2019 International Conference on Electrical, Computer and Communication Engineering (ECCE),
7-9 February, 2019

Design and Optimization of an Efficient Molybdenum Disulfide (MoS_2) Solar cell with Tin Sulfide BSF

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***Abstract*—Two-dimensional molybdenum disulfide (MoS_2) is a potential sunlight harvester due to low cost, layered type atomic structure, favorable electrical and optical properties. The performance of a molybdenum disulfide (MoS_2) photovoltaic cell is investigated by using the wxAMPS simulator. The hidden potentiality of MoS_2 is unfolded by using BSF strategy. The photoconversion efficiency is found 21.39% (J_{sc} = 29.89 mA/cm^2, V_{oc} = 0.841V and FF=0.856) for 1 µm MoS_2 absorber layer with 100 nm SnS BSF whereas in conventional structure, it is found 19.48% (V_{oc} = 0.826V, J_{sc} = 27.848 mA/cm^2, and FF = 0.846) without BSF for 1 µm MoS_2 absorber layer. The measured temperature coefficient (TC) is -0.047%/°C for conventional photovoltaic cell structure and -0.046%/°C for a modified structure with SnS BSF. It indicates the better thermal stability of the modified structure compared to the conventional structure.**

Keywords— Photovoltaic cell; Transition Metal Dichalcogenide; Back Surface Field; Thermally Stable.

I. INTRODUCTION

Energy is the key to the development and prosperity of a country. It is not possible to fully defend on fossil fuel from conventional sources of energy due to their negative impact on the environment and will run out in the near future. Renewable energy sources are not only environment friendly source of energy but also abundant in nature. Among diverse type of green energy sources, the contribution of solar energy in the field of renewable energy is most significant than others. It is also the cleanest and the most sufficient renewable energy source that are available in the earth.

MoS_2, WS_2, $MoSe_2$,WSe_2, TiS_2, $TiSe_2$ etc. are layered type transition metal dichalcogenide semiconductor material which have drawn attention as photovoltaic material from few decades .Among them MoS_2 is an indirect band gap material of 1.3 eV which has become a direct band gap material of 1.8 eV if it turns into a single atomic layer [1, 2]. The absorption coefficient of MoS_2 is close to 10^6 cm^{-1} which is similar between the thicknesses of few micro-meters to less than 100 Å [3].

In 2012, Shanmugan et al. observed the photovoltaic response of MoS_2 by fabricating a Schottky–barrier photovoltaic cell with the structure of ITO/MoS_2/Au which exhibits a PCE of 0.7% for the thickness of 110 nm of molybdenum disulfide and 1.8% for 220 nm thick molybdenum layer [4]. This identical team also fabricated ITO/TiO_2/MoS_2/P3HT/Au structure with power conversion efficiency of 1.3%, J_{sc} = 4.7 mA/cm^2 and V_{oc} = 0.56 V [5]. A hetero-junction photovoltaic cell structure of n-MoS_2 (monolayer)/p-Si is fabricated by Tsai et al. which exhibits a photo conversion efficiency of 5.23% with FF = 0.57, V_{oc} = 0.41 V and J_{sc} = 22.36 mA/cm^2 [6]. A solar cell structure of n-ZnO/n-CdS/p-MoS_2 was simulated Rashid et al. with conversion efficiency of 19.62% indicating MoS_2 as a potential absorber layer of solar cell [7].

A recognized way to ameliorate the proficiency of solar cell is the use of back surface field (BSF) between the rare contact material and absorber material which shorten the recombination loss. BSF do the function of electron reflector by creating an electric field. The moderation of conduction band barrier height width is done by incorporating a heavily doped back surface field of precise material to reflect the electron. The theoretical background of BSF is exposing it as a precise material for thin film technology [8].The back surface field technique is investigated in CdTe solar cell [9-16], CIGS solar cell [17, 18], $MoTe_2$ solar cell [19, 20] and AlSb solar cell [21] to enhance the performance of the photovoltaic cell.

The contribution of BSF technology in molybdenum disulfide (MoS_2) photovoltaic cell has been mastered in this work with a 100 nm thick Tin Sulfide (SnS) BSF material. Due to the favourable work function of SnS, ohmic contact formation becomes easier. It is also an earth abundant, low cost and environment friendly material. ZnSe exhibits superior performance than other window material due to it's widen band gap and ITO is evaluated as the best TCO material due it's extraordinary conductivity and transmittancy. A recently developed wxAMPS simulator is used for operating the numerical analysis of both conventional and modified structure.

II. NUMERICAL MODELING, MATERIAL PARAMETER AND SIMULATION

Numerical modeling of solar cell is a process for examining the prospect of ultra-thin MoS_2 photovoltaic cell for superior cell performance and improved thermal stability. It also

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checks the legitimacy of the modified photovoltaic cell formation. wxAMPS solar cell simulator has been used to design the solar cell in an efficient manner. It is an updated version of AMPS solar cell simulator with better interfaces and functions. Two tunneling models are incorporated in wxAMPS. They are intra-band tunneling [22] and trap assisted tunneling [23] where the most realistic result of the hetero-junction solar cell is provided by intra-band tunneling [24].

The conventional cell structure based on MoS_2 absorber layer generally consists of a window layer and TCO layer. The best suited and efficient window layer for MoS_2 absorber layer is ZnSe because of it has widen band gap and well bi-layer formation without serious defect. ITO is used as TCO layer for the most effective way of light passing with lower consumption of photon energy so that maximum photon energy can reach to the absorber layer for better cell performance. Nickel is used as back contact material for both conventional and modified cell structure.

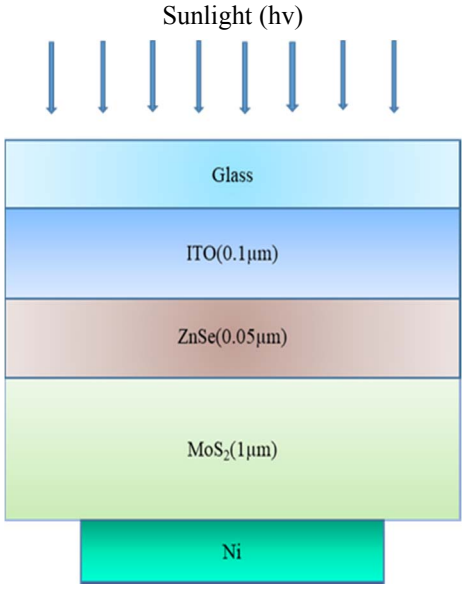

Fig. 1 Traditional MoS_2 photovoltaic cell structure

A SnS BSF material has been inserted between MoS_2 absorber material and Ni rare contact to observe the dominance of BSF strategy on the competence of molybdenum disulfide based cell structure. Photovoltaic cell without BSF layer, where absorber layer directly connected to the back contact faces back surface recombination and a barrier height problem. The cell performance is affected due to these problems. These problems can overcome by inserting a highly doped BSF material between rare contact and MoS_2 absorber layer. The BSF layer improves the cell performance than the conventional cell by reducing not only the recombination loss but also the barrier height of the bi-layer interface. Thus, for better cell performance modified cell structure with BSF layer is shown in Fig. 2.

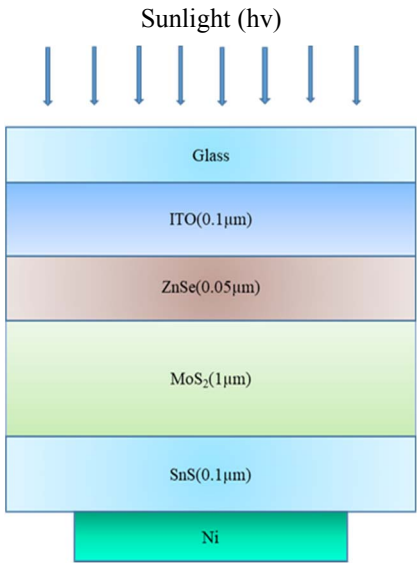

Fig. 2 Proposed structure of MoS_2 photovoltaic cell with SnS BSF

To simulate both conventional and proposed cell structures, electrical and optical properties of each layer are used from the experimental value and literature reviews and estimation in some cases [7, 21, 25, 26]. The electrical properties of different material used in simulation are demonstrated below in Table I for MoS_2 photovoltaic cell.

TABLE I ELECTRICAL PARAMETER OF THE DIFFERENT MATERIAL USED FOR SIMULATION

Parameters	**n-ITO**	**n-ZnSe**	**p-MoS_2**	**p-SnS**
Thickness(μm)	0.1	0.05	1	0.1
Bandgap E_g (eV)	3.6	2.58	1.29	1.25
Permittivity	9	9.2	13.6	12.5
Electron affinity χ (eV)	4.5	4.1	4.2	4.2
Density of States in conduction band N_c (cm^{-3})	2.22×10^{18}	1.5×10^{18}	2.22×10^{18}	1×10^{19}
Density of states in valance band N_v(cm^{-3})	1.8×10^{19}	1.8×10^{19}	1.8×10^{19}	4.13×10^{19}
Carrier concentration n, p(cm^{-3})	1×10^{18}	3×10^{19}	1×10^{17}	6×10^{18}
Hole mobility μp(cm^2/Vs)	25	28	150	100
Electron mobility μe(cm^2/Vs)	100	540	100	25

III. Results And Discussion

A. Absorber Layer Thickness Optimization

To get better cell performance, material preservation and thickness optimization of absorber layer are two main objectives of this research work. For conventional cell structure, the first step is to optimise the window layer thickness and then TCO layer. The thickness of window and TCO layer is diminished to 50 nm and 100 nm respectively by optimization. In the second step, thickness and doping concentration variation of absorber layer have been accomplished to observe the cell performance.

Through the numerical analysis effect of absorber layer on the performance of solar cell is observed for conventional solar cell structure with ITO/ZnSe/MoS_2. As the absorber layer is the main component of solar cell it is rule in the operation of solar cell is significant. The thickness of absorber layer is varied to examine the solar cell output parameters. With the increasing thickness of absorber layer power conversion efficiency is also in increasing trend significantly up to 1 µm and after this thickness of 1 µm solar cell performance does not increase satisfactorily with the increasing thickness of absorber layer. So it is considered as the optimum thickness of absorber layer.

B. Effect of SnS BSF Layer on the Cell Performance

A heavily doped SnS BSF layer is inserted between the absorber layer and back contact to overcome the recombination and, which will further increase the cell performance. In this analysis procedure, thickness of absorber layer is varied from 0.1 µm to 5 µm to investigate the cell performance without BSF and with 100 nm SnS BSF. Comparison without and with SnS BSF is shown below in Fig. 3 for absorber layer thickness variation.

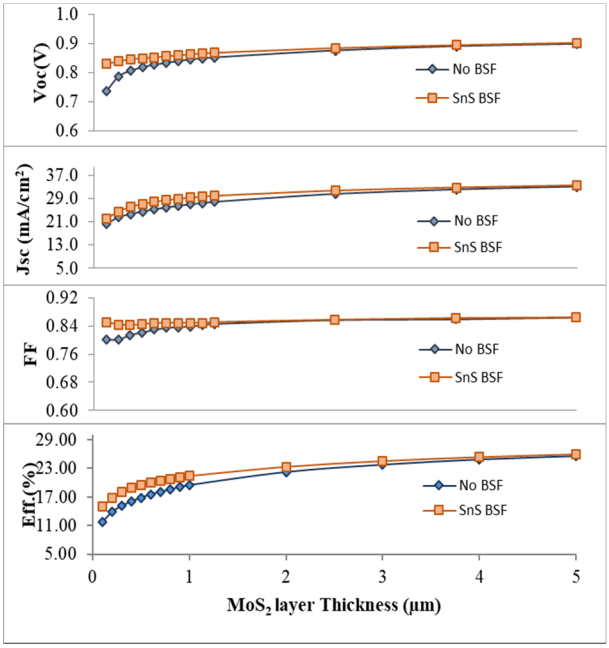

Fig. 3 Absorber layer thickness variation without BSF and with SnS BSF layer

From the above Fig. 3, it is evident that V_{oc}, J_{sc} and FF increases significantly up to "1 µm" due to the insertion of BSF layer between absorber layer and back contact than the conventional cell without BSF. Since the efficiency is the function of V_{oc}, J_{sc} and FF, the overall power conversion efficiency of the modified solar cell increases throughout the whole variation of thickness compared to the conventional solar cell. The modified cell structure is optimized with absorber layer 1 µm without affecting other layer parameters. Due to BSF layer incorporation absorber layer thickness is reduced from 5 µm to 1 µm by accommodating a little bit cell efficiency. Therefore 80% of absorber layer material preservation can be possible through this process. This preservation of absorber layer material can cause more and more generation of solar cell thus more electricity from solar cell. Consequently it will help to overcome the energy crisis in near future. Output parameters of both the conventional and proposed cell are given below in the Table II.

TABLE II PERFORMANCE PARAMETER OF NUMERICALLY SIMULATED CELL STRUCTURE WITH AND WITHOUT BSF

Parameter /cell structure	V_{oc} (V)	J_{sc} (mA/cm^2)	FF	η (%)
Base structure	0.826	27.84	0.846	19.48
With SnS BSF	0.841	29.89	0.850	21.39

The impact of SnS back surface field on the *J-V* curve is explored from Fig. 4. Both series resistance and shunt resistance have great impact on *J–V* characteristics curve as V_{oc}, J_{sc} and FF all of them are affected by their values.

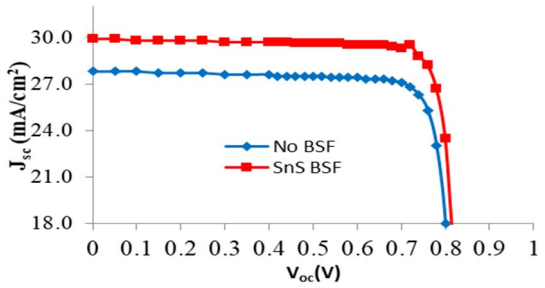

Fig. 4 Impact of BSF layer on J-V curve of MoS_2 solar cell

The J-V curve is shifted right for SnS BSF indicating the excellent performance of MoS_2 solar cell with the increased amount of open circuit voltage and short circuit current.

C. Effect of Doping Concentration of Absorber Layer

The performance of MoS_2 based solar cell has been examined for different doping concentration of the absorber layer. The doping concentration of MoS_2 has been varied in the range between 1×10^{12} cm^{-3} to 1×10^{19} cm^{-3} to explore the performance of MoS_2 solar cell with ZnSe window layer and ITO material for TCO layer.

The Fig. 5 shows the performance of MoS_2 based solar cell for different doping concentration. It can be concluded from the Fig. 5 that the fill factor remain almost constant throughout whole variation, where conversion efficiency, V_{oc} and J_{sc} remain almost constant up to 1×10^{16} cm^{-3}. After that conversion efficiency and J_{sc} is in decreasing trend and V_{oc} is in increasing trend. The electric field in the space charge region is increased with the increasing trend of doping concentration of the absorber layer which in turn increases the majority carrier's drift velocity. On the other hand, the higher doping concentration of absorber layer causes higher recombination losses of the minority carrier. The reason behind the reduction of efficiency after a certain doping concentration is the domination of the recombination rate of minority carriers over the drift velocity of majority carriers. The doping concentration of the absorber layer is optimized at 1×10^{17} cm^{-3} which is similar to reference structure [8].

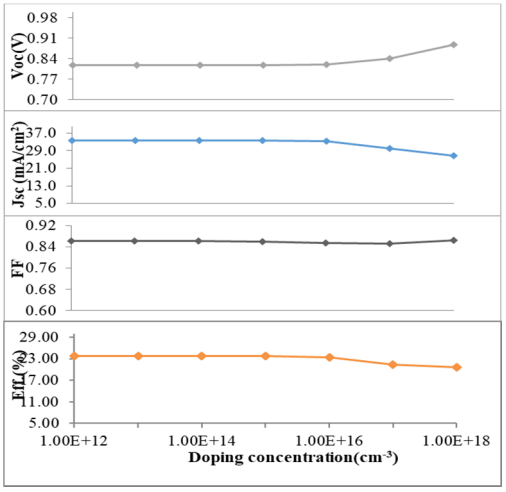

Fig. 5 Effect of doping concentration on the performance of MoS_2 solar cell

D. *Effects of Operating Temperature*

The thermal stability of the MoS_2 solar having no BSF layer and with BSF layer has been studied in the range between 25°C to 150°C for investigating the performance of the solar cell under different operating temperature.

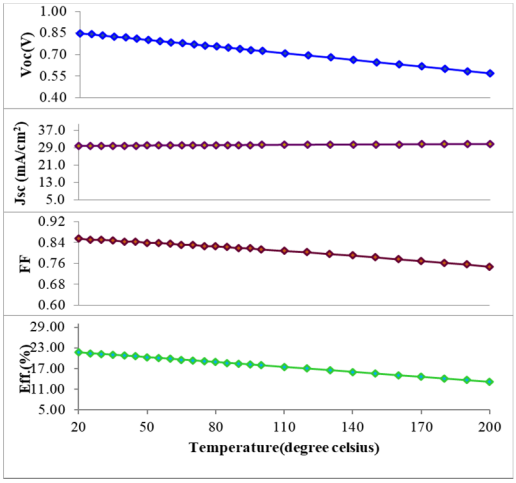

Fig. 6 Observation of performance parameters of MoS_2 photovoltaic cell under different operating temperature

It is observed from Fig. 6 that the reduction of efficiency of the MoS_2 photovoltaic cell is due the reduction of V_{oc} with the increment of temperature. It is further observed that J_{sc} is less affected by the temperature variation.

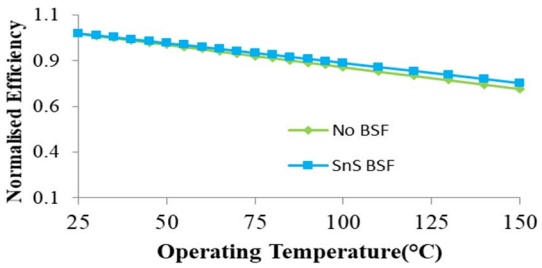

Fig. 7 Normalized efficiency comparison of the MoS_2 solar cell with and without BSF under different operating temperature

The temperature coefficient shows how solar cell power output changes with temperature variation. It is also an indicating parameter of thermal stability of solar cell. It is noticed from Fig. 7 that the performance of the both conventional structure and modified structure lessens almost linearly with the increase of temperature. The temperature coefficient is measured -0.047%/°C for conventional structure and -0.046%/°C for modified structure. It indicates the better thermal stability of the modified structure compared to the conventional structure.

D. *Effects on Quantum Efficiency*

The quantum efficiency is defined as the proportion of the quantity of the number of photon gathered by solar cell to the number of photon incident on it. Since every photon produces an electron hole pair, the ideal quantum efficiency should be 100%. But it doesn't happened in real cell cases due to different type of loss like buffer and window layer absorption, limitation of absorption of the absorber layer, deep penetration and recombination loss. The quantum efficiency of modified cell structure is shown in Fig .7 which has been inquired by wxAMPS solar cell simulator.

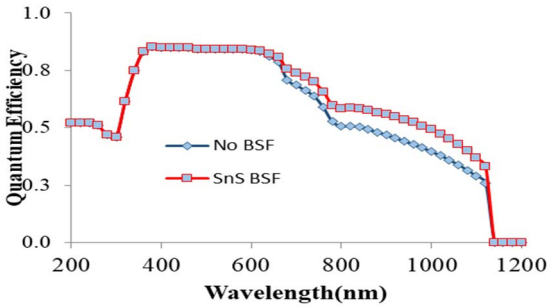

Fig. 8 Quantum efficiency vs. wavelength curve showing the effect of BSF layer

The Fig. 8 indicates the better quantum efficiency of modified structure with SnS BSF than conventional structure. The high absorption properties of SnS and reduction of recombination losses through the insertion of BSF layer, which improve the quantum efficiency as well as the overall performance of the modified structure.

IV. CONCLUSION

The performance of molybdenum disulfide (MoS_2) solar cell has been examined using BSF technology to design an efficient and thermally stable solar cell. Better cell performance has been achieved by using SnS BSF material between the absorber layer and back contact with power conversion efficiency of 21.39% and temperature coefficient (TC) of -0.046%/ºC compared to PCE of 19.48% and TC of -0.047%/°C for conventional structure.

ACKNOWLEDGMENT

This work has been supported by the Department of Electrical and Electronic Engineering (EEE) and Renewable Energy Laboratory (REL), Chittagong University of Engineering and Technology (CUET), Bangladesh.

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