Chalcogenide Letters Vol. 11, No. 8, August 2014, p. 397 - 403

PROSPECTS OF MOLYBDENUM DISULFIDE (MoS_2) AS AN ALTERNATIVE ABSORBER LAYER MATERIAL IN THIN FILM SOLAR CELLS FROM NUMERICAL MODELING

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Molybdenum Disulfide (MoS_2) is a potential low cost, alternative sunlight harvester for a possible replacement of the conventional photovoltaic materials. It is a suitable photovoltaic absorber material mainly due to its optimum optical and electrical properties. In this work, we numerically analyze both hetero-junction and homo-junction device structures of MoS_2 by 1D-Solar Cell Capacitance Simulator (SCAPS). Both n-ZnO/n-CdS/p-MoS_2 and n-MoS_2/p-MoS_2 show the conversion efficiencies above 19%. We also study various window layer materials to optimize the performance of the hetero-junction structure. The analysis includes the device stability as well operating temperature. The analyzed results indicate the feasible fabrication of high efficiency MoS_2 based solar cells.

(Received July 19, 2014; Accepted August 28, 2014)

Keywords: MoS_2, Thin Film Solar Cells, SCAPS, Absorber Layer, Electrical Performance, TMDC Materials.

1. Introduction

All the potential alternative photovoltaic (PV) materials, introduced recently, need to address three major issues: high efficiency, low cost and stability. Non-conventional MoS_2 is a layered type material under transition metal dichalcogenide (TMDC) compound; it has been under extensive research for the last few years due to the great potentiality of fabricating highly efficient solar cells [1, 2]. The structural lattice of MoS_2 consists of cations and anions with a naive arrangement [1]. It has an indirect band gap of 1.29 eV, while the direct transition starts at 1.6 eV [2, 3]. Layered MoS_2 thin films can be prepared by MOCVD, electro deposition, Pulsed Laser Deposition (PLD) and atomic layer deposition techniques. Its absorption coefficients are higher than 10^5 cm^{-1} for photon energy greater than 1.7 eV [4].

Photoconductive MoS_2 layers necessitate a texturization called type II, where the c-axis of the crystallites needs to be vertical to the plane of the substrate. When the c-axis of the crystallites is parallel to the plane of the substrate, they are not photoconductive and known as type I films. The band gap tuning of MoS_2 is possible by decreasing crystal thickness below 100 nm due to quantum confinement and calculations predict it to reach to 1.9 eV for a single monolayer. By increasing its size, the band gap transforms from indirect toward direct while the layer thickness attains a monolayer. Yet, the high lattice mismatch at the junction is anticipated to turn out high dislocation densities for some fabricated devices. Such dislocations act as minority carrier trapping centers. The optimum electrical performance can be achieved by allowing the formation of a buried junction p-MoS_2/n-MoS_2 near the surface of the MoS_2.

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Optimization of MoS_2 layer is recommended in practical implementation to further enhance the conversion efficiency [5]. In this research work, the main focus is to find out the best electrical performances of Molybdenum Disulfide (MoS_2) thin film solar cells with hetero-junction and homo-junction structures. Moreover, the effects of various operating temperatures along with various layer parameters have also been investigated.

2. Methodology

This numerical study was carried out by using a well-known simulator and being commonly used by many PV researchers named as SCAPS. It abbreviates as Solar Cell Capacitance Simulator and it is a one dimensional computer program for simulating the operation of thin film solar cells. This computer simulation program was developed by Department of Electronics and Information Systems (ELIS), a University of Gent, Belgium. In this work, default defect is used which is "neutral" defect type. Numerous significant parameters related to cell performance and others can be abstracted easily from this simulator such as recombination profiles, electric field distribution, individual carrier current densities, free and trapped carrier populations etc. Performance parameters of simulated solar cell were mainly witnessed to identify short circuit current (J_{sc}), open circuit voltage (V_{oc}), cell efficiency and fill factor in the presence of operating temperature.

The description of electronic properties related parameters and layer parameters used for simulation are shown in Table 1 and Table 2, respectively. In Fig. 1(a) and Fig. 1(b), the basic structure of the hetero-junction and homo-junction solar cell is illustrated respectively. All the material parameters are reviewed from literature and in some cases from reasonable estimation.

Table 1: General electronic properties of a layer

Eg	Energy bandgap (eV)
CHI	Electron affinity χ_e (eV)
EPS	Dielectric permittivity (relative) ε_r
NC	Effective density of states in conduction band ($1/cm^3$)
NV	Effective density of states in valance band ($1/cm^3$)
MUP	Hole band mobility μ_p (cm^2/Vs)
MUN	Electron band mobility μ_n (cm^2/Vs)
ND	Donor concentration ($1/cm^3$)
NA	Acceptor concentration ($1/cm^3$)

Table 2: Simulated layer properties

Layer	**ZnO**	**CdS**	**MoS_2**
Layer Thickness (μm)	0.2	0.05	1.0
EPS	9	9	13.6
MUN (cm^2/V-sec)	100	100	100
MUP (cm^2/V-sec)	25	25	150
NA ($1/cm^3$)	0	0	1.0E+17
ND ($1/cm^3$)	1.0E+18	1.0E+17	0
EG (eV)	3.3	2.4	1.29
NC ($1/cm^3$)	2.2E+18	2.2E+18	2.2E+18
NV ($1/cm^3$)	1.8E+19	1.8E+19	1.8E+19
CHI (eV)	4.45	4.2	4.2

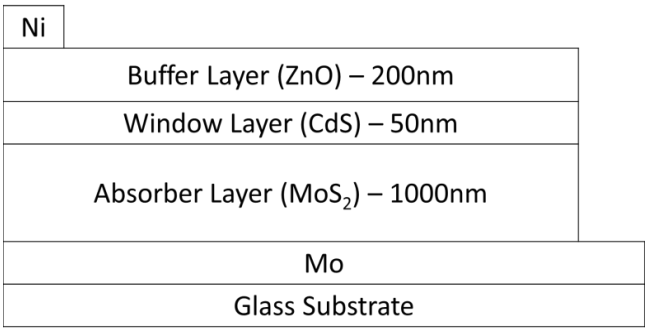

Fig. 1(a): Basic structure of the MoS_2 hetero-junction solar cells

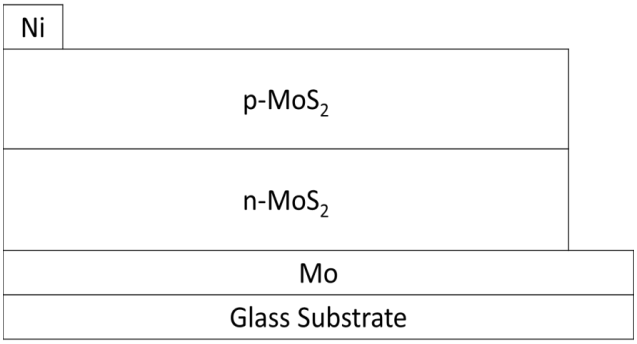

Fig. 1(b): Basic structure of the MoS_2 homo-junction solar cells

3. Result and discussions

3.1 Thickness variation effects of MoS_2

The layer thickness of MoS_2 has been varied from 0.50 μm to 2.0 μm and a highest efficiency of 22% is attained for 2.0 μm film (Fig. 2). A 50 nm thick buffer layer has been used to carry on the simulation work. However, it is really essential to optimize the growth process of the absorber layer since parallel growth to substrate is desirable. Increase in absorber layer means increase in p-type layer of the solar cells. This allows the longer wavelengths of the illumination to be collected which in turn contribute to Electron Hole Pair (EHP) generation. Therefore, the values for V_{oc} and J_{sc} have increased. It is also understood that both the V_{oc} and J_{sc} values will be reduced if the thickness of the absorber layer is reduced. This may be caused by insufficient absorption of the longer wavelength photons as well as the recombination process at the back contact of the solar cell with thinner layers. As the absorber layer thickness is reduced, the back contact will be very close to the depletion region. Thus electrons will be captured easily by the back contact interface which is full of recombination centers. If the absorber layer thickness is increased further than the optimum thickness of 1 μm, the conversion efficiency increases in a much slower rate. This is due to the EHP, which has to travel longer distances in a thicker absorber layer [6, 7].

Fig. 3 is showing spectral response of MoS_2 based solar cells. In the range of 350 nm to 500 nm regions, a very high quantum efficiency of around 90% is observed. These results depict that higher number of photons will be absorbed with the increment in absorber layer thickness. The high percentage of photon absorption will certainly perform a significant role to increase current density.

3.2 Effects of various buffer layers

To acquire optimum electrical performance, various latent buffer layers such as ZnS, InS, ZnO and ZnSe were examined during simulation. To make a good junction partner with a p-type absorber, a buffer material should be n-type or possibly intrinsic (i-type). The lattice constants of the absorber and buffer need to be matched to suppress the interfacial defects, which cause undesirable recombination of carriers. Moreover, these buffer materials are having sufficiently

widened band gaps. By considering all these aspects mentioned above, buffer layers have been chosen. Though ZnS consists of higher band gap, the efficiency is quite low which could happen due to the band offset in the conduction band of absorber layer material. Buffer thickness of 50 nm has been used for all the cases. An efficiency of 20.66% has been attained by using ZnO as buffer layer with MoS_2 as absorber layer. It is proposing that it might be a prospective alternative to CdS (Fig. 4).

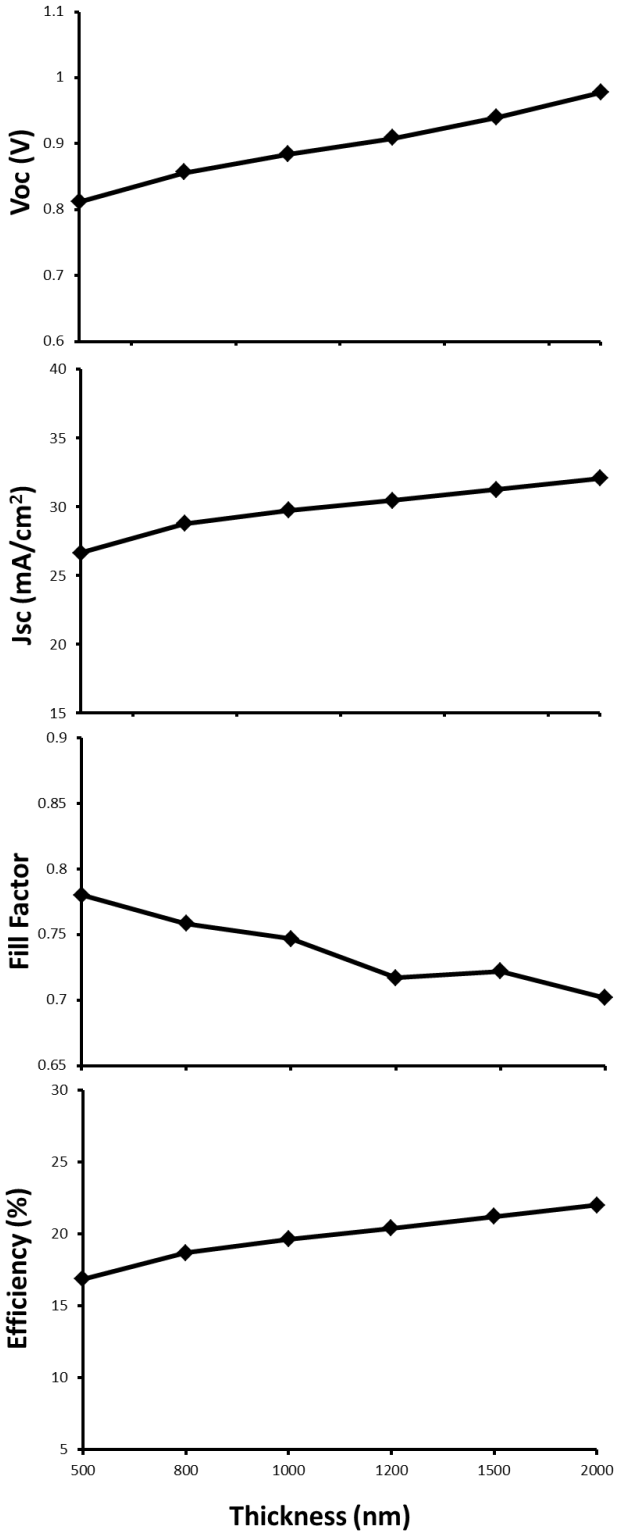

Fig. 2: Effects of various MoS_2 absorber layer thicknesses

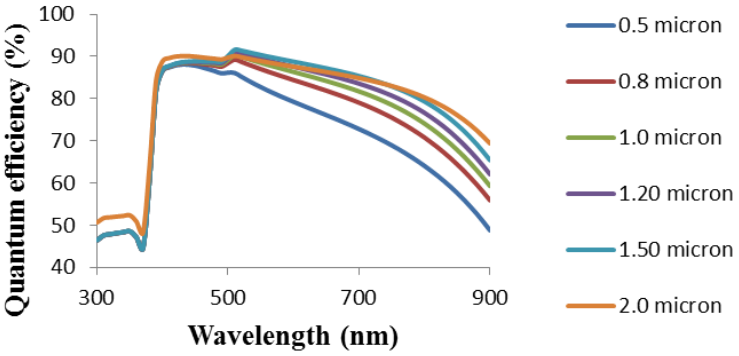

Fig. 3: Spectral response for different MoS_2 absorber layer thicknesses

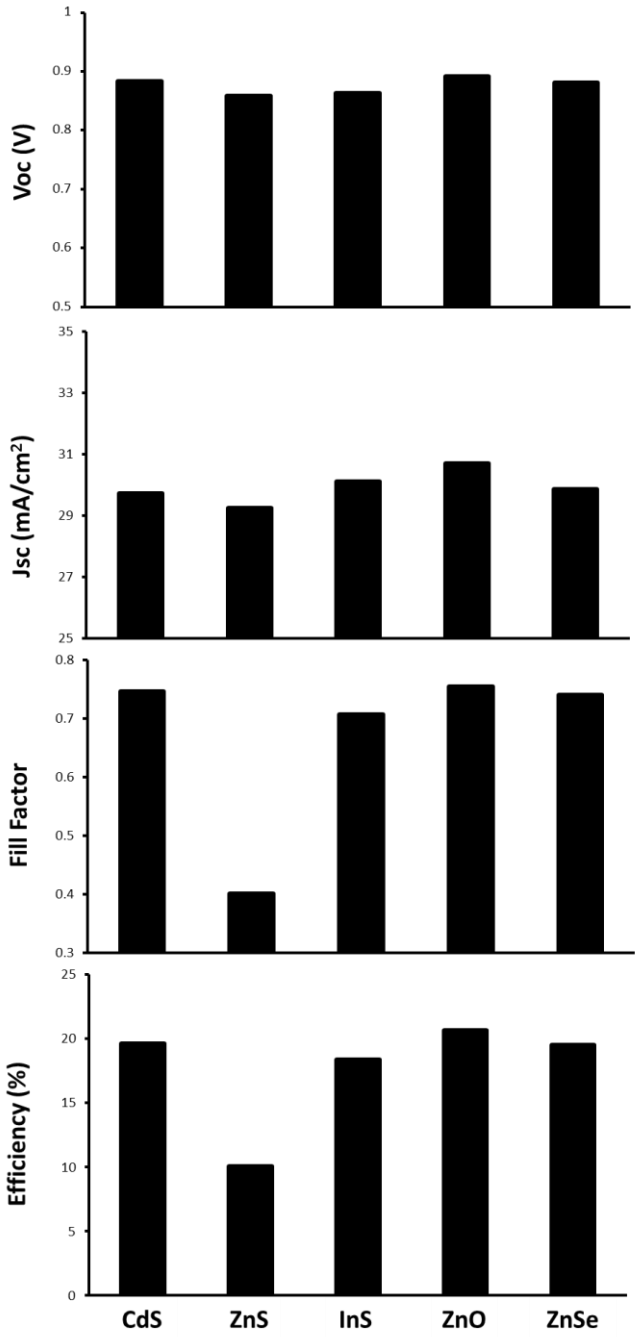

Fig. 4: Performance analysis of MoS_2 with various buffer layers

3.3 Temperature effects on MoS_2 solar cells

Operating temperature has a significant effect on the performance of the solar cells. In this work, a temperature of 300 K was fixed for most of the cases. From Fig. 5, it can be found that the overall efficiency is sternly affected by the operating temperature. The efficiency starts decreasing with the temperature rise, subsequently the carrier concentration; band gaps of materials; electron mobility and hole mobility would be affected. Energy bandgap becomes narrower at high temperature due to the thermal vibration and this will possibly speed up the recombination of electron hole pairs between conduction band and the valence band [6]. The band gap energy is unstable at high temperature which leads to higher rate of carrier recombination while roaming across the regions. Operating temperature has been varied between 300 K and 400 K to examine effects for MoS_2 based solar cells; whereby it is found higher operating temperature affects the MoS_2 based solar cells at the rate of –0.25%/^{o}C.

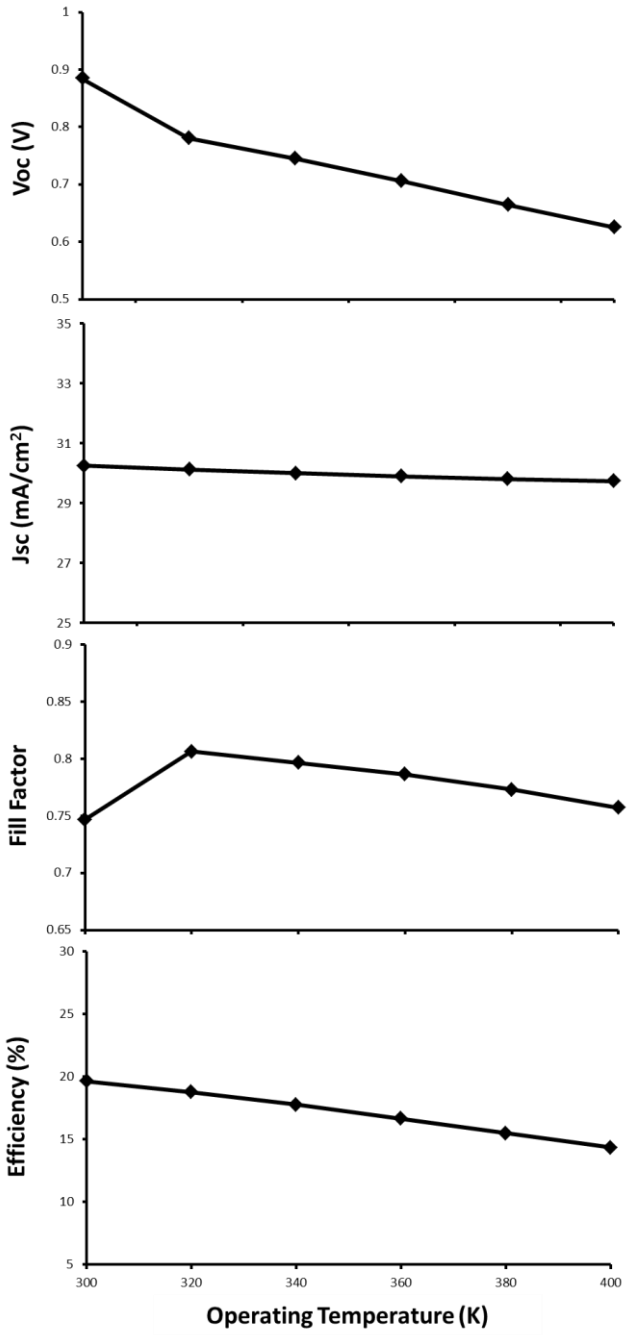

Fig. 5: Solar cell performance with different operating temperatures

3.4 Effects of Homo-junction structure

In this work, homo-junction structure is also evaluated for MoS_2 based solar cells. Significantly, a very much impressive result has been found. Homo-junction MoS_2 solar cells with device structure n-MoS_2/p-MoS_2 shows an efficiency of 26.1% with V_{oc} = 0.93 V, J_{sc} = 36.65 mA/cm^2 and a fill factor of 76.88%. However, doping investigation needs to be carried out to find out the feasible homo-junction fabrication.

4. Conclusion

The performance parameters of MoS_2 solar cells have been investigated in this study. The simulation results are clearly evident that MoS_2 based solar cells have notable performance range which is competitive with other existing thin film solar cells. The highest efficiency attained for hetero-junction MoS_2 solar cells is 19.62% and homo-junction is about 26.1% (V_{oc} = 0.93 V, J_{sc} = 36.65 mA/cm^2 and FF of 76.88%) with the preferable sub-micron thickness. However, the values might not be realistic at this point, but shows clear trend of improvement if proper optimization is done for all layers and associated parameters. Further numerical and practical studies are recommended especially in the field of interface defects which is proposed as the factor that degrades the solar cells performance.

Acknowledgment

The authors would like to acknowledge and thank University of Gent, Belgium for providing the SCAPS simulator programme used in this study and Qatar Environment and Energy Research Institute (QEERI) for their full support. Gratitude is also extended to Qatar Foundation for providing the research grant with the grant code NPRP 6-931-2-382.

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