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REGULAR ARTICLE

Establishment of the Prospective CZTGS Photovoltaic through the Optimization of Some Device Parameters

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In this work, numerical modelling and simulation of CZTGS thin film solar cells have been carried out using the Solar Cell Capacitance Simulator (SCAPS-1D). A device structure of AZO/CdS/CZTGS/Mo was modelled using this one-dimensional simulation program. The baseline model of the device gave an efficiency $\eta = 9.39$ %, a fill factor FF = 63.61 %, an open circuit voltage $V_{oc} = 0.86$ V, and a short circuit current $J_{sc} = 17.39$ mA/cm^2. The optimization process includes the variation of the absorber layer thickness, doping concentration, and device operating temperature. The optimal values of these parameters include an absorber layer thickness of 2.0 μm, a doping concentration of 1×10^{16} cm^{-3} at a thickness of 2.0 μm, and an operating temperature of 310 K with a back contact material work function of 5.0 eV. These values will provide essential information and guidelines for the development of a highly efficient and pro-mising CZTGS photovoltaics.

Keywords: CZTGS, Simulation, Efficiency, Thin film, Photovoltaic, Optimization.

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1. INTRODUCTION

The quest to develop Thin Film Photovoltaics (TFPVs) that could compete effectively and outshine the existing ones requires the use of a suitable absorber layer material. The absorber layer material must satisfy the globally recognized basic requirement of photovoltaic cells (PVs). This condition includes an abundance of constituent elements, non-toxic and cheap cost of production, and high conversion efficiency without material degradation [1, 2]. At present, a large number of absorber materials that could be used in photovoltaic energy conversion have been developed. However, from the technical point of view, only a few of them are stable and have been commercialized. The few ones that have made it to the commercial stage suffer from one major challenge or the other that has made its future in the photovoltaic industry look bleak. Prominent amongst these thin film solar cells are Cadmium Telluride (CdTe), Copper Zinc Tin Sulfo-Selenide (CZTSSe), Galium Arsenide and Copper Indium Gallium Sulfide (CIGS) [4]. The skyrocketing material cost and scarcity of indium and gallium give a major hindrance to the production of CIGS PVs, although it has attained an efficiency of 23.6% with high stability. Also, the toxicity of selenium in CZTSSe and cadmium in CdTe is another obstacle to their production, though CdTe PVs are stable with an efficiency of 21 % [4, 5]. The high cost of Ga and toxicity of As is a limiting factor to Gallium Arsenide solar cells.

One promising absorber material is the $Cu_2Zn(Sn,Ge)S_4$ (CZTGS) due to its high absorption coefficient, non-toxic nature, direct and optimal band gap. The choice of CZTGS lies in the fact that its physical properties can modified by changing the composition of Sn and Ge as well as S [6, 7]. Thus, making it a potential absorber material that can be used to overcome the impasse of the relatively low efficiency in CZTS thin film solar cells. As reported in the work of Umehara, several studies on the fabrication of CZTGS single crystals thin films and nanoparticles have been carried out. However, only a few papers have reported its solar cell performance [7]. Consequently, this research work will focus on using numerical modelling and simulation as a tool to establish the optimal absorber layer thickness, doping concentration and operating temperature of the CZTGS thin film solar cell. Results from this work will provide extremely valuable information in studying and fabricating CZTGS-based systems by scientists and engineers.

2. METHODOLOGY

Solar Cell Capacitance Simulator (SCAPS-1D) software, version 3.3.10 was used for numerical modelling and simulation studies in this research work. SCAPS is an application that uses the Gummel iteration scheme with Newton-Raphson sub-steps in solving the basic semiconductor equations [8, 9]. It has been used successfully in the modelling and simulation of thin film polycrystalline solar cells TFSC such as CdTe and CIGS which are already stable [10-11]. Also, SCAPS software has been reported in the literature for the modelling and

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simulation of CZTS thin film solar cells [9, 10]. Hence, the numerical simulation will be a crucial tool in studying the input to experimental optimization of the performance characteristics of CZTGS solar cells.

A numerical program with capabilities for modelling of photovoltaics must be able to solve the basic semiconductor equations. These semiconductor equations include the Poisson equation which relates the electrostatic potential to charge (Equation 1) and the continuity equations for electrons and holes (Equations 2 and 3) [10-13]. This set of equations results in a system of coupled differential equations which when solved using appropriate boundary conditions, the solar cell device parameters can be obtained.

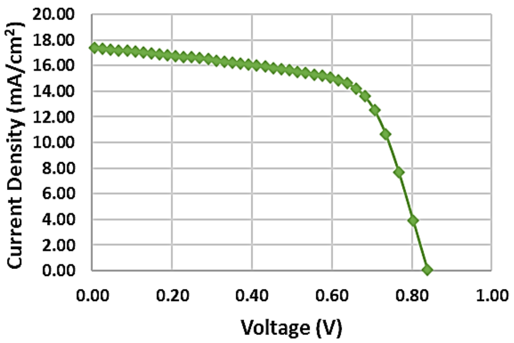


Fig. 1 – *J-V* plot of the base model of CZTGS solar cell

$$\frac{\partial}{\partial x}\left(\varepsilon_0\varepsilon_r\frac{\partial\Psi}{\partial x}\right)=-q\left(p-n+N_D^+-N_A^-+\frac{\rho}{q}\right) \quad (1)$$

$$-\left(\frac{1}{q}\right)\frac{\partial J_n}{\partial x}-U_n+G=\frac{\partial n}{\partial t} \quad (2)$$

$$-\left(\frac{1}{q}\right)\frac{\partial J_p}{\partial x}-U_p+G=\frac{\partial p}{\partial t} \quad (3)$$

Where Ψ is the electrostatic potential, ε_0 is the permittivity of free space and ε_r relative permittivity, ρ is the charge density of defects, n and p are the free carrier concentrations while N_D^+ and N_A^- are the densities of the ionized donors and acceptors, G is the generation rate, J_n and J_p are the electron and hole current densities.

The modelled device has a substrate structure which consists of ZnO:Al (window), CdS (buffer), CZTGS (absorber), and Molybdenum layers. The material and device parameters were obtained from theories, literature values and in some cases reasonable estimates were made where exact experimental values are not available [10, 13, 14].

3. RESULTS AND DISCUSSION

3.1 Modelling and Simulation of CZTGS Thin Film Solar Cell

The modelling and simulation of CZTGS cell was conducted using the baseline parameters. This simulation is based on the recently reported composition ratio of $Cu_2ZnSn_{0.8}Ge_{0.2}S_4$ which could give the best performance of the device [14]. The simulation of the device gave an efficiency (η) of 9.39 %, an open circuit voltage (V_{oc}) of 0.86 V, a short circuit current (J_{sc}) of 17.39 mA/cm² and a fill factor (FF) of 63.61 %. The corresponding J-V characteristics of this device are shown in Fig. 1.

3.2 Effect of Absorber Thickness of CZTGS on Device Performance

In this section, the effect of the device thickness is studied by increasing the absorber thickness from 0.4 µm-2.2 µm. It is observed that the J_{sc} increased non-linearly (Fig. 2a) and the V_{oc} shows almost a similar behaviour (Fig. 2b). The increase in the short circuit current as the thickness increases can be attributed to increased light absorption and carrier concentration. Beyond 2 µm, it is observed that the J_{sc} curve flattens out which indicates that all light is absorbed.

The fill factor increases as the thickness increases. However, beyond 1.0 µm the fill factor begins to degrade (Fig. 2c). The decrease in fill factor as the thickness increases can be attributed to an increase in resistance [15].

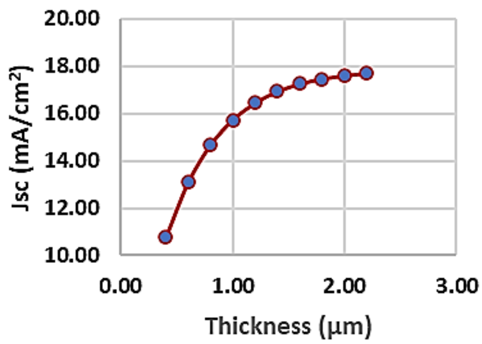


Fig. 2a – Effect of thickness on J_{sc}

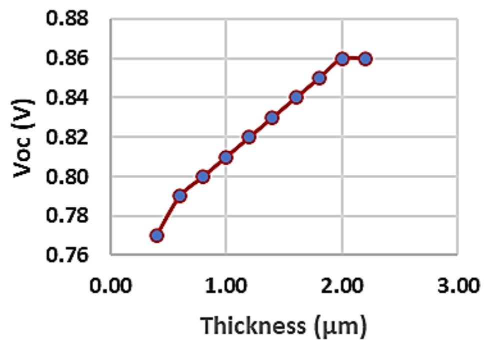


Fig. 2b – Effect of thickness on V_{oc}

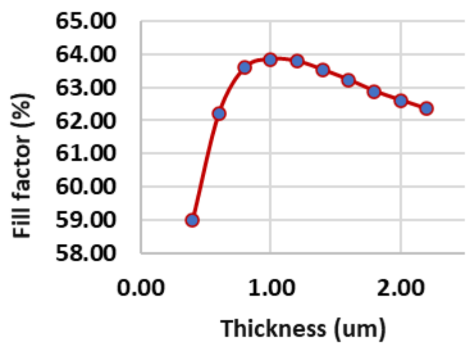


Fig. 2c – Effect of thickness on FF

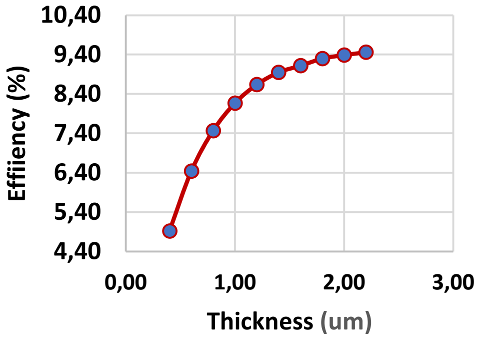
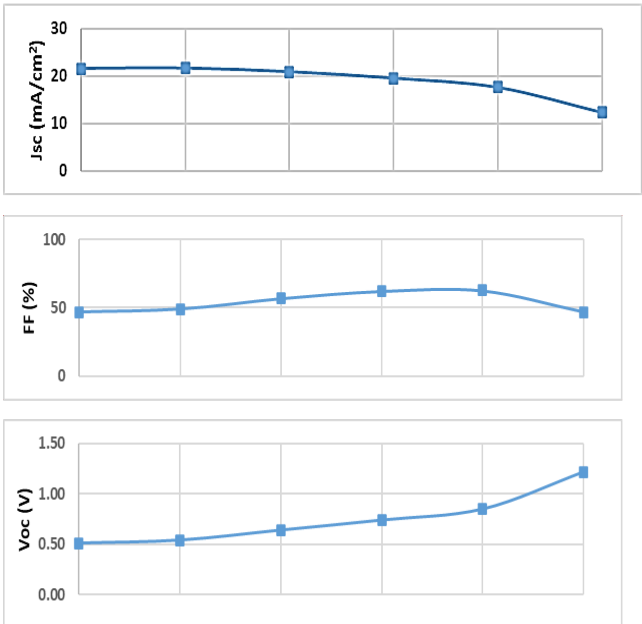


Fig. 2d – Effect of thickness on η

In the same vein, the efficiency is observed to increase steadily from 4.92 % to 9.40 % at a thickness of 2.0 µm. More photons with longer wavelengths can be collected in the CZTGS layer as the thickness increases [16]. Beyond this value of thickness, the increase in efficiency is no longer significant. Therefore, at a thickness of 2.0 µm for CZTGS, the performance of the device is optimized with a little trade-off of the fill factor.

3.3 Effect of Doping Concentration on CZTGS Thin Film Solar Cell

The effect of doping concentration on device performance was considered in this section. For the absorber layer, a doping concentration range of 1×10^{12} to 1×10^{17} cm^{-3} was considered. From Fig. 4, it was observed that the short circuit current decreased slightly as the concentration increased. Conversely, the open circuit voltage increased as the doping concentration increased. The degradation in J_{sc} as carrier concentration increases can be attributed to the rise in the recombination rate. The increase in V_{oc} is due to the rise in device saturation current thereby increasing electrical conductivity [17]. The fill factor and efficiency tend to increase with increasing concentration as well. Generally, the best device performance was observed at a doping concentration of 1×10^{16} cm^{-3}.



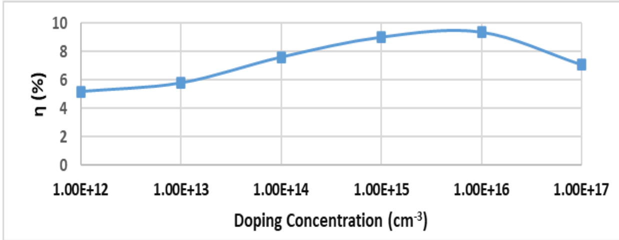


Fig. 4 – Effect of doping concentration on J_{sc}, V_{oc}, FF and η

3.4 Effect of Temperature Variation on CZTGS Solar Cell Performance

In most terrestrial applications, solar cells are generally exposed to temperatures varying from 283 K to 333 K. Consequently, theT operating temperature of CZTGS thin film solar cell was varied from 283 K-333 K with an incremental value of 10 K. The result shows that the values of the open circuit voltage decrease slightly as the temperature increases. This is due to increasing reverse saturation current density primary due to increase in the intrinsic carrier concentration [18].

Table 1 – Variation of temperature for CZTGS thin film solar cell

Temperature (K)	V_{oc} (V)	J_{sc} (mA/cm^2)	FF (%)	η (%)
283	0.86	17.46	62.11	9.29
293	0.85	17.56	62.42	9.36
303	0.85	17.64	62.68	9.41
313	0.85	17.72	62.89	9.45
323	0.85	17.80	63.06	9.49
333	0.85	17.87	63.18	9.52

Conversely, a slight increase is observed in the J_{sc} as the temperature increases as shown in Table 1. The increase in temperature decreases band gap of the semiconducting material, thus increasing the leakage current that enhances the short circuit current [19]. Fig. 5 shows that at a temperature of 310 K, the operating temperature is optimal. Also, the device performance indicates that it will be very stable for terrestrial applications.

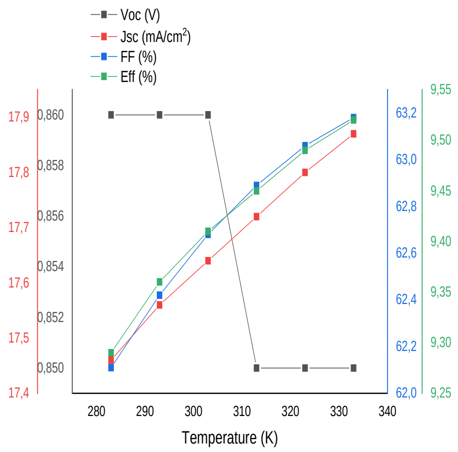


Fig. 5 – Temperature Effect on CZTGS Thin Film Solar Cell

4. CONCLUSION

One-dimensional numerical modelling and simulation of CZTGS thin film solar cell has been considered in this research work. The SCAPS simulation program was used to model and analyze AZO/CdS/CZTGS/Mo device structure. The optimal values of some of the device parameters was established in this work. Results showed the optimal values of these parameters include an absorber layer thickness of 2.0 μm, an acceptor concentration of 1×10^{16} cm^{-3} at a thickness of 2.0 μm, an operating temperature of 310 K and a back contact material with a work function of 5.0 eV. The values will provide essential information for the development and production of the promising and high efficient CZTGS thin film solar cells.

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Створення перспективної фотовольтаїки CZTGS шляхом оптимізації деяких параметрів пристрою

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У даній роботі чисельне моделювання та моделювання тонкоплівкових сонячних елементів CZTGS було виконано за допомогою симулятора ємності сонячних елементів (SCAPS-1D). Структура пристрою AZO/CdS/CZTGS/Mo змодельована за допомогою цієї одновимірної програми моделювання. Базова модель пристрою дала ефективність η = 9,39 %, коефіцієнт заповнення FF = 63,61 %, напругу холостого ходу V_{oc} = 0,86 В і струм короткого замикання J_{sc} = 17,39 мА/см^2. При процесі оптимізації змінюються товщини шару поглинача, концентрації легування та робоча температура пристрою. Оптимальні значення цих параметрів: товщина шару поглинача 2,0 мкм, концентрація легування $1 \cdot 10^{16}$ см$^{-3}$ при товщині 2,0 мкм і робоча температура 310 К з роботою виходу матеріалу тильного контакту 5,0 еВ. Такі значення нададуть важливу інформацію та вказівки для розробки високоефективної та перспективної фотоелектричної системи CZTGS.

Ключові слова: CZTGS, Симуляція, Ефективність, Тонка плівка, Фотовольтаїка, Оптимізація.