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Thin Film Dichalcogenide $MoSe_2$ Solar Cell with Optimized Design Parameters

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Abstract: *Efficient conversion of solar light into electricity is being investigated since long time past. Recent research on solar cell is motivated in a new direction with the use of dichalcogenide materials. We have studied here metal-dichalcogenide $MoSe_2$ solar cell. Design parameters are optimized to achieve maximum efficiency, better current density, high photo-voltage and improved fill factor.*

Keywords: *Chalcogenide, ITO layer, Back Surface Field, conversion efficiency, Shockley Queisser.*

I. Introduction

Solar energy reaching the Earth surface is so abundant that it surpasses our power needs by three orders of magnitude. Yet the existing issues and challenges are high conversion efficiency of the solar cells at low cost and of high durability. Contemporary silicon cells are mainly wafer based whereas recent thin film cells are only of a few micron thickness sufficient to absorb the entire radiant visible sunlight. Growing interest in the chalcogenide materials lies in relatively simple maneuvering the bandgap by controlling the concentration. Also, the recent development and realization of single layers of semiconducting metal-chalcogenide $MoSe_2$ have created interests to this material in harvesting efficient solar power conversion and to use in different optoelectronic devices. Like other 2D materials they also have amazing electronic and mechanical properties completely different from its 3D counterparts and so may find use in a host of novel thin film device applications. Direct gap semiconductors, like $MoSe_2$, are very much useful in solar cells and in other photonic devices because of relatively easier production and efficient exploitation of electron-hole pairs. Further, its relatively narrower bandgap of 1.5 eV, compared to the very common photo-catalytic material TiO2, matches well with the visible solar spectrum and infra-red light as well. This bandgap lies in between 1.0eV and 1.6eV and hence according to the Shockley-Queisser limit for the maximum theoretical efficiency of a solar cell, $MoSe_2$ is an important potential material to yield an efficient cell. Like any other chalcogenide based cells $MoSe_2$ also offer pretty long time durability and stability in power conversion efficiency. In our investigation of thin film $MoSe_2$ solar cell the entire process of solar conversion takes in three steps viz. (i) the solar quanta is absorbed in the base material acting also as a substrate (ii) generation of EHPs in the substrate and finally (iii) the carriers are separated by the built in field at junction.

II. Cell Modeling

To model the device we start with four different layers and an ITO layer. This ITO layer, made up of transparent TiO_2, is mainly used for the protection of the device from external hazards. The first layer is n+ doped $MoSe_2$ of thickness 0.1μm. Due to high absorption coefficient maximum amount of light is absorbed in minimum thickness. Also due to its high work function Schottky effect is avoided. The second layer is lightly n doped and its thickness is 0.1 μm which is very small due to high absorption coefficient. Main absorber layer of the device is the third layer. It is doped of with moderate level of p type material of thickness 4μm. which is much higher than the upper layer. Maximum absorption is done in this layer. Finally, the last layer is p+ doped. It creates a back surface field (BSF) to repel the minority electrons back to emitter.
A schematic of the model cell is shown in the Fig-1.

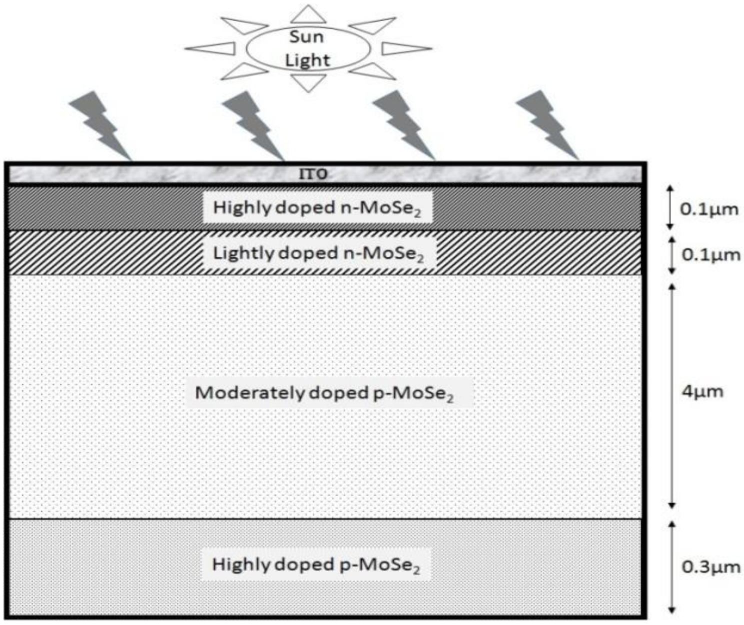

Fig 1: Schematic of the $MoSe_2$ solar cell

III. Cell Simulation

Performance of the solar cell in terms of its associate parameters is simulated by a simulator e.g. PC1D. The model cell is excited under sun light to generate solar power. Steady state intensity of 0.1 W/cm^2 from AM 1.5 light sources is used at a temperature of 25^{0}C [6-8].

IV. Results and discussions

1. Simulated results of open circuit voltage V_{OC} and short circuit current I_{SC} are found to be 0.49 V and -0.025 A respectively at the doping level and cell dimension optimization.
2. Overall percentage efficiency of our cell of 1 cm^2 area is calculated from the formula of

$$\eta = \frac{\text{output power (W)}}{\text{surface area (cm}^2) \times \text{intensity of light (W/cm}^2)} \times 100\%$$

and is found to be $\approx$ 12.1%

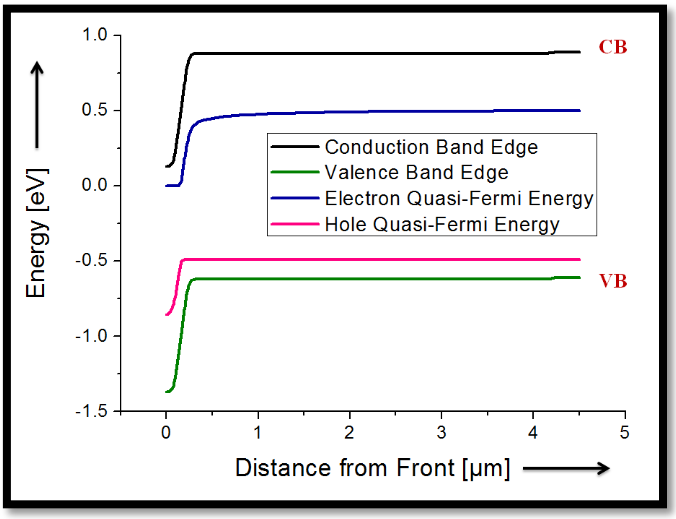

Fig 2: Energy band diagram of this $MoSe_2$ solar cell

For Fig-2 we represent the energy band structure of the solar cell. As the top two layers of this cell has been doped with n-type, so the conduction band edge is much closer to electron quasi Fermi level, than the valance band edge to the hole quasi Fermi level. Similarly, as bottom two layers has been doped with p-type, so the valance band edge is much closer to hole quasi Fermi level than the conduction band edge to the electron quasi Fermi level.

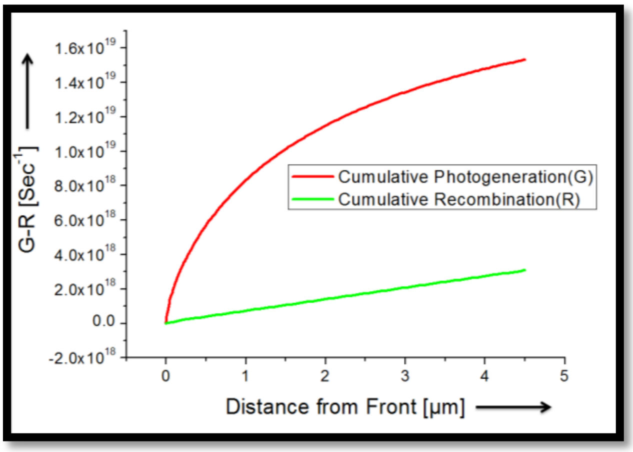

Fig 3: Generation & Recombination in this $MoSe_2$ Solar cell

The generation (G) and recombination (R) of carriers are shown in Fig-3. It is observed from the graph that photo-generation rate is much higher than the recombination rate and the separation between two curves are increased by moving deeper into the cell.

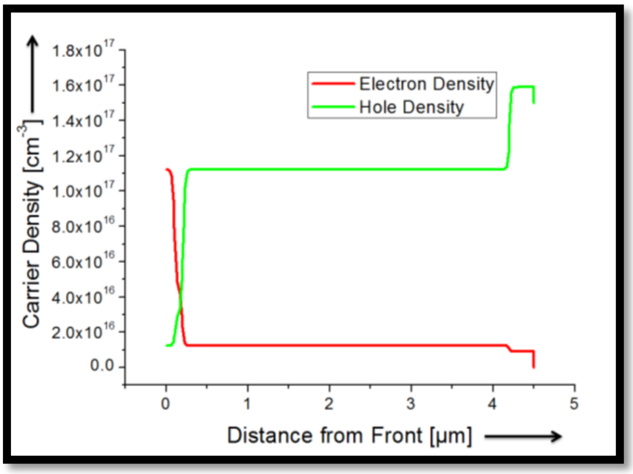

Fig 4: Carrier Densities in this $MoSe_2$ solar cell

Variation of carrier density with depth is depicted in Fig-4. It is noticed that the hole density is high in two bottom regions and low in the two top regions as compared to electron density because the top two regions are doped with n-type and bottom two regions are doped with p-type.

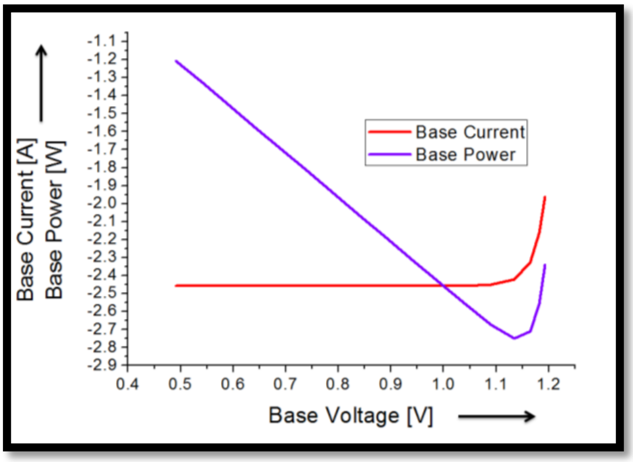

Fig 5: I-V curve and power curve of this $MoSe_2$ solar cell

The I-V characteristics and the power curve are plotted in Fig-5. As shown in the graph, the current curve is almost parallel to the x-axis due to the constant value of the short circuit current -0.02457 A. Whereas the power curve is keep on decreasing in negative direction because the solar cell always generate power. This negative power means, instead of consuming energy it generates solar energy.

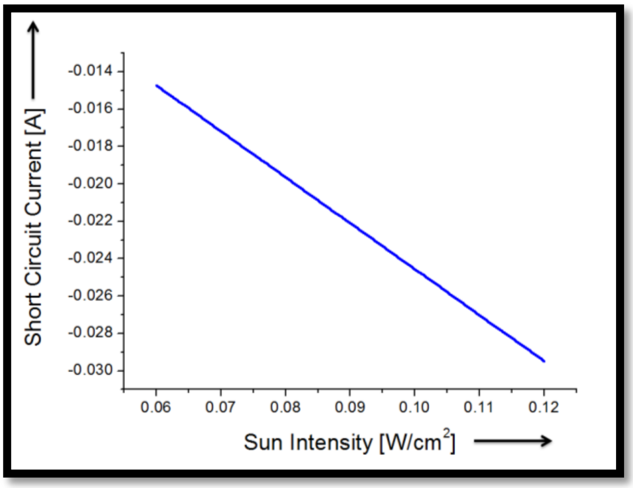

Fig 6: Short circuit current vs. solar radiation intensity

In the tropical countries the air mass coefficient is 1.5. In AM1.5 the sun intensity ranges from 0.068 W/cm^2 to 0.105 W/cm^2 [10]. Keeping this data in view, we have also shown the variations of short circuit current and open circuit voltage with solar variation intensity in Fig-6 and Fig-7 respectively. Short circuit current is seen to decrease and open circuit voltage to increase with solar radiation intensity.

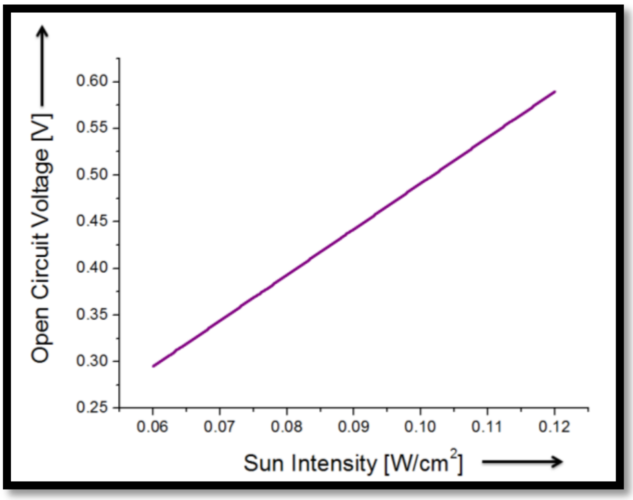

Fig 7: Open circuit voltage vs. solar radiation intensity

Here in this solar cell instead of using different substrate for different regions, we are using $MoSe_2$ as a substrate for all the regions. Some properties of $MoSe_2$ are given in the Table-1. As in this cell there are no hetero junctions present, that is why there is no need to worry about the lattice matching of the material. This cell has four regions with four different types of doping concentrations; those are mentioned in Table-2.

TABLE I. CHARACTERISTICS OF $MOSE_2$

Parameter	*Values*
Bandgap(eV)	1.5
Electron Affinity(eV)	4.45
Dielectric Permittivity(relative)	22.1
Electron mobility(cm^2/v-s)	55
Hole mobility(cm^2/v-s)	10
Refractive index	4.92

TABLE II. DOPING CONCENTRATIONS

Regions	*Type of doping*	*Thickness*	*Doping concentration*
Region-1	Highly doped n-type	0.1μm	1×10^{17} cm^{-3}
Region-2	Lightly doped n-type	0.1μm	1.5×10^{16} cm^{-3}
Region-3	Moderately doped p-type	4μm	1×10^{17} cm^{-3}
Region-4	Highly doped p-type	0.3μm	1.5×10^{17} cm^{-3}

V. Conclusion

The $MoSe_2$ solar cell is one of the most promising photovoltaic devices due to its relatively higher conversion efficiency (>12%) and low material cost. Also, the fabrication process is simpler due to the material homogeneity. Easy market availability of the material is an added advantage. The efficiency can further be enhanced to higher value by adding one top layer of silica powder [9]. This silica powder is used to trap the light and helps to send more light into the cell.

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