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A STUDY OF CZTS SOLAR CELL THROUGH NUMERICAL ANALYSIS

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ABSTRACT

The characteristics performance of the kieserite based Cu_2ZnSnS_4 based solar cell is investigated using a simulation program called Analysis of Microelectronic and Photonic Structures (AMPS). The cell structure is based on p-type Cu_2ZnSnS_4(CZTS) compound semiconductor as the absorber layer and ZnS as window layer. Al doped ZnO (AZO) is used as the transparent conductive oxide layer, which acts as the front contact of the cell. I study the influence of the operating temperature, doping concentration, thickness of the different layers. The band-gap variation of the absorber CZTS layer is also investigated. The thickness of the absorber layer is varied from 800 nm up to 3.5 µm and found substantial increase in the efficiency. The increased working temperature has a strong influence on the solar cell efficiency and the temperature coefficient is calculated to be about -0.17%/K. The highest efficiency is achieved by varying the carrier concentration profile of the absorber layer. All these simulation results will give some important guides for feasibly fabricating higher efficiency CZTS solar cells.

Key Words: CZTS, ZnS, AZO, AMPS-1D, Solar Cells

INTRODUCTION

Energy is a great issue for the development of society. Since the amount of fossil fuel is limited, a sustainable development of society requires the development of novel sustainable energy resources. In such a context, solar energy meets the requirement. Recently, Cu (In, Ga) Se2-based thin film solar cells have achieved efficiencies as high as 20.4 % in the lab scale [Lincot D, et al., BamiduroO,et al., Ribeaucourt L, et al.,Aksu S, et al.]

Over recent years, a good amount of efforts has been made to study the Cu2ZnSnS4 based thin-film solar cells [Moholkar, A., et al., Moritake, N., et al., Katagiri, et al.,Ennaoui, A., et al., Wang, K. et al., Katagiri, et al., Shin, B., et al., Seol, J. S., et al.]. Cu_2ZnSnS_4 is a quaternary semiconductor with excellent optical characteristics such as high absorption coefficient over 10^4 cm^{-1}, and a direct band gap value about 1.4 -1.5 eV, which is very close to the optimum band gap value of the single-junction solar cells. Moreover, all the chemical elements in CZTS are nontoxic and abundant. In comparison with other thin film solar cells, CZTS based solar cells are gradually becoming excellent low-cost alternatives. The CuZnSnS4-based thin film solar cells have achieved efficiency as high as 11.1 % using hydrazine-based processing CZTS absorbers [Scragg JJ, et al.].CZTS thin films have been prepared by various techniques such as spray pyrolysis [N.

Kamoun, et al.], thermal evaporation [T. Tanaka, et al.], sputtering [F.Y. Liu, et al.], chemical vapor deposition [K.Ramasamy, et. al.], electrochemical deposition [S. Ahmed, et al.], photochemical deposition [K. Moriya, et al.], screen printing [Z.H. Zhou, et al.], sol–gel method [K. Tanaka, et al.,].
In order to improve the CZTS cell efficiency and fully understand the performance of cells, it is necessary to systematically investigate the influence of the basic factors in the performance of the cells.

PROPERTIES OF CZTS

Copper zinc tin sulfide (CZTS) is a quaternary semiconducting compound which has received increasing interest since the late 2000s for applications in solar cells. The class of related materials includes other I_2-II-IV-VI_4 such as Copper Zinc Tin Selenide (CZTSe) and the Sulfur-Selenium alloy CZTSSe.

Some literature reports have identified CZTS in the related stannite structure, but conditions under which a stannite structure may occur are not yet clear. First-principle calculations show that the crystal energy is only 2.86 meV/atom higher for the stannite than kesterite structure suggesting that both forms can coexist. [Chen, S., et al.]

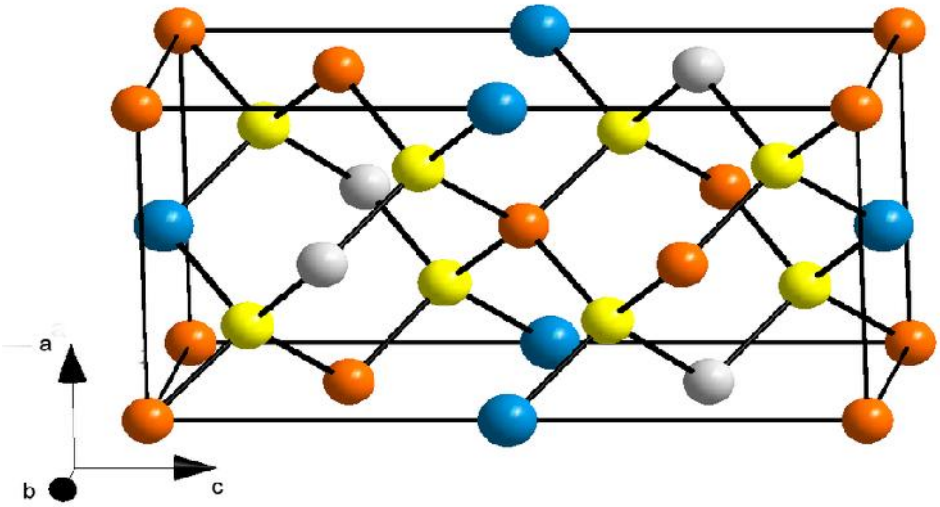

Figure 1: CZTS crystal structure. Orange: Cu, grey: Zn/Fe, blue: Sn, yellow: S.

Structural determination (via techniques like X-ray diffraction) is hindered by disorder of the Cu-Zn cations, which are the most common defect as predicted by theoretical calculations and confirmed by neutron scattering. The near random ordering of Cu and Zn may lead to misidentification of the structure.

Carrier concentrations and absorption coefficient of CZTS are similar to CIGS. Other properties such as carrier lifetime (and related diffusion length) are low (below 9 ns) for CZTS. This low carrier lifetime may be due to high density of active defects or recombination at grain boundaries.

Many secondary phases are possible in quaternary compounds like CZTS and their presence can affect the solar cell performance. Secondary phases can provide shunting current paths through the solar cell or act as recombination centers, both degrading solar cell performance. From the literature it appears that all secondary phases have a detrimental effect on CZTS performance,

and many of them are both hard to detect and commonly present. Common phases include ZnS, SnS, CuS, and Cu2SnS3. Identification of these phases is challenging by traditional methods like X-ray diffraction (XRD) due to the peak overlap of ZnS and Cu2SnS3 with CZTS. Other methods like Raman scattering are being explored to help characterize CZTS.

In this simulation study, Zinc Sulfide (ZnS) is used as the window layer. Zinc sulfide (ZnS) is a wide gap and direct transition semiconductor [L. I. Berger, B. P. Pamplin]. Consequently, it is a potentially important material to be used as an antireflection coating for heterojunction solar cells [W.H. Bloss, et al]. It is an important device material for the detection, emission and modulation of visible and near ultra violet light [Y.F. Nicolau, et el., E. Marquerdt, et al.]. In particular, ZnS is believed to be one of the most promising materials for photovoltaic cells, blue light emitting laser diodes [M. A. Hasse, et al.,] and thin film electroluminescent displays [K. Hirabayashi, H. Kozawaguchi].

MODELLING AND SIMULATION

Numerical simulation is an efficient way to predict the effect of changes in material properties, assess the potential merits of cell structures and then optimize the structure of cells. Therefore, in this work, a numerical simulation is performed by using AMPS-1D to achieve maximum efficiency of CZTS solar cell.

The AMPS-1D program has been developed for pragmatically simulate the electrical characteristics of multi-junction solar cells. It has been proven to be a very powerful tool in understanding device operation and physics for single crystal, poly-crystal and amorphous structures. To date, more than 200 groups worldwide have been using AMPS-1D for solar cell design [Hong Zhu, et al].

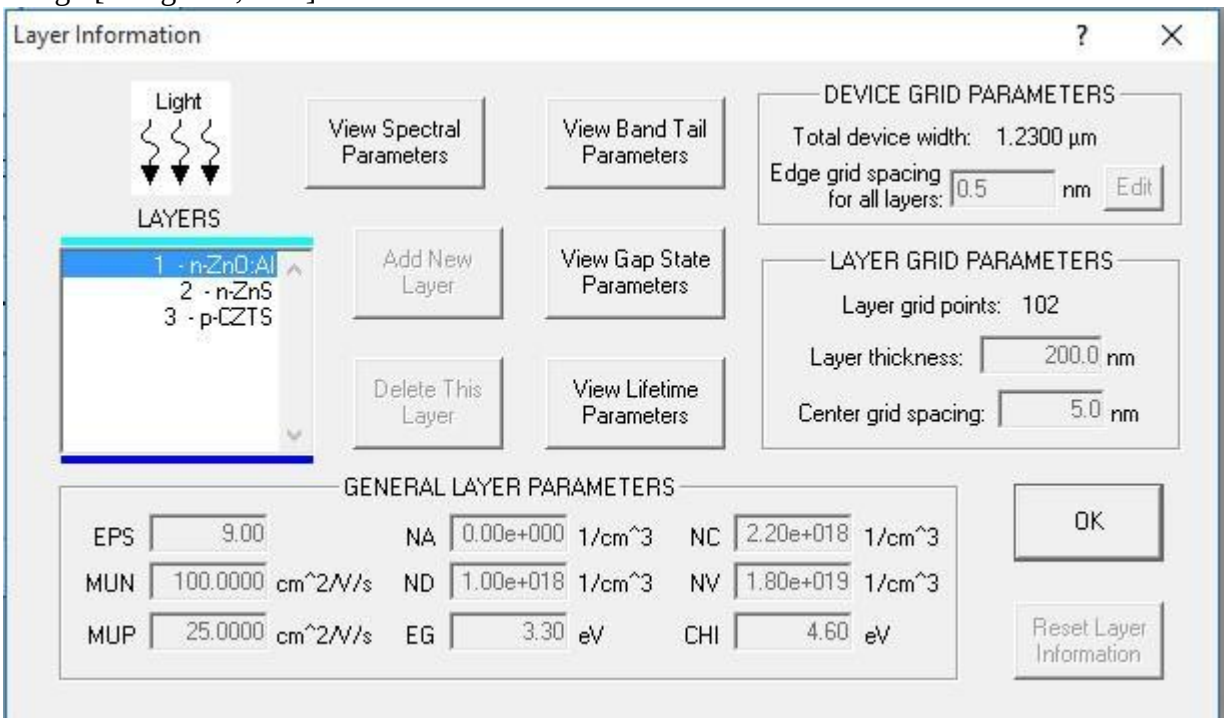

Figure 2: AMPS-1D simulation front panel contains the device and layer grid parameters, and general layer parameters

A three-layer device model of Aluminum doped ZnO, as TCO layer, ZnS as the window layer and CZTS as absorber layer (AZO/ZnS/CZTS) solar cell are investigated.

Figure -3: Simulated structure of AZO/ZnS/CZTS Solar Cell

I have started the simulation by taking default parameters of different layers and then changed the parameters within the acceptable limits to find out the optimum structure of the CZTS based solar Cell and hence the best efficiency configuration. Due to different composition of the constituent atoms the various parameters are not constant, rather they are variable within some acceptable limits which depends on the composition. In this simulation, I investigate the solar cell performance namely the efficiency (η%), short circuit current (Jsc), open circuit voltage (Voc), and Fill Factor (FF) by varying the thickness, bandgaps, doping concentration. I have also studied the effect of operating temperature on the solar cell performance. The Table I shows the description of all the parameters along with the variation used in this analysis, these parameters were selected based on literature, theory, experimental data, or in some cases, reasonable estimation.

AND DISCUSSION

The numerical analysis has been performed with an envision to find an optimum CZTS solar cell structure in terms of efficiency. The dependency of efficiency, short circuit current, open circuit voltage on device parameters like thickness, carrier concentration profile etc., are investigated first by using AMPS-1D. Fig -2 shows the simulated efficiency of the solar cell design using different TCO layers, whose specification was given to the Table-1.

TABLE 1 PARAMETERS USED IN SIMULATION

parameters	**n-ZnO:Al**	**n-CdS:O**	**p-CdTe**
W (μm)	0.1-0.8	0.01-0.1	1-3.5
ε/ε0	9	10	10
μ_n(cm^2/Vs)	100	100	100
μ_p(cm^2/Vs)	25	25	25
n, p (/cm^3)	1e15-1e20	9e15-9e20	2e15-2e20
E_g (eV)	3.30	3.40-3.94	0.94 - 1.6

Nc (/cm^3)	2.2e18	1.5e18	2.2e18
Nv (/cm^3)	1.8e19	1.8e18	1.8e19
χ (eV)	4.60	4.50	4.10

From figure-4(a), it is very clear that, the efficiency rises very steadily when thickness of the absorber layer increases. Maximum efficiency of about 21% is achieved for thickness about 3.5 µm. It is obvious because, as the thickness is increased, the absorption also increases, so the creation of electrons and holes in the absorber layer also increases. Eventually the short circuit current also increases as shown in the figure -4(b)

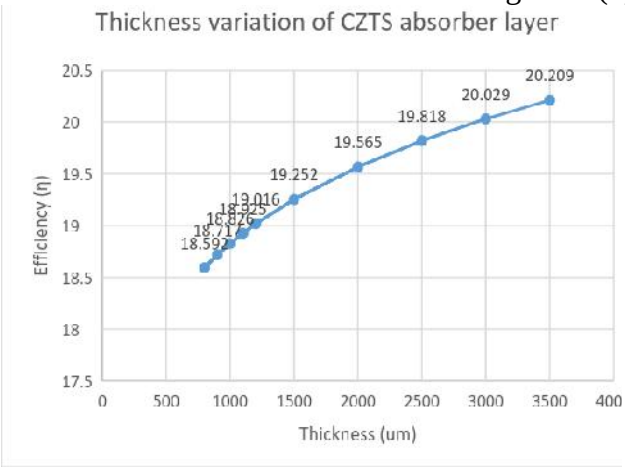

Figure 4-a: Efficiency variation due to the change of absorber layer thickness

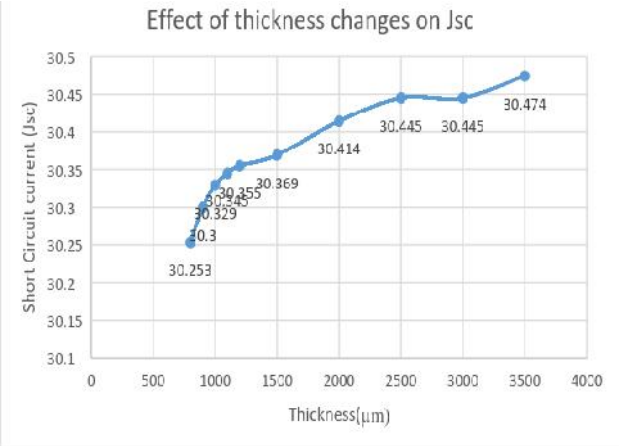

Figure -4(b): Short circuit current(Jsc) variation due to the change of absorber layer thickness

Figure -5 demonstrates how the efficiency changes with the increasing value of doping concentration. The maximum efficiency of about 40% is obtained with the p-type doping concentration of $2x10^{21}/cm^3$. And the most interesting part is at the doping level of $2x10^{22}/cm^3$, the efficiency drastically falls down only to 2.53%.

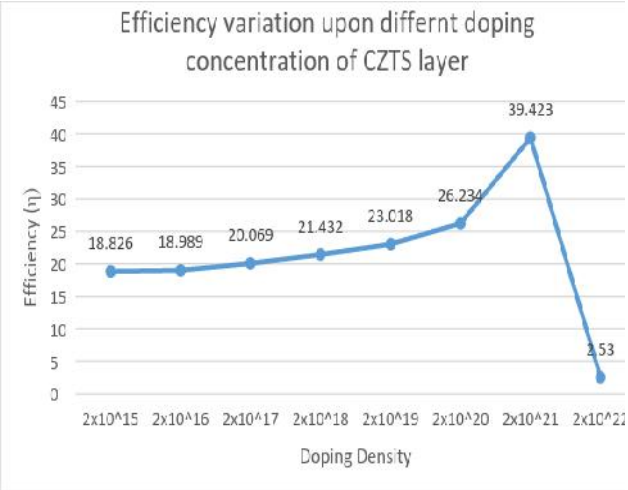

Figure -5: Efficiency and doping profile variation of CZTS absorber layer.

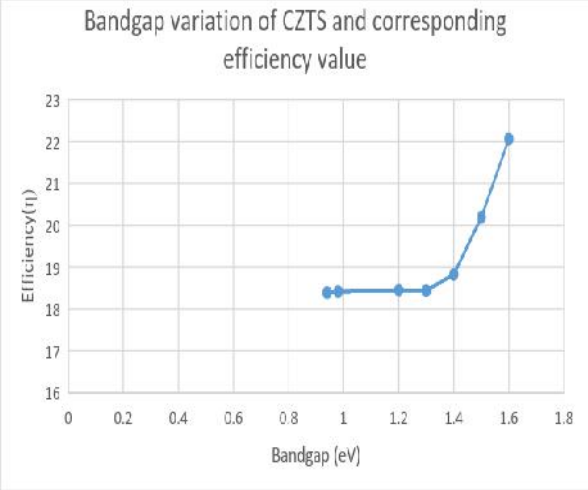

Figure- 6: Efficiency variation with the variation of bandgap(eV)

The band-gap of the absorber layer CZTS, is also a key factor for determining the efficiency of the solar cell, as it is shown in figure -6. It looks the efficiency of the cell under investigation is low at the lower band-gap regions (from 0.94 eV -1.4 eV), but it increases rapidly from 1.4 eV to 1.6 eV. As the optimum band-gap value of typical cell operation is ~ 1.5 eV. So efficiency increases in these ranges of the band-gap.

In this simulation environment, different material parameters of both window layer and transparent conductive oxides (TCO) layers are also investigated. The outcome of the changes is illustrated below –

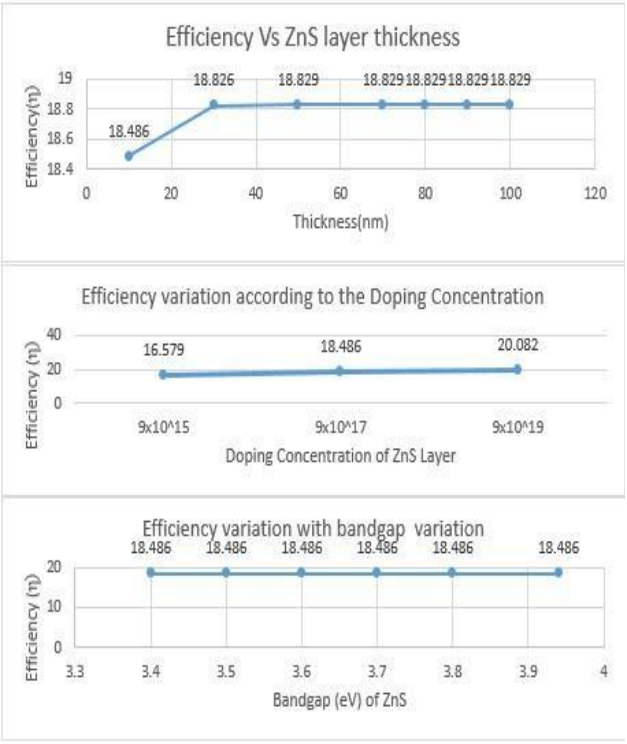

Figure- 7: Efficiency variation due to the changes of different material parameters of ZnS as window layer

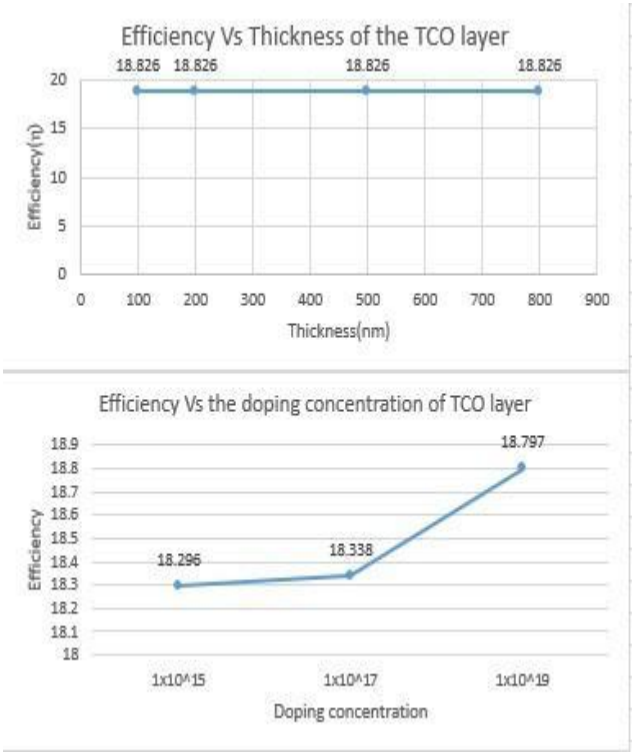

Figure-8: TCO layer Thickness and Carrier Concentration effect on overall efficiency of the cell

Figure -7 shows that, the changes of efficiency due to changes of different parameters of ZnS window layer and it is seen that, there is drastic changes of efficiency due to various thicknesses of ZnS layer as well as the changes of bandgap and doping concentration. The efficiency remains nearly constant despite of the changes of these material parameters.
The change of efficiency is found to be nearly zero as indicated in figure -8, due to the changes of the transparent conductive layer thickness. But for higher doping, the efficiency increases slowly with the increase of the concentration.

CONCLUSION

CZTS based thin film solar cells have attracted many researchers for their constituent material abundance in the earth's crust as well as the optimum value of material parameters like bandgap of about ~1.5 eV. It has large optical absorption coefficient is also an attracting quality factor. In this simulated work, maximum efficiency about 40% is achieved when the carrier concentration of the absorber layer is taken at the order of ~10^{21}. Thickness of the absorber also plays a very vital role in case of efficiency and found that if the thickness is increased, efficiency is also increased (about 31% for thickness of about 3.5~4 µm)

It has been found that, the bandgap of CZTS layer should be optimized to achieve higher efficiency value. In this work, maximum efficiency is observed at the bandgap of 1.6eV. Finally, by changing the thickness of the Transparent Conductive Oxide(TCO), the efficiency of the solar cell device may change.The understanding as well as the simulated results will also facilitate the investors to make choice on which technology to invest.

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