European Journal of Molecular & Clinical Medicine
ISSN 2515-8260 Volume 07, Issue 07, 2020

Numerical Simulation Of Sb_2S_3 Based Photovoltaic Cell

Ashutosh Kumar, D. Kumar

School of Chemical Engineering and Physical Sciences
Lovely Professional University, Punjab.

Abstract: ***Sb_2S_3 is emerged as potential candidate for the contemporary thin film solar cells. The optical properties such as band gap of 1.65 eV approximately, high absorption coefficient > 10^4 cm^{-1} etc. satisfy the quality an ideal absorber layer. In the current article, physical properties of Sb_2S_3 have been reviewed. To understand the architecture of Sb_2S_3 thin film solar cell, an attempt is made to simulate the device using one dimension solar capacitance simulator (1D-SCAPS) program. The simulation is carried out on the solar cell Glass/Mo/Sb_2S_3/CdS/i-ZnO/Al:ZnO. The efficiency calculated by the simulation is more than 11%.***

Keywords: Sb_2S_3, solar cell, SCAPS, JV-characteristics

1. Introduction

In modern world, there is a demand of a sustainable, renewable, cost efficiency and clean energy to reduce the major problems of global warming. The renewable energy sources are wind, geothermal, bio and solar energy. Among these harnessing solar energy has the great potential in various applications. In 1954, researcher Chapin, Fuller and Pearson have demonstrated first time silicon based solar cell with the efficiency of 4% at Bell Laboratories a first generation solar cell [1]. With the span of four decades, Si-solar cells have achieved more than 20% PV efficiency and consequently dominated PV market [2]. Despite of being high efficiency solar cells, Si-solar cells have not reached to the common house hold purposes due to the high cost. During the same period, CIGS and CdTe absorber based thin film solar cells have been developed. These cells have demonstrated PV efficiency more than 20% [3-6]. The cost of the thin film solar cell is comparatively lower than the Si-solar cell. The thin film solar cell have lots of technical issues such as low abundance of In and Te as well as toxic nature of Cd. Because of these issues, up scaling of CIGS and CdTe solar cells is a question. In order to overcome these issues, researcher are looking for alternate materials which is less toxic and easy to process at low cost with high efficiency.

Some researchers have find out some solar energy materials which is based on high light absorption and suitable physical properties to improve the efficiency of solar cell. A few materials explored for solar cell application is SnS [7], Cu_2O [8], Cu_2SnS_3 [9], Cu_2GeS_3 [10], GeSe [11], Sb_2S_3[12], Sb_2Se_3 [13] etc. These materials have shown appropriate physical properties suitable for PV cells. Among these, Sb_2S_3, Sb_2Se_3 absorber based solar cells have shown comparatively better PV efficiency about 6.5% which has drawn a significant attention by scientific society. In this article, numerical simulation studies on Sb_2S_3 solar cell have been discussed.

1.1 Crystal structure

Sb_2S_3 belongs to the orthorhombic family with space group P_{bnm}. The structure comprises an infinite long chain of $(Sb_4S_6)_n$ in ribbon form which is oriented along [001] direction. In the ribbon layer, Sb_2S_3 includes two trigonals (SbS_3) and two square pyramids (SbS_5). The bond length Sb-S is < 2.5 Å along [001] direction, 2.58 Å-3.25 Å along the [010] direction and 3.45 Å –3.74 Å along [100] direction [14]. The Sb-S atoms are held strongly along c-axis by

covalent bond whereas the ribbons along a-axis are weakly bonded through the van der Waals forces.

2.2 Electronic and optical properties

The electronic studies reveals that the valance band maxima is formed due to hybridization of Sb-5p, Sb-5s, and S-3p orbitals whereas conduction band minima is formed due to the antibonding Sb-5p and S-3p orbitals. The direct band gap and indirect band gap is estimated to be 1.84 eV and 1.76 eV respectively [11]. The absorption coefficient of Sb_2S_3 is in the range of 10^4 to 10^5 cm^{-1} for energy > 1.9 eV. Since the bond strength in Sb_2S_3 crystal is direction dependent, the bands are strongly dispersed along [001] and flat along [100] and [010]. Thus, the carriers are light along [001] and heavy along [100] and [010], the transport of charge carriers is anticipated to be anisotropic. The differences in bond energy and effective mass along different direction causes anisotropic behavior of electrical conductivity. The surfaces normal to (001) are defect free as it has low surface energy. The electronic and optical study show that Sb_2S_3 can be a potential absorber material for solar cells.

3.1 Sb_2S_3 based solar cell

In 1992, Savadogo and Mandal have developed photo electrochemical cell which demonstrated 2% efficiency with 40 mW/cm^2 illumination [15]. Chen et. al. have reported the maximum photovoltaic efficiency of planar Sb_2S_3 solar cell about 6.56%[16, 17-20] . This low efficiency predicts that an understanding from device aspect is to be developed. In order to understand the device structure, Sb_2S_3 solar cell architecture is simulated considering various physical parameters to achieve maximum device output.

In the present article device modelling is carried out by 1D-SCAPS program [18-20]. The solar cell configuration Glass/Mo/Sb_2S_3/CdS/i-ZnO/Al:ZnO is adopted in the substrate configuration (shown in Fig. 1). The physical properties of various layers of the device is presented in Table 1. The simulation is carried out at room temperature (300 K).

Table 1: Material properties used for the simulation of Sb_2S_3 solar cell.

	Sb_2S_3	CdS	ZnO	Al:ZnO
Thickness (μm)	1	0.05	0.05	0.3
Electron affinity (eV)	3.7	4.2	4.55	4.55
Band gap (eV)	1.6	2.4	3.3	3.3
Dielectric permittivity (relative)	7.08	9	8	8
CB DOS (N_C) (cm^{-3})	2.63×10^{19}	1.00×10^{18}	1.00×10^{18}	1.00×10^{18}
VB DOS (N_V) (cm^{-3})	6.25×10^{19}	1.00×10^{19}	8.00×10^{18}	8.00×10^{18}
e mobility (μ_e) ($cm^2/V/s$)	50	50	100	100
h mobility (μ_h) ($cm^2/V/s$)	10	20	20	20
Acceptor density (N_A) (cm^{-3})	5.00×10^{15}	----------	----------	----------
Donor density (N_D) (cm^{-3})	----------	1×10^{17}	1×10^{10}	1×10^{20}
Absorption (A) (cm^{-1} $eV^{1/2}$)	5×10^4	5×10^4	5×10^4	5×10^4
e thermal velocity ($V_{th,\ n}$) (cm/s)	10^7	10^7	10^7	10^7

h thermal velocity ($V_{th,\ h}$) (cm/s)	10^7	10^7	10^7	10^7

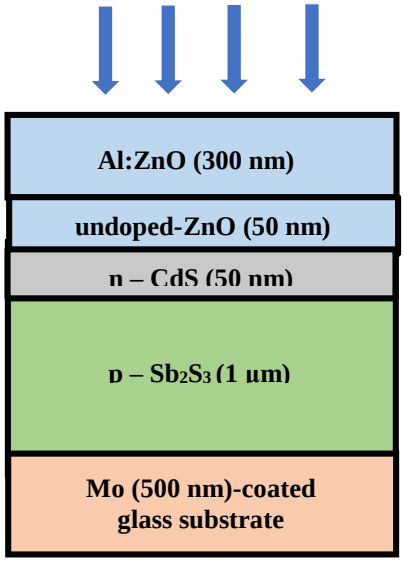

Fig. 1 Device structure of Sb_2S_3 solar cell.

3.2 Results and discussion

Fig. 2 (a) shows the simulation studies carried on the solar cell (shown in Fig. 1). The maximum power conversion efficiency of the simulated cell is 11.47%. The open circuit voltage (V_{OC}) and short circuit current is 967.36 mV and 19.18 mA/cm^2 respectively. The open circuit voltage achieved is very high which is expected due to the large splitting of quasi-Fermi levels across the pn-junction of Sb_2S_3 and CdS. The fill factor (FF) is 61.82 % which shows a better JV characteristics.

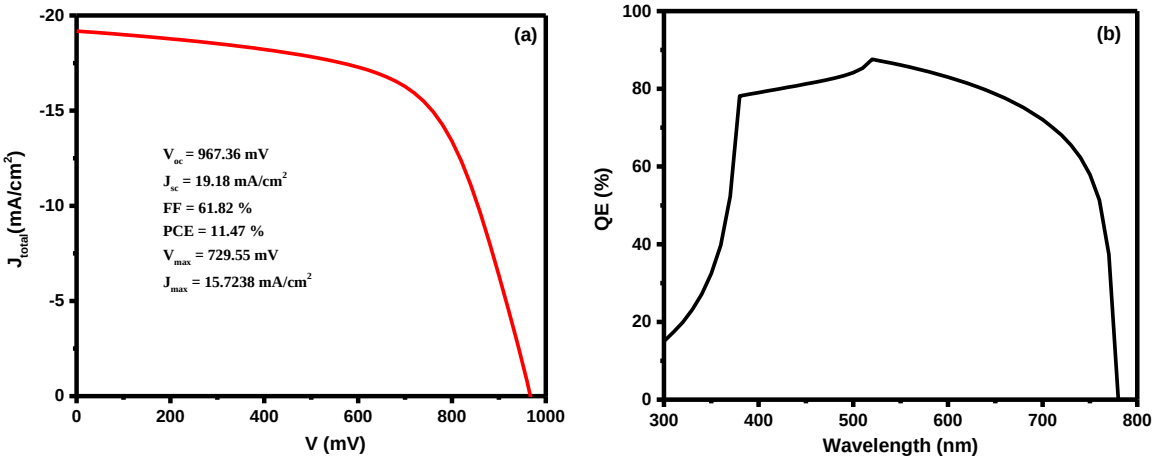

Fig. 2 Simulated (a) JV characteristics (under light illumination) and (b) quantum efficiency of Sb_2S_3 solar cell.

To understand the behavior of photogenerated charge carriers in the device, quantum efficiency of the device is simulated. The quantum efficiency of the Sb_2S_3 solar cell is illustrated in Fig. 2(b). The quantum efficiency, (number of charge carriers collected per photon incident), is more than 75% in visible range. The low quantum efficiency is due to the reflection losses. In the lower wavelength (< 380 nm) region the QE decreases due to the absorption of light in ZnO and CdS layers. QE also decreases sharply in the region of wavelength > 760 nm due to the transmission of photon through the Sb_2S_3 and consequently QE approached to zero. The absorption in the higher wavelength can be increased by

incorporating Se into Sb_2S_3 wherein the band gap of Sb_2S_3 reduces which results in increase of QE.

4. Summary

Sb_2S_3 is, a ternary chalcogenide compound, emerged as a potential absorber layer for thin film solar cell. The optical and electronic properties such as optimum band gap (~1.65 eV), high absorption coefficient (10^4-10^5 cm^{-1} in visible range), presence of low energy stable surfaces etc. show the suitability of the compound for thin film solar cell. The numerical simulation is carried out on the solar cell Glass/Mo/Sb_2S_2/CdS/i-ZnO/Al:ZnO using 1D-SCAPS program. The power conversion efficiency extracted from the modelled device is about 11.47% with J_{SC} = 19.18 mA/cm^2, V_{OC} = 967.36 mV and FF = 61.82%. Quantum efficiency of the modelled device is more than 75% in the visible range. The results demonstrate that Sb_2S_3 can be a promising absorber material for the thin film solar cells.

5. References

[1] Chapin D M, Fuller C S and Pearson G L 1954 A new silicon p-n junction photocell for converting solar radiation into electrical power *Journal of Applied Physics* **25** 676–7

[2] Louwen A, Van Sark W, Schropp R and Faaij A 2016 A cost roadmap for silicon heterojunction solar cells *Solar Energy Materials and Solar Cells* **147** 295–314

[3] Green M A, Emery K, Hishikawa Y, Warta W and Dunlop E D 2016 Solar cell efficiency tables (version 48) *Progress in Photovoltaics: Research and Applications* **24** 905–13

[4] Gupta, V. K., Sethi, B., Upadhyay, N., Kumar, S., Singh, R., & Singh, L. P. (2011). Iron (III) selective electrode based on S-methyl N-(methylcarbamoyloxy) thioacetimidate as a sensing material. *Int. J. Electrochem. Sci*, *6*, 650-663.

[5] Mukherjee, R., Lawes, G., & Nadgorny, B. (2014). Enhancement of high dielectric permittivity in CaCu3Ti4O12/RuO2 composites in the vicinity of the percolation threshold. Applied Physics Letters, *105*(7), 072901.

[6] Mukherjee, R. (2020). Electrical, thermal and elastic properties of methylammonium lead bromide single crystal. Bulletin of Materials Science, *43*(1), 1-5.

[7] Nair P K, Garcia-Angelmo A R and Nair M T S 2016 Cubic and orthorhombic SnS thin-film absorbers for tin sulfide solar cells *Physica Status Solidi (A) Applications and Materials Science* **213** 170–7

[8] Lee Y S, Chua D, Brandt R E, Siah S C, Li J V., Mailoa J P, Lee S W, Gordon R G and Buonassisi T 2014 Atomic layer deposited gallium oxide buffer layer enables 1.2 v open-circuit voltage in cuprous oxide solar cells *Advanced Materials* **26** 4704–10

[9] Berg D M, Djemour R, Gütay L, Zoppi G, Siebentritt S and Dale P J 2012 Thin film solar cells based on the ternary compound Cu2SnS3 *Thin Solid Films* **520** 6291–4

[10] Jin X, Zhang L, Jiang G, Liu W and Zhu C 2017 High open-circuit voltage of ternary Cu2GeS3 thin film solar cells from combustion synthesized Cu-Ge alloy *Solar Energy Materials and Solar Cells* **160** 319–27

[11] Xue D-J, Liu S-C, Dai C-M, Chen S, He C, Zhao L, Hu J-S and Wan L-J 2017 GeSe thin-film solar cells fabricated by self-regulated rapid thermal sublimation *Journal of the American Chemical Society* **139** 958–65

[12] Moon S-J, Itzhaik Y, Yum J-H, Zakeeruddin S M, Hodes G and Grätzel M 2010 Sb2S3-based mesoscopic solar cell using an organic hole conductor *The Journal of Physical Chemistry Letters* **1** 1524–7

[13] Liu X, Xiao X, Yang Y, Xue D, Li D, Chen C, Lu S, Gao L, He Y and Beard M C 2017 Enhanced Sb2Se3 solar cell performance through theory-guided defect control *Progress in Photovoltaics: Research and Applications* **25** 861–70

[14] Kondrotas R, Chen C and Tang J 2018 Sb2S3 solar cells *Joule* **2** 857–78

[15] Savadogo O and Mandal K C 1992 Studies on new chemically deposited photoconducting antimony trisulphide thin films *Solar energy materials and solar cells* **26** 117–36
[16] Jiang C, Tang R, Wang X, Ju H, Chen G and Chen T 2019 Alkali Metals Doping for High-Performance Planar Heterojunction Sb2S3 Solar Cells *Solar RRL* **3** 1800272
[17] Laha, S. S., Mukherjee, R., & Lawes, G. (2014). Interactions and magnetic relaxation in boron doped Mn3O4 nanoparticles. *Materials Research Express*, *1*(2), 025032.
[18] Burgelman M, Decock K, Khelifi S and Abass A 2013 Advanced electrical simulation of thin film solar cells *Thin Solid Films* **535** 296–301
[19] Ahmadi, M. H., Ghazvini, M., Sadeghzadeh, M., Alhuyi Nazari, M., Kumar, R., Naeimi, A., & Ming, T. (2018). Solar power technology for electricity generation: A critical review. *Energy Science & Engineering*, *6*(5), 340-361.
[20] Mukherjee, R. (2020). Electrical, thermal and elastic properties of methylammonium lead bromide single crystal. Bulletin of Materials Science, *43*(1), 1-5.