ENHANCED PHOTON CONVERSION EFFICIENCY IN ULTRA-SLIM P-a-SiC:H/I-a-Si:H/N-a-Si:H HETERO-STRUCTURE PHOTOVOLTAIC CELL USING SUITABLE P-TYPE TCO/HTM LAYERS

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***Abstract*—**This paper demonstrates the performance improvement of a very thin (410 nm thick) P-a-SiC:H/I-a-Si:H/N-a-Si:H heterojunction solar cell simulated using SCAPS-1D software, a very commonly encountered mathematical simulation program used for modeling variegated solar cells structures. Our PIN heterojunctoin solar cell comprises of two distinct consecutive P+ layers, $CuAlO_2$ as Transparent conducting oxide (TCO), and $SrCu_2O_2$ as Hole-transport material (HTM) layer, a window layer (P- type amorphous-Silicon-Carbon (a-SiC:H)), an absorber (intrinsic (I) hydrogenated amorphous-Silicon (a-Si:H)), n-type a-Si:H and ZnO as the bottom layer before the back contact. It can be realized that insertion of these TCO and HTM on PIN enhances the conduction of charge carriers to the contacts and thus serves as an efficient carrier conduit. This eventually increases the efficacy of the ohmic contact and also provides the effect of back surface field. Corollary, we observe the better efficiency at optimized thickness, band gap and doping concentration of each layer from our proposed heterostructure, which leads to an outstanding view of the transport mechanism and revelation of the role of a suitable TCO and an opposite HTM on the performance of PIN heterostructure solar cell based on a-Si:H. The best photon conversion efficiency (PCE) from our P-a-SiC:H/I-a-Si:H/N-a-Si:H heterojunction solar cells is achieved as 21.4%.

***Keywords*—**a-Si:H, a-SiC:H, heterojunctoin solar cells, HTM, PCE, TCO.

I. INTRODUCTION

Owing to some promising features such as high optical absorption coefficient, substantially reduced cost, many-meters-long large-scale fabrication with less challenging techniques (regardless of the substrates' types at temperature below 600^{o}C, even glass can be utilized as substrate), and non-toxicity, thin film amorphous-Silicon photovoltaic (PV) cells have always been considered as an attractive choice for the research community of renewable technology [1-5].

In line with this, energy-bandgap (E_g) tunability is considered as a pertinent feature for amorphous silicon PV cells. Variation of the E_g of amorphous silicon alloys are made wide-ranged by changing the percentage of elemental-substance (hydrogen, carbon, and germanium, etc.) into the amorphous silicon. Therefore, in latest years, hydrogenated amorphous-Silicon (a-Si:H) and its compounds grow into a favorable candidates for PV applications. The inclusion of a-Si:H alloys (a-SiC:H, a-SiGe:H, etc) offer a decent solution to enhance a-Si:H solar cell performance [6-7]. The alloys that are used most in PV cells are amorphous-Silicon-Carbon (a-SiC:H) and amorphous-Silicon-Germanium (a-SiGe:H). The a-SiC:H compound with wider E_g is typically utilized as a window layer for abating the optical loss. While due to narrow bandgap, a-Si:H and a-SiGe:H compounds are extensively used as intrinsic layer, and thus expected to play a vital part in the performance enhancement in a-Si:H based cells. It is worth mentioning that the photon conversion efficiency (PCE) of a-Si:H PV cells has evolved to surpass 12% for single junction, 13-14.6% for tandem or multijunction PV cells [7]. Mainly, the key stumbling block of a-Si:H solar cell is yet the small PCE compared to the rest of the existing PV technologies, mostly owing to the large number of electronic energy states within the E_g, that even augments at the exposure of heat/sun and thus results in the deterioration of PCE which is known as the established Straeber-Wronski Effect (SWE) [8].

Therefore, for improvement of efficiency in cell technology, detail understanding and optimum usage of individual layer of PV cells are regarded as one of the critical matters. Likewise, inclusion of effective tunnel recombination junction in tandem cells, mobility of charge carriers, concentration of impurity added, surface qualities of the electron and hole transport materials

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(ETM & HTM) and their proper alignment of energy bands with absorber [9-11], all are the decisive aspects for effective passage or collection of the charge carriers to the metal contacts (front and back). This is simply possible if the work-function of front contact material is almost identical or marginally larger than conduction band edge of the transport layer. Corollary, larger work-function presumably yields an ohmic contact for holes and electrostatic barrier for electrons in HTM. Cell performance also worsens if the recombination mechanism is not addressed properly as accumulated charges will intrude the electric field inside the cell. Therefore proper Tunnel junction or recombination layer is imperative to maintain the current flow through an entire heterojunction cell.

Again, talking about the transparent conducting oxide (TCO), HTM, ETM layers in PV cells, it is needless to mention that these are merely semiconductor capable of converting a fraction of solar spectrum into illumination current. Also these are indispensable in solar cells as photoelectrodes due to their appropriate properties such as abundance with suitable E_g and affinity, wide surface-area, and flexibility of processing in diverse forms. Till now several processing methodologies and advancement have been carried out largely based on absorber layer than the other layers. However, the other layers can also augment the performance of the PV cells through controlling the specific dynamics of carriers along the complete conduit starting from the absorber to the external contacts/electrodes.

In this circumstance, our structure targets to explore all the pertinent performance features through simulation focusing on improving the conversion efficiency of a typical PIN heterojunction hydrogenated amorphous-Silicon (P-a-SiC:H/I-a-Si:H/N-a-Si:H) with the inclusion of a p-type transparent conducting oxide of $CuAlO_2$, and a HTM layer of $SrCu_2O_2$ and thereafter also through the variations of thicknesses, series resistance, defect densities, doping concentrations, and E_g of every PIN layers. We hope and surmise, this learning will benefit the researchers in this field of renewable energy, considering optimization and evolution of the prevailing PIN PV cells together with the comprehension of the starring role of the transport layer on the performance of the heterojunctions at the same time.

II. Methodology, Simulation and Structural Details of Proposed Cell

In this work the modelling and simulation are performed using the popular SCAPS-1D simulation program/software. We intended to elevate the performance of the proposed cell through optimization of thickness, energy gap, defect densities and doping concentrations of the window, absorber/intrinsic, conducting oxides and transport layers for attaining maximum possible PCE under 1.5 AM solar irradiance and at a temperature of 300 K.

The properties of all requisite design parameters used for calculating the carrier dynamics and transport equations of the structure are given in Table-I and II that have been collected from existing established literatures [12-14].

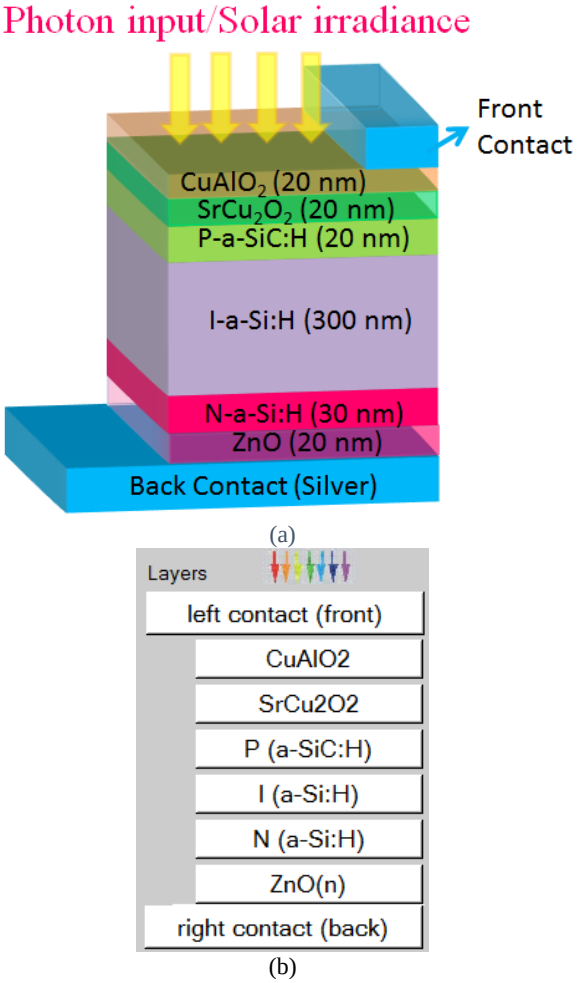

Fig. 1. (a) Schematic depiction of proposed heterojunction PV cells at optimized thickness of all layers. (b) A screen-shot of the layout from SCAPS-1D simulation software.

In Fig. 1, the structural details of our proposed PIN P-a-SiC:H /I-a-Si:H /N-a-Si:H heterojunction solar cell is shown elucidately. In our optimized structure, a-Si:H is inserted as N-type (30 nm thick), a-SiC:H is used as P-type (20 nm thick) layers at the top and the intrinsic a-Si:H (300 nm thick) is sandwiched as the absorber layer. Above the P-type a-SiC:H, 20 nm thick $SrCu_2O_2$ is used as HTM and another 20 nm of $CuAlO_2$ is used as P-type TCO on the very top attached to the front contact. Also,

a 20 nm of N-type ZnO is added right beneath the N-type a-Si:H connected to the back contact to offer low electrical losses (low series resistance) and optical losses. The total thickness of the entire structure becomes only 410 nm as a whole.

TABLE I
PARAMETERS OF KEY MATERIALS UTILIZED AS PIN

Parameters	N-a-Si:H	I-a-Si:H	P-a-SiC:H
E_g(eV)	1.8	1.8	1.90
χ (eV)	3.8	3.8	3.7
ε_r	11.9	11.9	11.9
N_C (cm^{-3})	2.50×10^{20}	2.50×10^{20}	2.50×10^{20}
N_v (cm^{-3})	2.50×10^{20}	2.50×10^{20}	2.50×10^{20}
μ_n (cm^2/Vs)	2.00×10^{1}	2.00×10^{1}	1.00×10^{1}
μ_p (cm^2/Vs)	2.00×10^{0}	2.00×10^{0}	1.00×10^{0}
N_D (cm^{-3})	0	0	0
N_A (cm^{-3})	8.00×10^{18}	0	2.9×10^{18}

TABLE II
PARAMETERS OF MATERIALS USED AS TCO AND HTM

Parameters	ZnO (n)	$SrCu_2O_2$	$CuAlO_2$
Thickness (µm)	0.02	0.02	0.02
E_g(eV)	3.37	3.3	3.60
χ (eV)	4.35	2.2	2.500
ε_r	10	9.7	60.000
N_C (cm^{-3})	2.22×10^{18}	2.20×10^{18}	2.20×10^{18}
N_v (cm^{-3})	1.78×10^{18}	1.80×10^{19}	1.80×10^{19}
μ_n (cm^2/Vs)	1.00×10^{2}	1.00×10^{-1}	2.00×10^{0}
μ_p (cm^2/Vs)	5.00×10^{1}	4.60×10^{-1}	8.60×10^{0}
N_D (cm^{-3})	1.00×10^{20}	0	0
N_A (cm^{-3})	0	3.68×10^{18}	3.80×10^{18}

A. *The optical Properties of a-Si:H*

The pertinent optical properties of a-Si:H is its absorption coefficient, E_g and refractive index. The E_g of it is determined as the minimum band-gap also referred as mobility gap between extended conduction and valence band that typically lies in the range of 1.7 to 1.8 eV for a good quality of a-Si:H. However, the optical E_g increases as the concentration of H increases [15]. The inclusion of Ge in a-Si:H reduced the E_g, while alloying with C (a-SiC:H) results in widening the gap that can be tuned to as high as 2 eV [16].

B. *The significance of a-SiC:H in PIN a-Si PV Cell*

The inclusion of large band gap of a-SiC:H as top/window layer is essential to heighten the absorption in typical PIN solar cell based a-Si:H, owing to their great conductivity, and wider range of optical E_g suitable for photon soaking [17-18]. But it is not preferably used as absorber because its defect density is high. In a-SiC:H, the optoelectronic priorities and thickness are the major parameters that needed to be optimized for better performance of PIN cells. Corollary, the attachment of suitable absorber (intrinsic) layer at the interface of P-I can play a vital role in upgrading the crossing-junction of p-i-n solar cell and lessening the recombination at P-I domain. In this context, P-I interface of p-a-SiC:H /I-a-Si:H is suitably matched in PIN solar cells based on a-Si:H.

III. RESULTS AND DISCUSSIONS

A successful PV cell demands two basic requirements: (i) the current generated throughout heterojunctions will be almost equal and (ii) the cell will have lowest electrical resistance and optical losses possible. These requirements can be controlled by varying band-gap, thickness, and defect of absorber layer and by adding suitable transport layer [17-19].

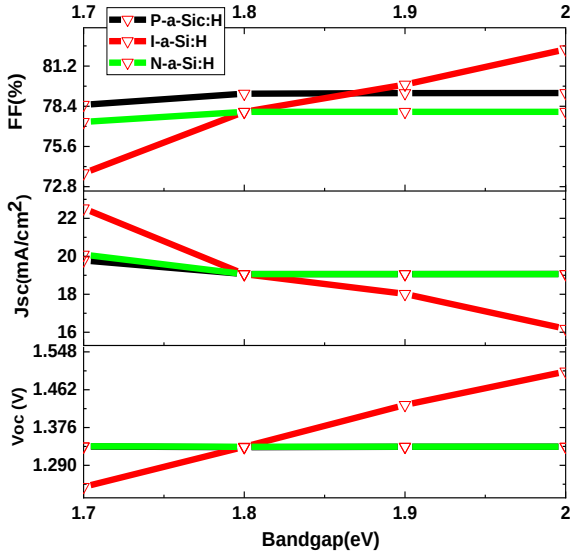

Fig. 1. Fill-Factor (FF), J_{sc} (short circuit current density), and open circuit voltage V_{oc}, as a function of band-gap varied from 1.7 to 2 eV for all P, I and N-layers.

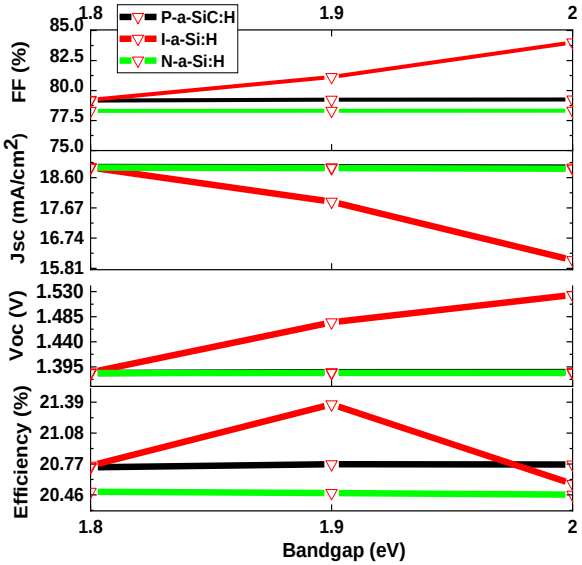

Fig. 2. Fill-Factor (FF), Jsc (short circuit current density) open circuit voltage V_{oc}, and efficiency (%) as a function of E_g of the P, I and N-layers varied from 1.8 to 2 eV.

It has been revealed almost an era ago that the a-Si:H gives higher efficiency if light enters into the PIN PV cell from P-type window [3]. Since in PIN, intrinsic (I) layer works as absorber layer, the carriers mostly generates here, experienced the field, and they (electrons/holes) are swept/run towards the N-side/P-side of the structure. The low thickness of I-layer would provide high electric field, but will soak lesser number of carriers. Therefore, thickness, band-gap, and defect of I-layer are considered important design parameters.

Our simulation, as shown in Fig. 1, shows the effect of varying band-gap (E_g) on the performance of the cell such as FF, J_{sc} and V_{oc} for the P, I and L-layer each. Since for a good quality of a-Si:H the E_g can vary from 1.7 to 2 eV, we intend to see the effect for this particular range. We can see from the Fig.1 that as the E_g is increased the FF, and V_{oc} is increased, while J_{sc} is decreased, which is very typical. It is conspicuous from the result that 1.8 eV is the optimized E_g of the a-Si:H as I and N-layers. Next, from Fig. 2 we can also observe the effect of E_g on the efficiency together with other factors giving emphasis on the range from 1.8 to 2 eV, particularly for P-type a-SiC:H as window. We can see that for P-type a-SiC:H, 1.9 eV is the optimized E_g at which highest efficiency can be attained.

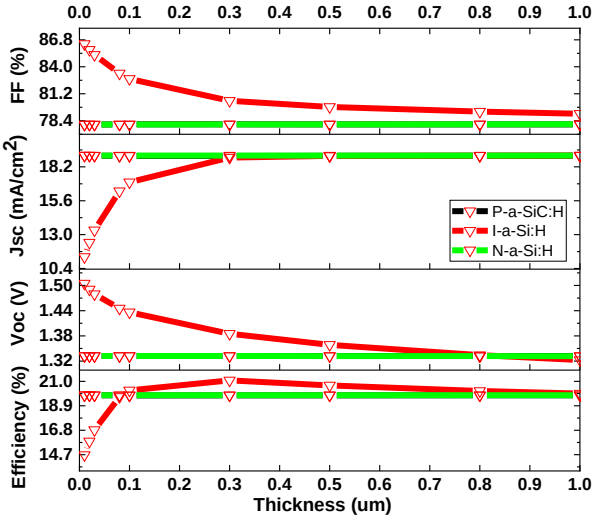

Fig. 3. The effect of the variation of thickness of each layer from 1 nm to 1000 nm on Fill-Factor (FF), J_{sc} (short circuit current density) open circuit voltage V_{oc}, and efficiency (%) of the entire structure.

Then we observe the effect of thickness, defect and doping densities on our structure as depicted in Fig. 3, 4 and 5, consecutively. Our simulation results reveal that the efficiency increases linearly by increasing the thickness of absorber I-layer from 1 to 100 nm and gradually becomes maximum at 300 nm (Fig. 3). Thereafter the efficiency starts to decrease slowly again. As we know that the photon absorption is expected to increase with increasing thickness, however, it is also known that much larger thickness will affect the electric field and therefore we see the optimized thickness of the I-layer of the PIN structure is 300 nm.

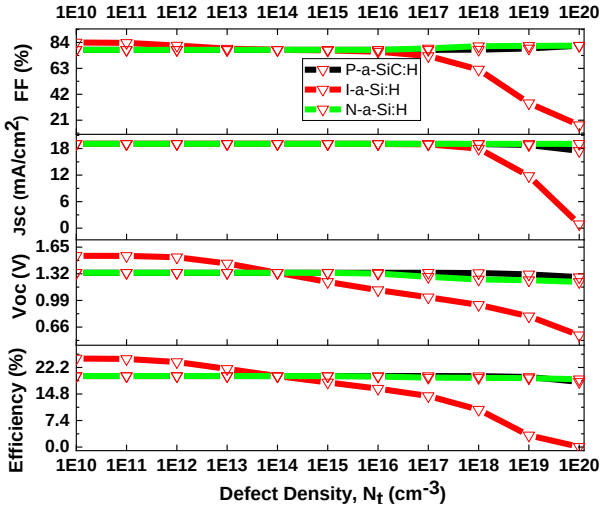

Fig. 4. Fill-Factor (FF), J_{sc} (short circuit current density) open circuit voltage V_{oc}, and efficiency (%) as a function of defect density N_t (cm^{-3}) of all layers.

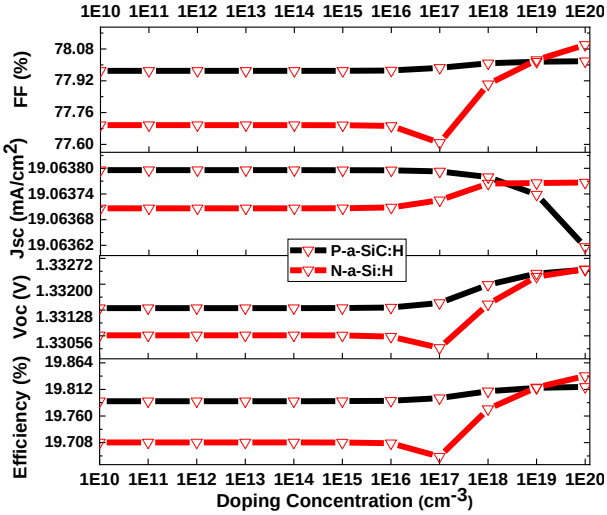

Fig. 5. The variation of doping concentration on the performance parameters (Fill-Factor (FF), J_{sc} (short circuit current density) open circuit voltage V_{oc}, and efficiency (%)) of all layers.

The P-type a-SiC:H layer shows the same dependence as the N-type a-Si:H layer with the variation of thickness on the performance. The P-layer thickness is chosen as 20 nm, whereas for N layer thickness is selected slightly thicker as 30 nm with an N+ ZnO layer right beneath with a thickness of 20 nm for maintaining series resistance as low as possible. Thus the overall height of total N layers is decided as 50

nm, while the total P layers is best optimized as 60 nm including the 20 nm of P+ type $SrCu_2O_2$ HTM and P+-type $CuAlO_2$ TCO of 20 nm above the P-type a-SiC:H window.

We also explore the effect of defect density. We can see from the Fig. 4 that, particularly the defect density of I-a-Si:H strongly disturbs the performance of the cell and charge transport by introducing the non-uniform electric field profile. Also the optimization of our structure to choose suitable doping densities of relevant P and N layers are depicted in Fig. 5.

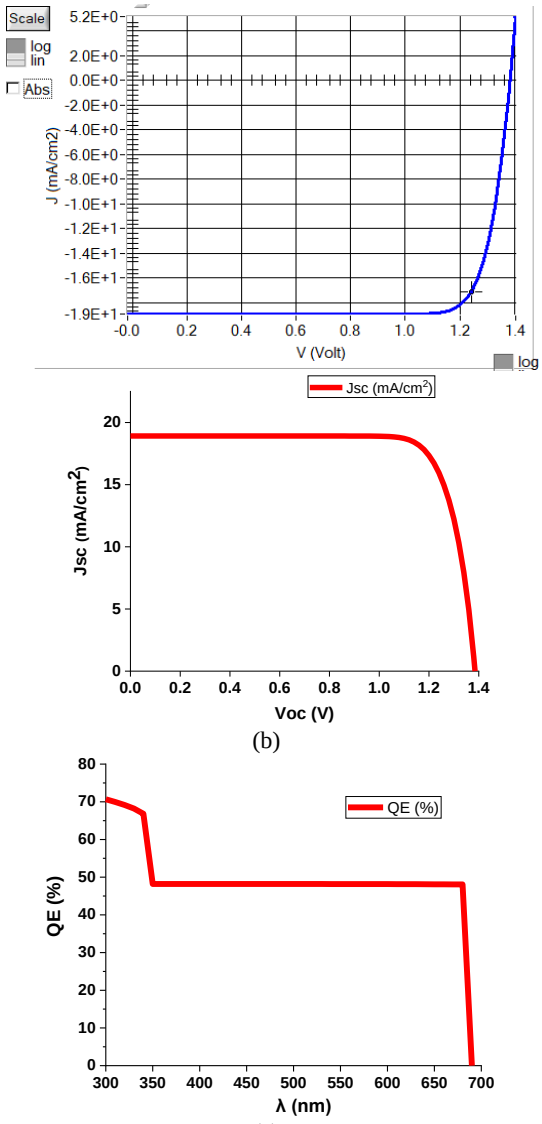

Fig. 6. (a) The screen-shot of the I-V curve from SCAPS-1D after simulation of the optimized PIN (P-a-SiC:H/I-a-Si:H/N-a-Si:H) heterojunction solar cell including P+ type $SrCu_2O_2$ HTM and P+-type $CuAlO_2$ TCO (b) The plotted I-V characteristics of the optimized PIN (P-a-SiC:H/I-a-Si:H/N-a-Si:H) heterojunction solar cell including P+ type $SrCu_2O_2$ HTM and P+-type $CuAlO_2$ TCO. (c) The quantum efficiency (QE (%)) of the PV cell as a function of wavelength.

Finally, the I-V characteristics and quantum efficiency of the optimized structure of P-a-SiC:H/I-a-Si:H/N-a-Si:H heterojunction solar cell including P+ type $SrCu_2O_2$ HTM and P+-type $CuAlO_2$ TCO, and a similar P-a-SiC:H/I-a-Si:H/N-a-Si:H heterojunction without the P+ type $SrCu_2O_2$ HTM and P+-type $CuAlO_2$ TCO are shown in Fig. 6, and Fig. 7, respectively for the readers understanding. It reveals that without HTM and TCO, the efficiency reduced 2% from our proposed cell with HTM and TCO.

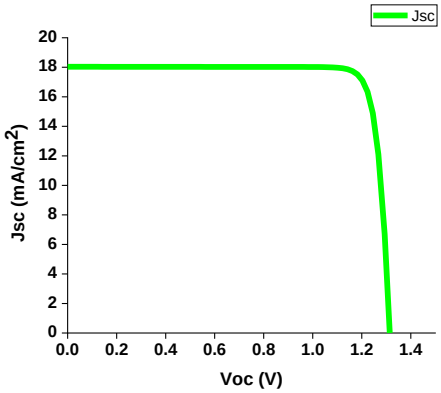

Fig. 7. The I-V characteristics of the PIN (P-a-SiC:H/I-a-Si:H/N-a-Si:H) heterojunction solar cell without HTM and TCO.

In a nutshell, the optimization of our overall structure is accredited to the favorable effect on the performance of the PV cell, specifically achieving the V_{oc} of 1.4 V, PCE of 21.4% and short-circuit current of 19.01 mA/cm^2 without any significant defeat in FF as 81.06%.

IV. Conclusion

In this effort, a systematic analysis on an ultra-slim (410 nm) heterojunction PIN P-a-SiC:H/I-a-Si:H/N-a-Si:H PV cell is designed and simulated using SCAPS-1D simulator. At first place, the PV cell were simulated and optimized with the variation of band diagram, thickness, defect densities and doping concentrations of P-type a-SiC:H as window layer at P-I interface, a-Si:H as absorber I and N-type layers. The highest PCE is achieved to be 21.4% implementing $SrCu_2O_2$ as HTM layer and $CuAlO_2$ as suitable P-type TCO which provide suitable back surface-fields as well. Simulation results reveal that they have significant contribution in achieving such a high efficiency. At 1.5 AM solar irradiance, the proposed cell structure with HTM and TCO layers achieved an open-circuit voltage of 1.4 V, a short-circuit current density of 19.01 mA/cm^2, and a fill factor of 81.06% and the corresponding overall conversion efficiency of 21.4%. The same structure without TCO and HTM produces an open-circuit voltage of 1.3 V, a short-circuit current density of 18 mA/cm^2, and the reduction of efficiency of 2% than that of the previous one.

REFERENCES

[1] K. L. chopra and S. R. Das, "Thin Film Solar cell", *Springer*, New York, USA, 1983.
[2] S. Adachi, "Optical Constants of Crystalline and Amorphous Semiconductors," *Kluwer Academic Publishers*, Boston, 1999.
[3] X. Deng, and E. A. Schiff, "Amorphous Silicon-Based Solar Cells', in A. Luque and S. Hegedus (eds), *Handbook of Photovoltaic Science and engineering*, John Wiley &Sons, Chichester, 2003.
[4] P. A. Basore, "Pilot Production of Thin Film Crystalline Silicon on Glass Module", *in Proc. 29th IEEE Photovoltaic Specialist Conference*, 2002, pp. 49–52.
[5] S. Schicho, *Amorphous And Microcrystalline Silicon Applied In Very Thin Tandem Solar Cells*, Forschungszentrum Jülich, 2011.
[6] A. Terakawa, M. Shima, K. Sayama, H. Tarui, H. Nishiwaki, S. Tsuda, "Optimization of a-SiGe:H Alloy Composition for Stable Solar Cells", *Jpn. J. Appl. Phys.* Vol. 34, p. 1741, 1995.
[7] M. Stuckelberger, R. Biron, N. Wyrsch, F. Haug, C. Ballif, "Review: Progress in solar cells from hydrogenated amorphous silicon", *Renewable and Sustainable Energy Reviews*, vol. 76, pp. 1497–1523, 2017.
[8] D. L. Staebler and C. R. Wronski, "Reversible Conductivity Change in Discharged Produced Amorphous Silicon", *Appl. Phys. Lett.*, Vol. 31, p. 292, 1997.
[9] J. Even, L. Pedesseau, O. Durand, M. Modreanu, G. Huyberechts, B. Servet, O. Chaix-Pluchery, "Vibrational properties of $SrCu_2O_2$ studied via Density Functional Theory calculations and compared to Raman and infrared spectroscopy measurements", *Thin Solid Films*, vol. 541, pp. 113–116, 2013.
[10] K. R. Adhikari, S. Gurung, B. K. Bhattarai, and B. M. Soucase, "Comparative study on $MAPbI_3$ based solar cells using different electron transporting materials", *Phys. Status Solidi C*, vol. 13, No. 1, pp. 13–17, 2016.
[11] H. Kawazoe, M. Yasukawa, H. Hyodo, M. Kurita, H. Yanagi & H. Hosono, "P-type electrical conduction in transparent thin films of $CuAlO_2$", *Nature*, vol. 389, p. 939–942, 1997.
[12] A. Idda, L. Ayat and N. Dahbi, Improving the Performance of Hydrogenated Amorphous Silicon Solar Cell Using a-SiGe:H Alloy, Journal of Ovonic Research, vol. 15, No. 5, pp. 271–278, 2019.
[13] N. A. Jahan, M. M. U. Karim and M. M. Hossain, "A High Efficiency Ultra Thin (1.8 μm) CdS/CdTe p-i-n Solar Cell with CdTe and Si as BSF layer", Advances in Science, *Technology and Engineering Systems J.* vol. 3, pp. 213-217, 2018.
[14] H. Yuehui, Z. Xiangwen, Q. Minghao, W. Lifu, Z. Tao, and X. Yaojiang, "Simulation analysis of the effects of a back surface field on a p-a-Si:H/n-c-Si/n+-a-Si:H heterojunction solar cell", *J. Semicond.* vol. 30, pp. 064006–064010, 2009.
[15] T. Hama, Y. Okamato, Y. Hamakawa, and T. Matsubara, "Hydrogen Content Dependance of the Optical Energy Gap in a-Si:H", J. Non-Cryst. Solids, vol. 8, pp.141–150, 2000.
[16] D. Girginoudi and A. Thanailakis, "The effect of hydrogen content on the optoelectronic properties of amorphous siliconcarbide films", *J. Appl. Phys.* vol. 69, pp. 1490–1493, 1991.
[17] T. Dinh, D. V. Dao, H-P. Phan, L. Wang, A. Qamar, N-T. Nguyen, P. Tanner, and M. Rybachuk, "Charge transport and activation energy of amorphous silicon carbide thin film on quartz at elevated temperature", *Appl. Phys. Exp.* vol. 8, pp. 061303–061307, 2015.
[18] M. W. M. van Cleef, F. A. Rubinelli, R. Rizzoli, R. Pinghini, R.E. I. Schropp and W. F. van der Weg," Amorphous Silicon Carbide/Crystalline Silicon Heterojunction Solar Cells: A Comprehensive Study of the Photocarrier Collection", *Jpn. J. Appl. Phys.* vol. 37, pp. 3926–3932, 1998.
[19] C. S. Solanki, "Solar Photovoltaics: Fundamentals, Technologies And Applications", *PHI Learning Pvt. Ltd.*, Delhi, May 9, 2015.

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