Journal of Materials, Processes and Environment
December edition. Vol.4. N°2. (2016)
ISSN : 2335-1020

Simulation study and analysis of $ZnO/SiO_2/Si$ SIS heterojunction solar cell

N. Ziani[1], F. Bouaraba[1], M.S. Belkaid[1]

[1.] Laboratoire des Technologies Avancées de Génie Electrique (LATAGE), Département d'Electronique, Université Mouloud MAMMERI de Tizi-Ouzou, Algérie

ABSTRACT — In this paper simulation study with the design evaluation of n-ZnO/SiO_2/p-Si and n-ZnO/SiO_2/n-Si heterojunction solar cells using two dimensional numerical computer aided design tool (TCAD). A program in ATLAS simulator from SILVACO international has been developed. The device performance is evaluated by implementing special models (i.e., surface recombinations, thermionic field emission tunneling model for carrier transport at the heterojunction etc) at the semiconductor-semiconductor interfaces. A current density of 22,15 mA/cm^2, open circuit voltage of 0,46 V and fill factor of 31% was achieved for n-ZnO/SiO_2/p-Si heterojunction. Contrary to n-ZnO/SiO_2/p-Si structure, n-ZnO/SiO_2/n-Si SIS heterojunction shows poor photovoltaic response and low Voc because higher barrier height for the ZnO/SiO_2/n-Si. Simulation results give dark current of the order of 10^{-11} A for both types of structures.

Keywords: *Simulation, solar cell, $ZnO/SiO_2/Si$, SIS heterojunction, Atlas silvaco.*

I. Introduction

As shown in a previous paper, semiconductor-insulator-semiconductor (SIS) diodes have certain features which make them more attractive for solar energy conversion than conventional Schottky diode, metal-insulator-semiconductor (MIS), or heterojunction structures [1]. The SIS structure is potentially more stable and theoretically more efficient than either a Schottky or an MIS structure. The origins of this potential superiority are the suppression of majority-carrier tunneling in the high potential barrier region of the SIS structure, and the existence of a thin interface layer which minimizes the amount and impact of interface states. This results in an extensive choice of the p-n junction partner with a matching band gap in the front layer. In addition, the top semiconductor thin film can serve as an antireflection coating, a low-resistance window, as well as the collector layer of the junction [2].

Corresponding author: Nora Ziani
Research field: Materials and Environment
E-mail: nziani14@gmail.com

Moreover, the SIS structure with a wide gap semiconductor as the top layer eliminates the surface dead layer associated with homojunction devices. This absence of absorption in the surface dead layer improves the ultraviolet response.

In a device such as the SIS diode, the two semiconductors are separated by an interfacial layer. The insulator is sufficiently thin (10-30 Å) so that current transport through the interface is by tunneling. While the tunneling process is sensitive, to a degree, to the sharp of the barrier, it is charge transport in the semiconductors that determines the I-V characteristics. The tunneling serves largely to provide an ``ohmic contact" [3].

The inversed Si surface provides a supply of minority carriers which can tunnel into the TCO ($J_{CT}= A^*T^2 \exp(-q\Phi_B/kT)\exp(-(q\Phi Td)^{1/2})$). ZnO layers are very frequently used as window layers in photovoltaic solar cells [4]. With a wide bandgap, high transparency and low resistivity material, it can be used as a window layer and simultaneously heterojunction partner for heterojunction based solar cells [5-6-7]. This double role of ZnO material in heterojunction solar cells offers some advantages such as an excellent blue light response, simple processing steps, low processing temperatures, and non toxicity virtue. Using ZnO over Si provides a window for photon transfer, gives a higher built in potential to increase the open circuit voltage Vco and seems to passivate the surface and grain boundary defects to reduce the dark current [8] and hence increase in the Vco.

The main purpose of this work is to thoroughly investigate the design investigation of n-ZnO/SiO_2/p-Si and n-ZnO/SiO_2/n-Si based SIS heterojunction solar cells using two dimensional numerical simulation and the true potential of ZnO/SiO_2/p-Si heterojunction solar cells**.**

II. Simulation

A simulation program for proposed ZnO/SiO_2/p-Si and ZnO/SiO_2/n-Si heterojunction solar cells structure has been developed in ATLAS simulator from SILVACO international to obtain various electrical and optical characteristics. Fig. 1 shows the structure of the ZnO/SiO_2/Si hetero-structure which is a type II alignment hetero-junction according to Anderson model [9].

Thickness of ZnO, SiO_2 and Si is 300 nm, 0.3 nm and 300µm respectively. Light is assumed to be falling from the top of the heterojunction. After defining the physical structure of device, material properties of ZnO and Si has been defined.

The set of material properties which are required for simulation includes the values of bandgap, electron affinity, dielectric constant, conduction band densities, valance band densities and electron/hole mobilities. Table 1 shows set of parameters that has been taken into consideration for the simulation of heterojunction cell. Doping is considered uniform for all the regions. The Gummel Newton iteration method has been used to improve the efficiency of iteration. Concentration dependent model for mobility calculation and surface recombination mechanism at contacts has been considered in the simulation. For calculation of dark current AUGER, Band-to-Band and SRH model of recombination mechanisms have been considered. The heterostructures have been treated with the affinity rule to divide the difference in band gap. Transport across the interfaces is modeled with thermionic emission and tunneling.

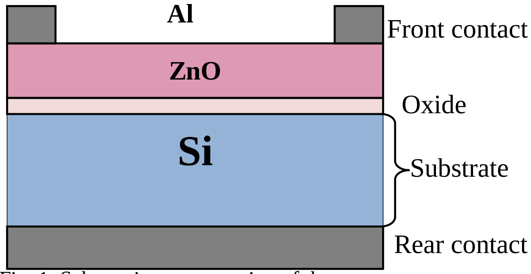

Fig. 1 Schematic representation of the sample structure.

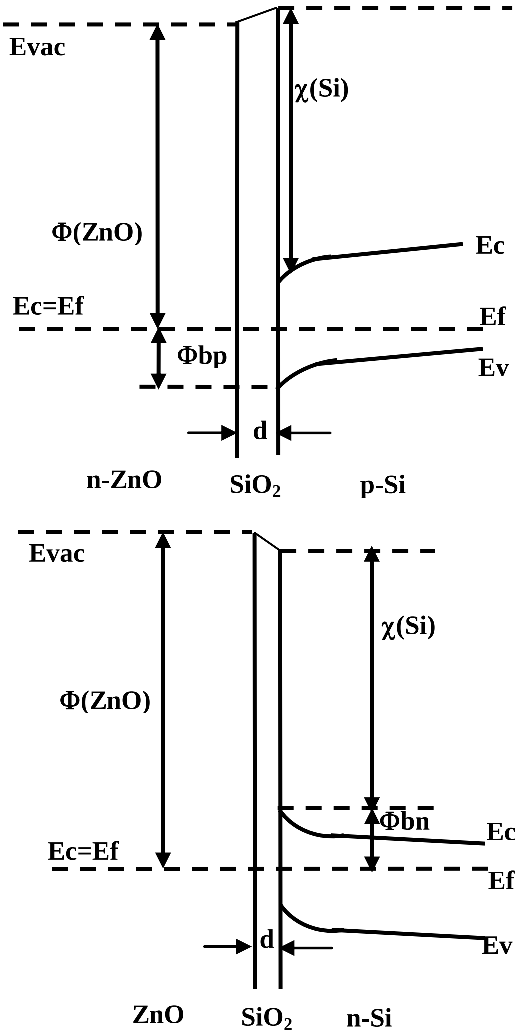

Fig. 2 Band gap structure of ZnO/SiO_2/Si SIS heterojunction to n-type and p-type silicon.

Energy band diagram of ZnO/SiO_2/p-Si and ZnO/SiO_2/n-Si heterojunctions is illustrated in Fig. 3. Φ_{ZnO} and Φ_{Si} are the ZnO-to-SiO_2 and Si-to-SiO_2 barrier heights related to the work functions of ZnO and Si, respectively. While the heterojunction is under illumination, the light-generated current is primarily due to the photoexcited electron-hole pairs in the Si. Φ_B is the barrier height which dominates the open-circuit voltage (Voc) of the photovoltaic devices. However, there are interface states exist at ZnO/SiO_2 and SiO_2/Si interfaces, which directly affect the performance of SIS solar cells.

III. Results and discussion

In these section simulation results of $ZnO/SiO_2/Si$ SIS heterojunction solar cells has been presented. Fig. 3 presents the schematic energy-band diagram of the n-ZnO/SiO_2/p-Si and n-ZnO/SiO_2/n-Si SIS heterojunction structure. Barrier heights can be read out from the band diagrams, and the values obtained are ϕ_{bn}=0.52eV and ϕ_{bp}=0.48 eV on n-type and p-type, respectively, when using electron concentration N_d=10^{20} cm^{-3} for the ZnO, as here.

Table 1.Modeling parameters used In the Simulation.

	ZnO	*Si*
Effective density of states in the conduction band Nc [cm^{-3}]	2.8e19	2.8 e19
Effective density of states in the valance band Nv [cm^{-3}]	2.8e19	1.04 e18
Dielectric constants (ε)	8.5	11.9
μ_n (cm^2/V.s)	100	1350
μ_p (cm^2/V.s)	2500	480
τ_n [sec]	10e-3	1000
τ_p [sec]	10^{-6}	100
Doping [cm^{-3}]	1.e20	1.e15
Bandgap (Eg) [eV]	3.3	1.12
Electron affinity χ [eV]	4.65	4.05

For both type of structures, without considering lattice mismatch between two materials, Anderson model (or so called electron affinity model) is used in this work which directly relates the conduction band discontinuity with the electron affinity difference of the two semiconductor materials. An ultra-thin SiO_2 layer with the thickness about 3.0A° can be seen at the interface between the Si substrate and ZnO layer. In addition to the microstructure and properties of ZnO layers, the geometry of SiO_2 layer is known to affect the tunneling current and, hence, is correlated to the SIS device performance.

Fig. 4 shows the current-voltage characteristic of the $ZnO/SiO_2/Si$ heterojunctions measured in the dark. The I-V curves of the devices show fairly good rectifying behavior for both types of substrates. Under dark conditions dark current of the order of 10^{-11} A is obtained for the device on both n- and p-Si.

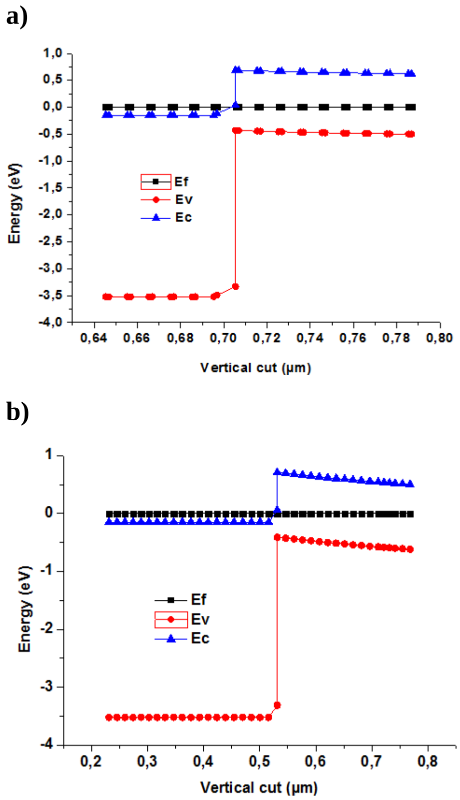

Fig. 3. Simulated band structure for the ZnO/SiO_2/p-Si heterostructure (a) and ZnO/SiO_2/n-Si (b).

Based on the dark current as a function of the applied bias, the characteristics can be described by the standard diode equation:

$$I= I_s [\exp (qV/nk_BT) – 1] \quad (1)$$

I_s is the reverse saturation current, n is the diode ideality factor, k is the Boltzmann constant and T is the absolute temperature.

I_s, determined by extrapolating the straight line of ln I to V = 0, is given by

$$I_s=A^*AT^2 \exp (-\Phi_{bn,p}/kT) \quad (2)$$

where A is the contact area, A^* is the Richardson constant of Si and $\Phi_{bn,p}$ is the effective barrier height.

Fig. 5 presents the I–V characteristics for the SIS devices measured under the AM1.5 illumination condition. Typical good rectifying and photoelectric behavior were observed for the device on both n- and p-Si. The dark leakage current is small, whereas its

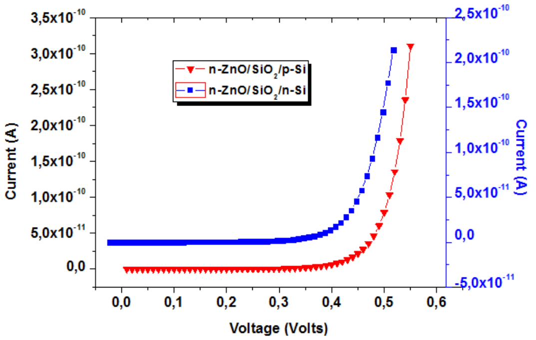

Fig. 4 I-V curve of the SIS heterojunctions devices in the dark.

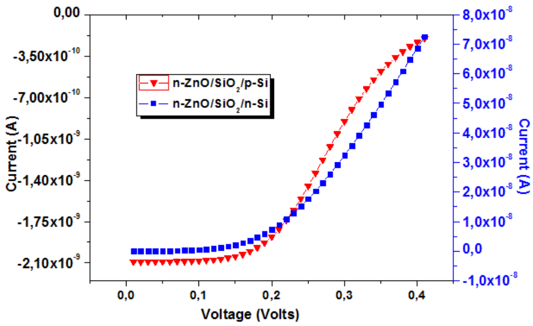

Fig. 5 I-V characteristic of SIS heterojunctions devices measured at the AM1.5 illumination condition.

photocurrent generated under illumination is much higher. Under bias conditions the photocurrent caused by the ZnO surfaces exposed to illumination by AM1.5 solar spectrum was obviously much larger than the dark current. For example, when the bias is 0.2 V, the dark current is only 10^{-11} A, whereas the photocurrent reaches 10^{-8} A under illumination. It is generally understood that the photoelectric effect results from the light-induced electron generation at the area of the Si, particularly near the heterojunction interface [10]. Light is absorbed in the Si layer and generated electrons and holes drift to ZnO side and Si side. So the photocurrents are consequently obtained [11].

Since the ZnO films are highly transparent T> 90 % in the visible region, the visible light passes through ZnO films and is absorbed primarily in the underlying Si, generating electron-hole pairs, responsible for the observed photocurrent under bias conditions [12].

On the other hand, the UV photons are mainly absorbed in the ZnO layer and the photogenerated electrons drift towards the positive electrode through the depleted ZnO region. Consequently, the current increases linearly as the reverse bias increases.

The photovoltaic characteristics including Voc, Jsc and fill factor (FF) of the ZnO/ SiO_2/Si devices derived from the I-V are listed in Table2.

The Voc of SIS solar cells is mainly determined by the barrier height (denoted as Φ_B) related to the difference between the work functions of the ZnO layer and Si substrate.

Table 2. Photovoltaic characteristics including open-circuit voltage (Voc), short circuit current density (Jsc), and fill factor (FF) of ZnO/SiO_2/Si devices.

SIS structure	***Voc(V)***	***Jsc(mAc m^{-2})***	***FF(%)***
ZnO/SiO_2/n-Si	0.015	0.02	24.70
ZnO/SiO_2/p-Si	0.46	22.15	31.05

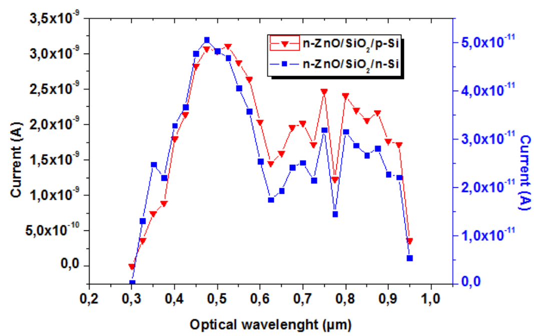

Fig. 5 Photocurrent spectra of the SIS heterojunction solar cells.

For the photoresponse spectra, photocurrents (Iph) are measured when the ZnO/SiO_2/Si diodes are irradiated from the ZnO side. The photoresponse curve shows that the photocurrent increases with increasing the light energy (i.e. decreasing wavelength) and becomes the maximum for a light of wavelength 480 nm and thereafter decreases sharply as the UV region is approached.

It can be deduced from the results obtained in this work that the transport of carriers in the

$ZnO/SiO_2/Si$ heterojunction is dominated by the insulating SiO_2 layer.

Contrary to ZnO/SiO_2/p-Si structure, ZnO/SiO_2/n-Si heterojunction shows poor photovoltaic response and low Voc because higher barrier height for the ZnO/SiO_2/n-Si.

IV. Conclusion

This work demonstrates a theoretical design assessment using two dimensional numerical simulations form SIS solar cells consist of ultra thin SiO_2 layers covered p and n-type Si substrates and n-ZnO films.

The best n-ZnO/SiO_2/p-Si device exhibits the open-circuit voltage, short-circuit current density and fill factor of this device are 0.46 V, 22.15 mA/cm^2 and 31.05 %, respectively. ZnO/SiO_2/n-Si SIS heterojunction shows poor photovoltaic response and low Voc because higher barrier height.

References

[1] R. Singh, K. Rajkanan, D.E. Brodie, J.H. Morgan, *IEEE Transactions on Electron Devices 27 (1980)* 656-662.

[2] S. Ashok, P.P. Sharma, S.J. Fonash, IEEE Transactions on Electron Devices 27 (1980) 725-730.

[3] K.K. Ng, H.C. Card, *IEEE Transactions on Electron Devices 27 (1980)* 716-724.

[4] Wilson W. Wenas, Syarif Riyadi, *Solar Energy Materials and Solar Cells 90 (2006)* 3261-3267.

[5] Tingfang Yen et aI., "Current transport in ZnO/Si heterojunctions for low-cost solar cells", *4th photovo/taic energy conversion conference (2006)* 1653-1656.

[6] D. G. Baik and S. M. Cho, "Application of sol-gel derived films for ZnOln-Si junction solar cells.", *Thin Solid Films, Vol. 354 (1999)* 227-231.

[7] Zhang Wei-Ying et aI., "Dependence of photovoltaic property of ZnO/Si heterojunction solar cell on thickness of ZnO films", *Chin. Phys. Lett. Vol. 25 No. 5(2008)* 1829-1831.

[8] Dengyuan Song, Armin G. Aberle, James Xia, *Applied Surface Science 195 (2002)* 291-296.

[9] C. Periasamy and P. Chakrabarti, ”Large-Area and Nanoscale n-Zno/p-Si Heterojunction Photodetectors”, *J. Vac. Sci. Technol. B,* ***29,*** *051206 (2011).*

[10] S. Mridha, M. Dutta, Durga Basak, *Journal of Materials Science: Materials in Electronics 20 (2009)* 376-379.

[11] I. S. Jeong, Jae Hoon Kim, Seongil Im, *Applied Physics Letter 83 (2003)* 2946-2948.

[12] J.Y. Lee, Y.S. Choi, J.H. Kim, M.O. Park, S. Im, *Thin Solid Films 403-404 (2002)* 553-557.