZnO based thin film solar cell has been studied and optimized. Also the effect of doping concentration of n-ZnO layer on efficiency of the device has been studied and optimized.

2. PROPOSED DEVICE STRUCTURE

Crystalline silicon was doped with p-type of impurity with the doping concentration of 1×10^{15} and ZnO is doped with n-type impurity with the doping concentration of 1×10^{20}. A very thin layer of intrinsic Zinc Oxide (ZnO) is sandwiched between p-Si and n-ZnO and slightly n-type doped with concentration of 1×10^{12}.

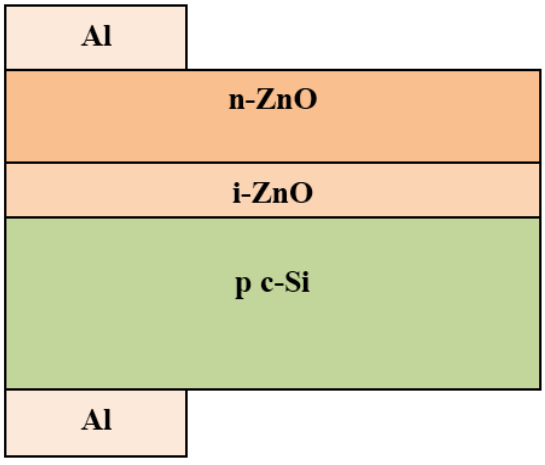

Figure 1: Schematic Structure of ZnO/cSi based single heterojunction used in simulation.

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Intrinsic ZnO layer provides high electric field to separate exciton pair at cathode and anode. Aluminum electrode is used on top and bottom. The device structure is shown in Figure **1**.

3. DEVICE SIMULATION

For our modeling and simulation study, a commercially available device simulator ATLAS was used which is a physically based, numerical device simulator [10-14]. ATLAS from SILVACO international, is a physics-based, two and three dimensional device simulator that predicts the device's electrical behavior and enables the design of microelectronic devices. It also provides significant insight into the mechanisms involved in device operation in that it can provide a two dimensional profile of carrier concentration, electric potential profiles, electric field lines and current density profiles [10-14]. A complete documentation of ATLAS can be found in the available manual from Silvaco International [30]. The set of fundamental equations solved by ATLAS are Poisson's equation, the continuity equations and the transport equations. The solution of Poisson's equation and continuity equation that are a set of coupled, partial differential equations which is solved numerically with the help of ATLAS software for obtaining terminal characteristics of the microelectronic devices is as below [10-14]

Poisson's Equation

Poisson's Equation provides relation between variations in the electrostatic potential and local charge density of electrons and holes. It is mathematically described by the following relation [10-14]

$$\nabla.(\varepsilon\nabla\psi) = -\rho \tag{1a}$$

$$\nabla.(\varepsilon\nabla\psi) = -q\left(p - n + N_d^+ - N_a^-\right) \tag{1b}$$

where ψ is the electrostatic potential, ρ is the local space charge density, ε is the local permittivity of the semiconductor (F/cm), N_d^+ is the ionized donor density (cm^{-3}), p is the hole density (cm^{-3}), n is the electron density (cm^{-3}) and N_a^- is the ionized acceptor density (cm^{-3}). The reference potential is still considered to be the intrinsic Fermi potential for ATLAS simulation [30]. Exposure to crystal defects, which can be caused by the presence of dangling bonds at the interface, or through impurities in the substrate semiconductor material. The presence of these defect centers or traps on the semiconductor substrate can significantly affect the electrical characteristics of the device. To account for the trapped charge, Poisson's equations are modified by adding an additional term Q_T, representing trapped charge given in (1c) [10-14].

$$\nabla.(\varepsilon\nabla\psi) = -q\left(p - n + N_d^+ - N_a^-\right) - Q_T \tag{1c}$$

where $Q_T = q\left(N_{tD}^+ + N_{tA}^-\right)$.Here N_{tD}^+ and N_{tA}^- are ionized density of donor like traps and ionized density of accepter like traps respectively.

Continuity Equations

For electrons and holes, the continuity equations are defined as follows [10-14]

$$\frac{\partial n}{\partial t} = \frac{1}{q}\nabla.J_n + G_n - R_n \tag{2}$$

$$\frac{\partial p}{\partial t} = -\frac{1}{q}\nabla.J_p + G_p - R_p \tag{3}$$

where n and p are the electron and hole concentrations, J_n and J_p are the electron and hole current densities, G_n (R_n) and G_p (R_p) are the generation (recombination) rates for the electrons and holes, respectively and q is the fundamental electronic charge.

Transport Equations

The drift-diffusion model is described as follows [10-14]

$$J_n = qn\mu_n E_n + qD_n\nabla n \tag{4}$$

$$J_p = qn\mu_p E_p - qD_p\nabla p \tag{5}$$

where μ_n and μ_p are the electron and hole mobilities, D_n and D_p are the electron and hole diffusion

Table 1: Parameter Used During Simulation

Parameter Used	Value
Thickness of n-ZnO layer	0.20 micron
Thickness of p-type i-ZnO layer	0.01 micron
Thickness of p-Si layer	49.79 micron
n-type doping [cm^{-3}]	1×10^{20}
p-type doing [cm^{-3}]	1×10^{15}
Bandgap of ZnO [eV]	3.37
Bandgap of Si [eV]	1.12
Affinity of ZnO [eV]	4.65
Affinity of Si [eV]	4.05
NC300 [cm^{-3}]	9×10^{18}

constants, E_n and E_p are the local electric fields for electrons and holes, respectively, and ∇_n and ∇_p are the three dimensional spatial gradient of n and p.

Parameters used in simulation are given in the following table.

4. RESULTS AND DISCUSSION

After simulation of above described solar cell following results were obtained: Figure **2**. Shows I-V characteristics in dark and illuminated condition of the n-ZnO/i-ZnO/p-Si p-i-n heterojunction solar cell. Figure **3** shows the spectral response of the solar cell. Figure **4** shows the variation of internal and external quantum efficiency of the solar cell with wavelength. Function1 represents external quantum efficiency and function 2 represents internal quantum efficiency of the solar cell under discussion. About 99% internal quantum efficiency is achieved in UV region and 90% internal quantum efficiency is achieved in visible region. External quantum efficiency is about 90% in UV region and 80% in visible region.

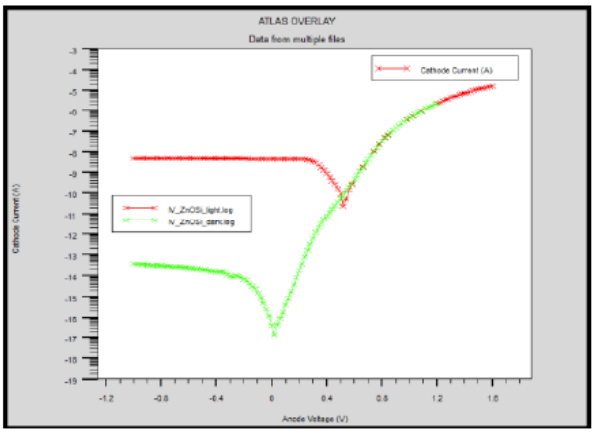

Figure 2: I-V characteristics in dark and illuminated condition of the n-ZnO/i-ZnO/p-Si p-i-n heterojunction solar cell.

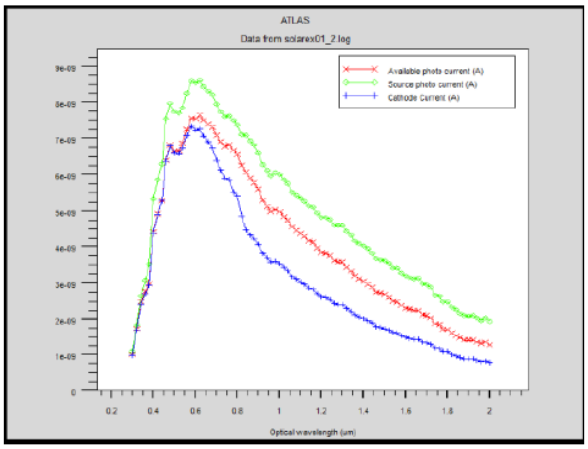

Figure 3: Spectral response of the solar cell.

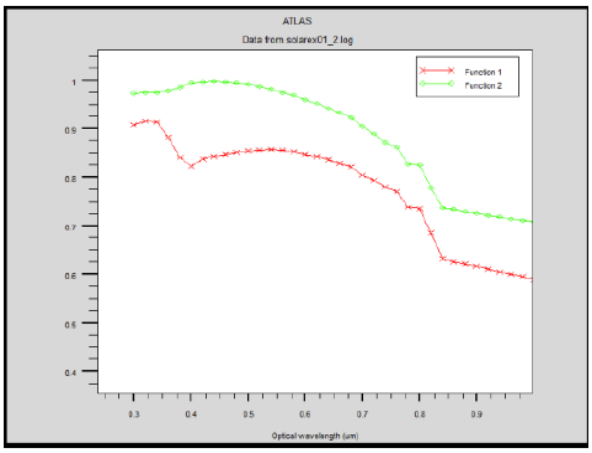

Figure 4: variation of internal and external quantum efficiency of the solar cell with wavelength.

A. Effect of Thickness of i-ZnO on Output Parameters

In the proposed device structure intrinsic layer inserted between n-ZnO and p-Si creates high electric field that contributes in separation of electron-hole pair at junction hence reduces the recombination loss. This intrinsic layer contributes in enhancing the efficiency. Effect of thickness of intrinsic layer on efficiency has been studied and data are as follows:

Figure **5:** shows variation of efficiency of solar cell with intrinsic layer thickness of the solar cell.

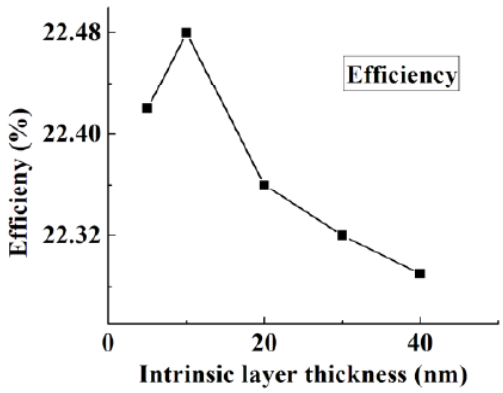

Figure 5: Graph of Efficiency vs thickness of i-ZnO.

B. Effect of doping concentration of n-ZnO layer on Output Parameters

Doping concentration of n-ZnO layer also affect the efficiency of the device. Study has been done to optimize the doping concentration of n-ZnO by simulating the device structure for different doping concentrations. Output recorded for different doping concentration is as follows:

Table 2: Variation in Efficiency with Respect to I-Zno Thickness

S. No	Thickness of intrinsic Layer (nm)	V_{oc} (V)	I_{sc} (A)	FF	P_{max} (W)	I_m(A)	V_m (V)	η (%)
1.	5	0.468	4.28×10^{-9}	76.80	1.5×10^{-9}	4.01×10^{-9}	0.379	22.42
2.	10	0.463	4.3×10^{-9}	76.98	1.5×10^{-9}	4.01×10^{-9}	0.38	22.48
3.	20	0.463	4.27×10^{-9}	76.72	1.5×10^{-9}	4.00×10^{-9}	0.38	22.36
4.	30	0.463	4.27×10^{-9}	76.63	1.5×10^{-9}	3.99×10^{-9}	0.379	22.32
5.	40	0.463	4.26×10^{-9}	76.53	1.5×10^{-9}	3.98×10^{-9}	0.38	22.29

Table 3: Effect on Doping on Efficiency

S. N.	Doping (Cm^{-3})	V_{oc} (V)	I_{sc} (A)	FF	P_{max} (W)	I_m (A)	V_m (V)	η (%)
1	1×10^{17}	0.463	4.26×10^{-9}	76.52	1.51×10^{-9}	4.03×10^{-9}	0.38	22.26
2	1×10^{18}	0.463	4.27×10^{-9}	76.72	1.520×10^{-9}	4.00×10^{-9}	0.38	22.35
3	1×10^{19}	0.463	4.27×10^{-9}	76.72	1.52×10^{-9}	4.00×10^{-9}	0.38	22.37
4	1×10^{20}	0.46	4.30×10^{-9}	76.98	1.53×10^{-9}	4.02×10^{-9}	0.38	22.48
5	1×10^{21}	0.46	4.28×10^{-9}	76.70	1.52×10^{-9}	4.00×10^{-9}	0.38	22.30

Figure **6** shows the variation of efficiency with n-ZnO layer doping.

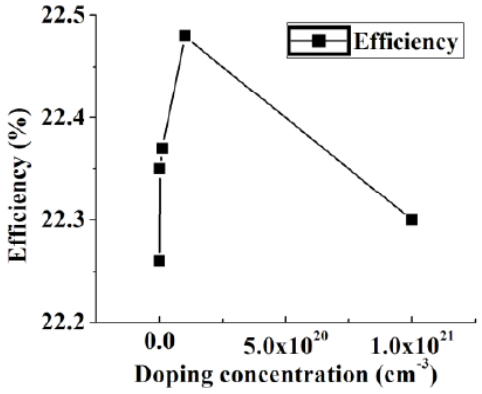

Figure 6: Variation in Efficiency with n-ZnO layer Doping.

On the basis of above presented database the designing parameter of proposed device structure is optimized as follows:

As we can see from above tables that the maximum efficiency is obtained for thickness of 10 nm of i-ZnO layer and other output parameters such as fill factor, maximum power, open circuit voltage, short circuit current, maximum voltage, maximum current remains almost constant. Hence the value of thickness of intrinsic layer is optimized to 10 nm. Similarly, the doping of n-ZnO is optimized to 10×10^{20}.

Table 4: Optimized Parameters

Parameter Used	Value
Thickness of n-ZnO layer	0.20 micron
Thickness of p-type i-ZnO layer	0.01 micron
Thickness of p-Si layer	49.79 micron
n-type doping [cm^{-3}]	1×10^{20}
p-type doing [cm^{-3}]	1×10^{15}

CONCLUSION

By the simulation of proposed structure of n-ZnO/i-ZnO/Si p-i-n heterojunction solar cell, Open Circuit Voltage (V_{oc}) of 0.463 V, Short Circuit Current (I_{sc}) is 4.3×10^{-9} Ampere, Fill Factor (FF) is 76.98%, Maximum Voltage (V_{max}) is 0.38 V, Maximum Current (I_{max}) is 4.024×10^{-9} A and overall efficiency is 22.48% was achieved. It has been also observed that the proposed device structure absorbs more in Ultra-Violet (UV) region. Proposed device structure is comparatively smaller in size hence cost effective too. Tandem solar cell structure for proposed device can also be designed and analyzed for better efficiency. This structure can also be analyzed with anti-reflection coating on top and reflecting coating at bottom.

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