Enhancement the Performance of Molybdenum Telluride Solar Cells with Zinc Telluride BSF

Mrinmoy Dey^{1, 2*}, Maitry Dey³, M. A. Matin^{1, 2} and Nowshad Amin^{4, 5}

¹Department of Electrical and Electronic Engineering, Chittagong University of Engineering and Technology,

Chittagong-4349, Bangladesh

²Renewable Energy Laboratory (REL), Chittagong University of Engineering and Technology,

Chittagong-4349, Bangladesh

³Department of Electrical and Electronic Engineering, Premier University,

Chittagong-4203, Bangladesh

⁴Solar Energy Research Institute (SERI), The National University of Malaysia,

43600 Bangi, Selangor, Malaysia

⁵Department of Electrical, Electronic and Systems Engineering, The National University of Malaysia,

43600 Bangi, Selangor, Malaysia

*mrinmoycuet@gmail.com

Abstract—The binary semiconductor compound Molybdenum telluride (MoTe₂) is For high efficiency and better thermal stability, Molybdenum telluride (MoTe₂) is considered as potential solar cell. AMPS (Analysis of Microelectronic and Photonic Structures) simulator is used to investigate the cell performance parameters for ultra-thin MoTe₂ PV cell. In this research work, it has been explored that the cell conversion efficiency of MoTe₂ PV cell is improved with the insertion of Zinc Telluride (ZnTe) as back surface field (BSF) above the back contact metal. The highest conversion efficiency of 25.29% was found for ZnTe BSF with only 0.7 μ m of absorber layer whereas it was 17.06% for no BSF with 1 μ m thickness of absorber layer. The thermal stability of MoTe₂ PV cell with ZnTe BSF showed better stability.

Keywords— Thermal Stability, Ultra-thin, MoTe₂, Photovoltaic cell, AMPS, ZnTe BSF.

I. INTRODUCTION

Molybdenum Ditelluride (MoTe₂) is commonly known as Molybdenum Telluride and it is considered by the researchers as potential candidate for cost effective, highly efficient, stable PV cells and green energy for thin film technology in earth. Subsequently, some research groups are doing extensive research work to explore the hidden potentiality on MoTe₂ PV cells. The binary semiconductor material MoTe₂ has direct band gap 1.1 eV and the work function is 4.7 eV [1]. The percentage of mass distribution for MoTe₂ material is 27.32% molybdenum (Mo) and 72.68% tellurium (Te).

The higher performance of PV cell, preservation of absorber layer material and better thermal stability are the challenges for $MoTe_2$ PV cell research work. During the production of efficient $MoTe_2$ PV cells, tellurium pressure or

vapour is often play significant role. In this study, Cadmium Sulphide (CdS) window layer is selected with MoTe₂ as absorber layer to form CdS/MoTe₂ PV cells. In this research work, the possibility of ultra-thin MoTe₂ PV cell is investigated with the addition of potential BSF layer at the back contact for higher performance and better cell stability. Many research groups are researching extensively on CdTe solar cells to explore the hidden potentiality by the insertion of back surface field between the absorber layer and back contact metal. The performance of CdS/CdTe solar cell is improved through adding ZnTe BSF discussed by Dey et. al [2], ZnTe BSF as discussed by Dey et. al [3], GeTe BSF as discussed by Dey et. al [4], PbTe BSF as discussed by Matin and Dey [5] and SnTe BSF as discussed by Dey et. al [6]. The insertion of suitable BSF layer placement between the back contact and absorber layer in the proposed cell showed better performance to design this ultra-thin high performance MoTe₂ PV cell.

In this research work, numerical analysis is done by well known AMPS simulator to examine the performance of ultrathin CdS/MoTe₂ cell structure with ZnTe BSF layer to explore the hidden potentiality of MoTe₂ PV cells with improved cell performance parameters. Both the higher cell conversion efficiency (25.08%) and better thermal stability were achieved in the modified proposed cell structure (SnO₂/Zn₂SnO₄/CdS/MoTe₂/ZnTe/Ni) with less than 1 μ m of absorber layer.

II. MODELING AND SIMULATION

To represent the complicated system in a simplified mode, PV cell model is supportive by avoiding the non useful features. Consequently, all the significant parameters are considered and the non important ones are ignored, then a good model can be constructed for analysis. AMPS-1D simulator is widely used more than 200 research groups for designing PV cell structure [7]. The conventional structure of CdS/MoTe₂ PV cell is shown in Fig. 1 for numerical analysis to investigate the different parameters of cell performance.



Fig.1 Modeling of conventional MoTe₂ PV cell

In this research work, the model of conventional $MoTe_2 PV$ cell consists of Stannic Oxide (SnO_2) as TCO (Transparent conducting oxide) layer, Zinc Stannate (Zn_2SnO_4) as buffer layer, CdS as window layer and finally $MoTe_2$ as absorber layer. The hidden potentially of CdS/MoTe₂ cell structure can be explored by adding the potential ZnTe BSF layer in between absorber layer and back contact metal.



Fig.2 Proposed cell structure of MoTe₂ PV cell

In this study, the used materials with different parameters are shown in Table I which are chosen based on experimental data, literature values or in some cases reasonable estimations [3, 8, 9].

TABLE I	THE MATERIAL PARAMETERS USED FOR THE NUMERICAL
	ANALYSIS OF THE PROPOSED CELLS

Parameters	n-CdS	p-MoTe ₂	p-ZnTe
Thickness, W (µm)	0.01-0.1	0.1-10	0.1
Permittivity, ε/ε0	9	13	14
Electron mobility, $\mu c (cm^2/Vs)$	350	110	70
Hole mobility, μp (cm ² /Vs)	50	426	50
Carrier concentration, n, p (cm ⁻³)	1×10 ¹⁷	1×10 ¹⁷	7.5×10 ¹⁹
Band gap, Eg (eV)	2.42	1.10	2.25
Density of state in conduction band, Nc (cm ⁻³)	1.8×10 ¹⁹	1×10 ¹⁵	7.5×10 ¹⁷
Density of state in valence band, Nv (cm ⁻³)	2.4×10 ¹⁸	1×10 ¹⁷	1.5×10 ¹⁹
Electron affinity, χ (eV)	4.50	4.20	3.65

III. RESULTS AND DISCUSSION

A. Optimization of Conventional Cell

The numerical analysis was done by AMPS-1D simulator in conventional CdS/MoTe₂ PV cell to optimize the thickness of CdS window layer as well as thickness and doping concentration of MoTe₂ absorber layer to overcome the challenges of thin film PV cells. Fig. 3 shows the variation of thickness for CdS window layer from 10 nm to 100nm to investigate the performance of MoTe₂ PV cells without BSF layer. From the numerical analysis considering the conversion efficiency and current technology, CdS layer is reduced to 70 nm in the cell structure of CdS/MoTe₂ PV cell for optimization of window layer along with 500 nm TCO layer and 100 nm Zn₂SnO₄ buffer layer.



Fig.3 Effect of the CdS thickness variation on cell performance of the conventional cell

The main challenge of thin film PV cell is to preserve the absorber layer material for GW range solar power generation. Fig. 4 illustrates the thickness variation of absorber layer from 100 nm to 10 μ m to examine the performance of MoTe₂ PV cells. The MoTe₂ absorber layer is optimized to 1 μ m with 500 nm TCO layer, 100 nm Zn₂SnO₄ buffer layer and 70 nm CdS window layer in the CdS/MoTe₂ PV cell structure to design in ultra-thin range.



Fig.4 Effect of the $MoTe_2$ thickness variation on cell performance of the conventional cell

The performance parameters of PV cell are depends on the amount of doping concentration. The effect of doping concentration variation for absorber layer is shown in Fig. 5. For this purpose, the doping concentration of MoTe₂ layer is varied from 10^{13} cm⁻³ to 10^{17} cm⁻³ and the highest cell conversion efficiency is found for higher doping concentration of 10^{17} cm⁻³ which is now practically achievable.



Fig.5 Effect of the doping concentration of $MoTe_2$ on cell performance of the conventional cell

B. Effects of ZnTe BSF Insertion

In this research work, the conventional MoTe₂ PV cell is modified into proposed cell which consists of SnO₂ layer, Zn₂SnO₄ buffer layer, CdS window layer as well as 1 μ m thickness of absorber layer with 10¹⁷ cm⁻³ doping concentration. The modification of conventional cell is completed by adding a high band gap material ZnTe (*Eg* = 2.25 eV) of 100 nm thickness placed above the back contact metal to improve the cell conversion efficiency, thermal stability and preserve the absorber layer also by reducing back surface recombination velocity in between the absorber and BSF layer. Table II shows the effects of ZnTe BSF insertion on MoTe₂ PV cell with 1 μ m thickness of absorber layer. With the insertion of ZnTe BSF layer, the magnitude of cell performance parameters is higher compared to conventional cell structure.

TABLE II THE OUTPUT PARAMETERS OF PROPOSED CELL WITHOUT BSF LAYER AND WITH BSF LAYER

Structure/ parameters	V _{oc} (V)	Jsc (mA/cm ²)	FF	Eff. (%)
Base case	0.98	23.740	0.730	17.06
ZnTe BSF	1.07	27.91	0.842	25.16

Numerical analysis has been done in the proposed cell to investigate the possibility to lower thickness of absorber layer. The simulation results are shown in Fig. 6 that the cell performance parameters are varied with the variation of absorber layer thickness from 0.1 μ m to 5 μ m. It is depicted in Fig. 6 that the cell conversion efficiency is getting increased in the 1 μ m range of absorber layer with highly doped ZnTe BSF. This is because for the improved values of open circuit voltage, fill factor and current density.



Fig.6 Variation of absorber layer thickness in the proposed cell with ZnTe $\ensuremath{\mathsf{BSF}}$

It is found from the numerical analysis that the conversion efficiency is 17.06% for conventional structure of MoTe₂ PV cell without BSF layer. The highest conversion efficiency 25.29% (FF = 0.847, *Voc* = 1.08 V and *Jsc* = 27.61 mA/cm²) is achieved at only 0.7 μ m of absorber layer with 100 nm of ZnTe BSF layer which is approximately 8% greater than the conventional cell structure. These results of cell performance with the addition of ZnTe BSF layer are agreeable to the related published work [8]. The cell performance is improved by reducing back surface recombination velocity through highly doped p-type BSF layer.

C. Effects of Operating Temperature

The thermal stability is important parameter for PV cell and it is determined by the performance of cell under higher operating temperature. In this case, the operating temperature plays a significant role to test the cell performance parameters of the proposed cell with compared to conventional cell structure. From the numerical analysis, the potentiality of ZnTe BSF layer insertion in the proposed cell structure of CdS/MoTe₂ PV cell is observed. The effect of operating temperature is shown in Fig. 7 for both MoTe₂ PV cell without and with ZnTe BSF. The performance of MoTe₂ PV cell is examined for both without and with ZnTe BSF at operating temperature ranging from 25°C to 160°C. The cell performance parameters are decreased at higher operating temperature and the degradation of conversion efficiency is decreased in the proposed MoTe₂ PV cell by adding the potential ZnTe BSF.



Fig. 7 Effect of temperature on cell performances of $MoTe_2$ cell with and without ZnTe BSF

The normalized efficiency has been calculated for $MoTe_2$ PV cell with and without ZnTe BSF. Fig. 8 shows that the normalized efficiency is decreased at higher operating temperature for both cases. In case of no BSF insertion in $MoTe_2$ PV cell, the normalized efficiency is linearly decreased with the increased of operating temperature ranging from

25°C to 105°C. By adding the ZnTe BSF, the normalized efficiency of the proposed cell is almost constant in the operating temperature ranging from 25°C to 55°C with a TC of 0.24%/°C and then from 55°C to 105°C the normalized efficiency is linearly decreased at a temperature co-efficient of -0.34%/°C which shows better stability in the proposed with ZnTe layer.



Fig. 8 Effect of operating temperature on normalized efficiency

IV. CONCLUSION

The effect of ZnTe BSF insertion has been investigated in the proposed ultra-thin MoTe₂ PV cell to achieve higher cell conversion efficiency with lower thickness of absorber layer. The performance of MoTe₂ PV cell with ZnTe BSF showed best cell conversion efficiency of 25.29% (FF = 0.847, *Voc* = 1.08 V and *Jsc* = 27.61 mA/cm²) at 0.7 µm thickness of MoTe₂ absorber layer. The cell conversion efficiency of baseline case MoTe₂ PV cell is 17.06% (FF = 0.730, *Voc* = 0.98 V and *Jsc* = 23.74 mA/cm²) without ZnTe BSF layer. With the addition of ZnTe BSF, the conversion efficiency is increased upto 8%. Moreover, the thermal stability is better at higher operating temperature in case of ZnTe BSF placing between the absorber layer and back contact metal.

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