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Numerical Simulation for Enhancement of output Performance of WS_2 based Thin Film Solar Cells

Sobab Khan[1], Mudasar Rashid[2], Waqas Rahim[3], Muhammad Aitezaz Hussain,[4] Ahtasham Rahim[5],
[1,2,4,5]Department of Renewable Energy Engineering
[3]Department of Electrical Engineering
[3]CECOS University of IT and Emerging Sciences
[1,2,4,5]Center For Advanced.Studies in Energy University of Engineering and Tecnology Peshawar 25000, Pakistan
mrsobabkhan@gmail.com[1] mudasar_uetian@yahoo.com[2], engr_waqasrahim@hotmail.com[3], aitizazk36@gmail.com[4], khanshami361@gmail.com[5]

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***Abstract*—**In this paper , Tungsten Disulfide is utilized for the development of an efficient model, using SCAPS one dimensional Simulator. Performance of the developed model is compared with other thin film solar cells currently under study. An efficient solar cell model with comparable photovoltaic parameters to the recent thin film models is obtained. Taking ZnO window layer material, ZnSe as buffer layer material, WS2 as absorption layer material and Mg as back surface field with back reflector a 20% efficient, design with 0.9Voc, 25 mA/cm2 current density and fill factor of 85% is developed.

***Keywords*—** Sustainable, Photovoltaic, Simulator, Back Surface field, Reflector.

I. INTRODUCTION

Energy has become essential in economic growth in any country and a key element to relieve from poverty. Global energy structure is in the stage of seizure in the current scenario. Venery for sustainable power to meet the ever-growing world's energy demand has encouraged photovoltaic community to emphasis on renewable energy field in particular. Renewable energy sources are in abundance in nature such as wind, hydro power, biomass and the energy form the sun. Solar energy is the most abundant, inexhaustible and clean of all the renewable energy resources till date. The power from sun intercepted by the earth is about 1.8 × 1011 MW, which is many times larger than the present rate of all the energy consumption. Photovoltaic technology is one of the finest ways to harness the solar power. Photovoltaic conversion is the direct conversion of sunlight into electricity without any heat engine to interfere. Photovoltaic devices are rugged and simple in design requiring very little maintenance and their biggest advantage being their construction as stand-alone systems to give outputs from microwatts to megawatts. Hence they are used for power source, water pumping, remote buildings, solar home systems, communications, satellites and space vehicles, reverse osmosis plants, and for even megawatt scale power plants. With such a vast array of applications, the demand for photovoltaics is increasing every year. A huge amount of research work has been made in solar energy in particular and scientists are investigating particular in thin films because of their cost verses energy efficiency.

A. Thin Films Technology

Thin films greatly reduce the amount of semiconductor material required for each cell when compared to silicon wafers and hence lowers the cost of production of photovoltaic cells. Gallium arsenide (GaAs), copper, cadmium telluride (CdTe) indium diselenide (CuInSe2) and titanium dioxide (TiO2) are materials that have been mostly used for thin film PV cells. Barnett et al. investigated that solar cells utilizing thin-film polycrystalline silicon can achieve photovoltaic power conversion efficiencies greater than 19% as a result of light trapping and back surface passivation with optimum silicon thickness [1]. Aberle reviewed the most promising thin-film c-Si PV technologies that have emerged during the last 10 years and found that three different thin-film c-Si PV technologies (SLIVER, hybrid, CSG) can be transferred to industrial production]. compared epitaxial growth of silicon thin film on double porous sacrificial layers obtained by liquid or vapor phase epitaxy (LPE or VPE) and found that mobility and diffusion length are slightly higher with VPE compared to LPE fabricating solar cells using a detached film obtained with VPE and without any surface passivation treatment or antireflective coating, exhibits an efficiency of 4.2% with a fill factor of 0.69 [2]. Sagan et al. studied reflection high-energy electron diffraction (RHEED) pattern of CdTe and HgCdTe thin films grown on Si by pulse laser deposition [3]. Solanki et al. described a process of transferring thin porous silicon layers (PSL) onto a ceramic substrate like alumina [4]. Powalla et al. assessed that all existing thin-film PV technologies, especially the Cu(In,Ga)Se2 (CIGS)-based technology, have a high cost reduction potential at high production volumes projecting futuristic challenge to combine high production volumes with high throughput, sufficient yield and superior quality to achieve efficiencies of above 11% and a maximum of 12.7% [6]. Hollingsworth et al. demonstrated based on thin-film fabrication studies that ternary single source precursors can be used in either a hot, or cold-wall spray chemical vapor deposition reactor, for depositing CuInS2, CuGaS2 and CuGaInS2 at reduced temperature (400–450◦C), which display good electrical and optical properties suitable for photovoltaic devices [6]. Ito et al. presented techniques of TiO2 film fabrication for dye-sensitized solar cells that consists of pre-treatment of the working photo electrode by TiCl4, variations in layer thickness of the transparent nanocrystalline-TiO2 and application of a topcoat light-scattering layer as well as the adhesion of an anti-reflecting film to the electrode's surface resulting in a conversion efficiency of global air mass 1.5 (AM 1.5, 1000 W/m2) solar light to electric power over 10% [7]. Messina et al. presented a methodology to deposit Sb2S3 thin films of 500–600 nm in thickness that are adequate for use in photovoltaic structures from a single bath along with the differences in the film thickness and improvement in the crystallinity and photoconductivity upon annealing the film in nitrogen [8]. Liehr et al. proposed Microwave Plasma Enhanced Chemical Vapour Deposition (PECVD) of thin films when highest deposition rates and/or high fragmentation of precursor material is desirable for photovoltaic applications [9]. Sathyamoorthy et al. discussed the electrical transport properties of flash evaporated Zinc Phthalocyanine thin films and studied the DC conduction mechanism in these films (Al–ZnPc–Al structure) at different temperatures along with the field dependence behavior on activation energy and possible conduction mechanism in the ZnPc films under DC field [10]. 4.6. Some other solar cells Mainz et al. demonstrated that rapid thermal sulphurisation of sputtered Cu/In precursor layers is suitable for industrial production of thin film photovoltaic modules [11].Yoosuf et al. investigated the effect of sulfurization temperature and time on the growth, structural, electrical and photoelectrical properties of b-In2S3 films [12]. Nishioka et al. evaluated the temperature dependences of the electrical characteristics of InGaP/InGaAs/Ge triple junction solar cells under concentration and found that for these solar cells, conversion efficiency decreased with increasing temperature, and increased with increasing concentration ratio owing to an increase in open-circuit voltage (Voc) [13]. Antolín et al. investigated the photocurrent produced by double-absorption of sub band gap photons predicted by the IBSC model that has been measured in QD-IBSCs (Quantum dot-Intermediate band solar cells) fabricated with InAs/GaAs material using a modulated technique with two light beams [14]. Woods et al. discussed the performance, testing, and problems of copper indium aluminum diselenide (CIAS) thin-film devices with CIAS co-evaporated in a large-area moving substrate deposition system on transparent back contact technology [15]. Phani et al. described the titania solar cells that converts sunlight directly into electricity through a process similar to photosynthesis and has performance advantages over other solar cells, which include the ability to perform well in low light and shade, and to perform consistently well over a wide range of temperatures and low cost [16]. Grätzel proposed the dye-sensitized nanocrystal line electrochemical photovoltaic system that has become a validated and credible competitor to solid-state junction devices for the conversion of solar energy into electricity and it's the prototype of a series of optoelectronic and energy technology devices exploiting the specific characteristics of this innovative structure for oxide and ceramic semiconductor films with an incident photon (standard AM 1.5) to current conversion efficiencies (IPCE) over 10% [17]. WS2 is a layer type semiconductor that exhibits similar structured materials like graphite or mica [18]. It is well known as transition-metal Dichalcogenides (TMDC) like MoS2, MoS(Se)2, WS2 and WS(Se)2, which are all potential semiconductors. TMDCs particularly MoS2 and WS2 raised special concern to photovoltaic community as absorber layer material in thin-film solar cells [19]. This is due to their suitable bandgaps (1-2 eV) and the very high absorption coefficients which is over 105 cm–1 [19]. Though single crystals of this material have been extensively studied for optical equipment; only a few studies have been carried out on the photovoltaic properties of thin film. About 30 years ago, TMDCs were studied as semiconductors for solar cells with a liquid electrode [20].To fabricate thin-film solar cells, polycrystalline WS2 films were used for the last one decades [21]. Numerical simulation is a primary step to determine the optimize structure of a solar cells. Presently, there is a lack of numerical simulation report about WS2 solar cells. Therefore, with a view to develop high efficiency, earth abundant WS2 solar cell; a numerical simulation based on SCAPS-1D.

II. SIMULATION AND MODELLING

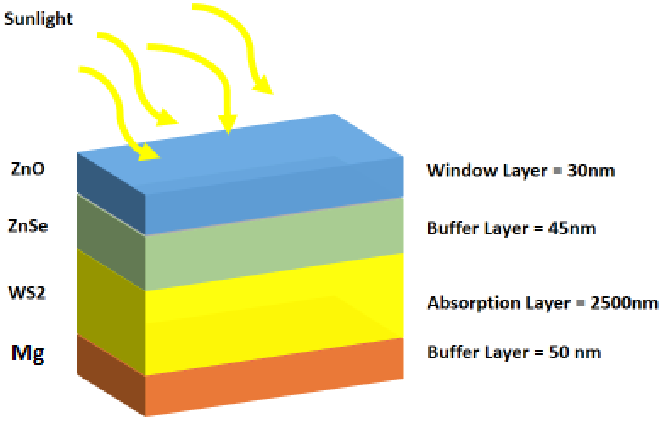


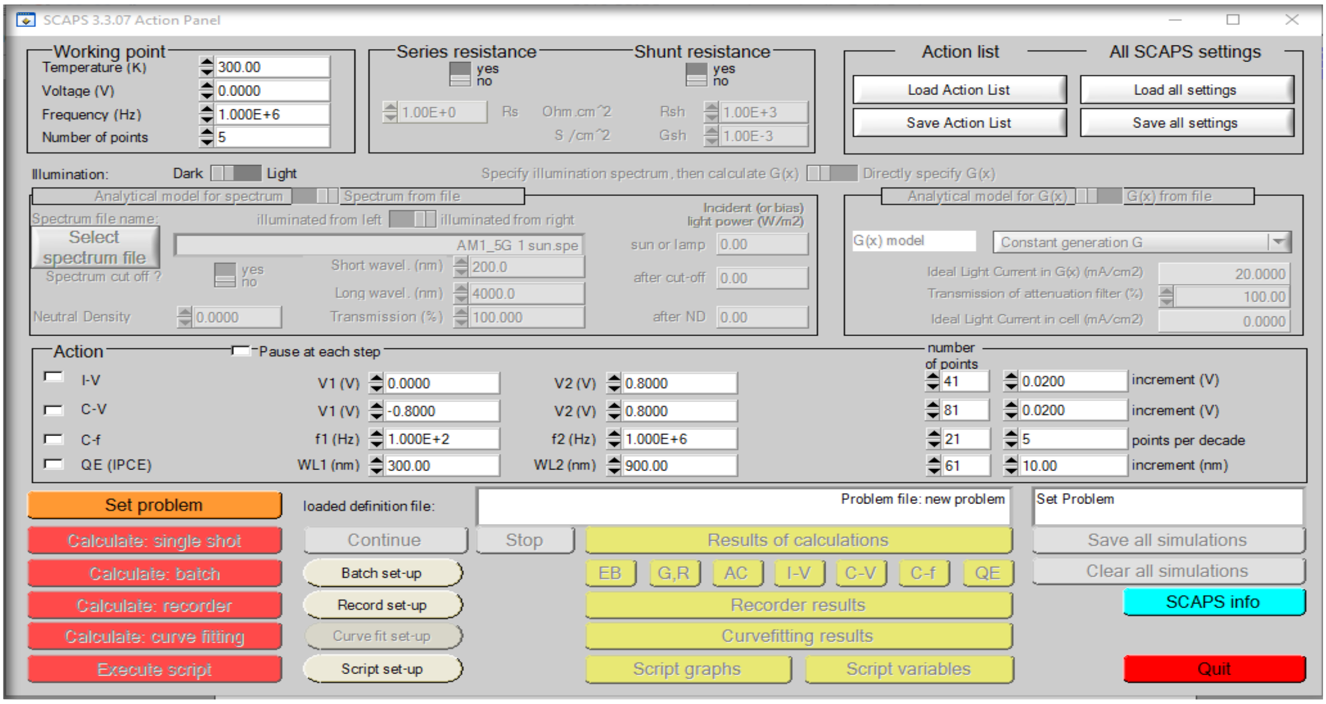
Figure 1: Proposed Model

The WS2 absorption based modal is consist of four layers The window layer having thickness of 30nm is made of ZnO material, which is a promising candidate because it provides low series resistance, permits high optical transmission and electrical conduction, and cheaper in cost than other optical or Mg materials [22]. The buffer layer having thickness 45nm is made of ZnSe material, which has a wide bandgap of 2.42 eV and has good electrical properties, and is better in electrical transmission [23, 24]. The active layer having thickness of 2500nm has also a wide bandgap and is responsible to trap highly energetic photons. For trapping and absorbing the remaining low energy photons a narrow band gap material having thickness 50nm, made of Mg is deposited at the bottom surface, which is available in a large amount, mostly non-toxic, requires low temperature and low cost substrate [25]. The electro optical parameters of the materials used in the model are given in table 1.

Table 1: Photo Electric Properties of Materials

S. No	Parameters	ZnO	ZnSe	WS2	Mg
1	Thickness (nm)	130	50	3000	300
2	Permittivity (Ɛr)	8	8	12.6	4
3	Electron-Affinity (eV)	4.5	3.9	3.3	2.1
4	Bandgap (eV)	3.3	2.4	1.15	3
5	Density of States Nc (cm^{-3})	2.20E+14	2.20E+14	2.20E+14	2.20E+14
6	Density of States Nv (cm^{-3})	1.80E+15	1.80E+15	1.80E+15	1.80E+15
7	Electron Mobility (cm^2/Vs)	80	80	80	2.00E-5
8	Hole Mobility (cm^2/Vs)	25	25	25	2.00E-5
9	Donor Concentration ($1/cm^3$)	1.00E+18	1.80E+17	0	0
10	Accepter Concentration ($1/cm^3$)	0	0	1.00E+16	2.00E+16

All the simulations are performed in solar cell capacitance simulator (SCAPS, ver 3.3.07) developed by University of Gent, Belgium. SCAPS is a one-dimensional solar cell device simulator, which is freely available to the Photovoltaics research community. Compared to other simulation tools SCAPS has the ability to accurately calculate the open-circuit voltage, current density, fill factor, quantum efficiency, capacitance voltage and frequency spectroscopy, power conversion efficiency, generation and recombination profiles, heterojunction energy band structure, distribution of electric field, spectral behavior, light bias, and temperature, respectively



Temperature (K) 300.00
Voltage (V) 0.0000
Frequency (Hz) 1.000E+6
Number of points 5

Rs 1.00E+0 Ohm.cm^2
Rsh 1.00E+3
Gsh 1.00E-3 S /cm^2

AM1_5G 1 sun.spe
Short wavel. (nm) 200.0
Long wavel. (nm) 4000.0
Transmission (%) 100.000
Neutral Density 0.0000

Incident (or bias) light power (W/m2)
sun or lamp 0.00
after cut-off 0.00
after ND 0.00

G(x) model: Constant generation G
Ideal Light Current in G(x) (mA/cm2) 20.0000
Transmission of attenuation filter (%) 100.00
Ideal Light Current in cell (mA/cm2) 0.0000

☐ I-V	V1 (V)	0.0000	V2 (V)	0.8000	41	0.0200 increment (V)
☐ C-V	V1 (V)	-0.8000	V2 (V)	0.8000	81	0.0200 increment (V)
☐ C-f	f1 (Hz)	1.000E+2	f2 (Hz)	1.000E+6	21	5 points per decade
☐ QE (IPCE)	WL1 (nm)	300.00	WL2 (nm)	900.00	61	10.00 increment (nm)

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Figure 2: Dedicated Panels of SCAPS-1D

III. RESULTS AND DISCUSSION

After simulating the model on SCAPS 1D simulator it was found that WS2 is excellent material for thin film applications as it is found having comparable properties to that of perovskites and cigs solar cells. The voltage verses current characteristics of perovskite and cigs solar cells were compared with that of proposed thin film model and quantum efficiency curves of the models were also compared. Following characteristic curves were obtained as a result of software simulations.

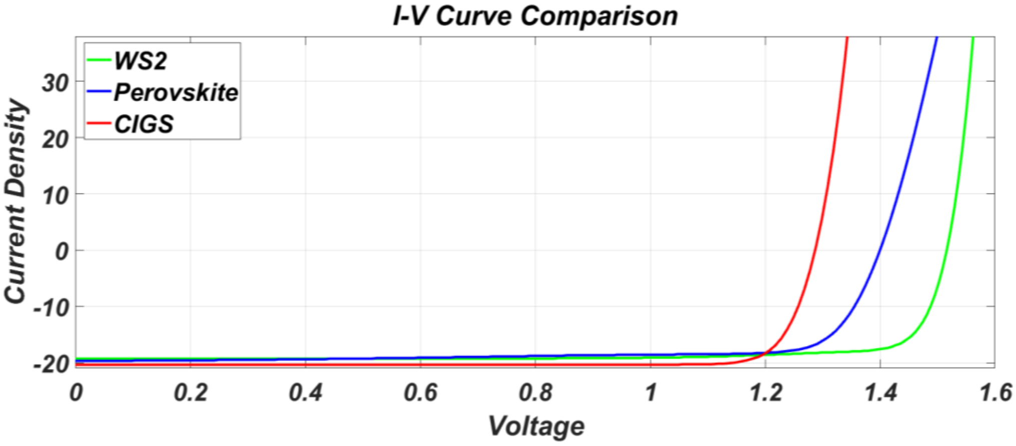

Figure 3: VI Characteristic Curves Comparison

Figure 3 describes that WS2 shows better characteristic properties as compared to perovskite and cigs based solar cells in term of open circuit voltage but relatively low current densities. These parameter describe the efficiency and fill factor of solar cells. Similarly quantum efficiency curves of the models are also obtained using SCAPS 1D simulator and MATLAB. Following quantum efficiency curve is obtained using the above mentioned materials.

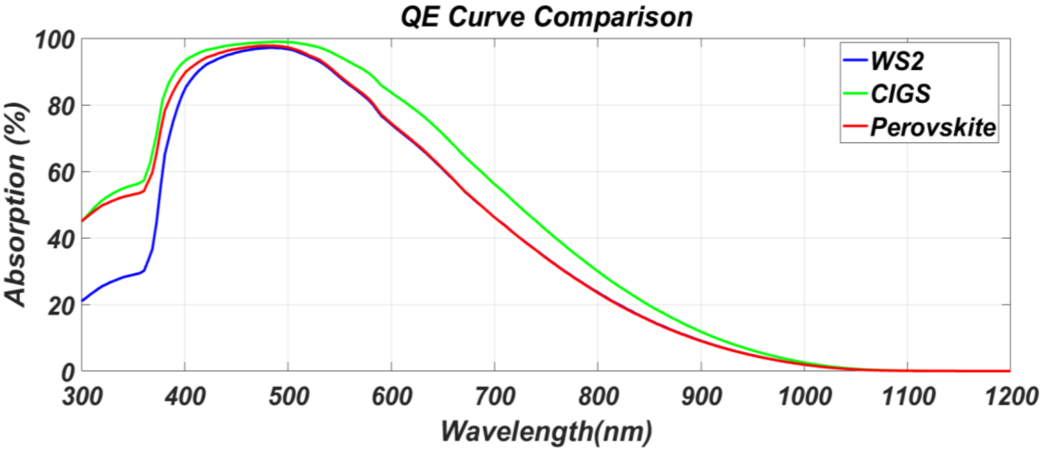

Figure 4: Quantum Efficiency Curv

Figure 4 shows comparison characteristic curves of the models representing quantum efficiency verses wavelength of incident light. Quantum efficiency of WS2 lies in between that of cigs and perovskite.

Table 2: Photo-Electric Parameters of the proposed model

Material	**Voc** *(eV)*	**Jsc** *(mAcm^{-2})*	**Efficiency** *(%)*	**Fill Factor** *(%)*
Reference CIGS	0.86	30.56	21.0	84
Reference Perovskite	1.32	20.5	21.2	80
Proposed WS_2 based Model	0.9	25.5	20	85

CONCLUSION

Tungsten disulfide is a good alternative for cigs and perovskite in thin films as an absorbing material because of its better photo electric parameters. Moreover WS2 is inexpensive and nontoxic material. It provides better open circuit voltage (Voc), short circuit currents (Jsc), efficiency (ŋ) and fill factors (FF). Three dimensional modelling of the proposed model open gates for research community in photovoltaics to investigate WS2 for electricity generation.

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