

**MODELLING OF THE SOLAR CELL BASED ON  $\text{Cu}_2\text{SnS}_3$  THIN FILM PRODUCED BY SPRAY PYROLYSIS****Serap YIGIT GEZGIN<sup>1</sup>**  **Ilhan CANDAN<sup>2</sup>**  **Silan BATURAY<sup>2</sup>**  **Hamdi Sukur KILIC<sup>1,3,4,\*</sup>** <sup>1</sup> Department of Physics, Faculty of Science, University of Selçuk, 42031 Selçuklu, Konya, Turkey<sup>2</sup> Department of Physics, Faculty of Science, Dicle University, Diyarbakir, Turkey<sup>3</sup> Directorate of High Technology Research and Application Center, University of Selçuk, 42031 Selçuklu, Konya, Turkey<sup>4</sup> Directorate of Laser-Induced Proton Therapy Application and Research Center, University of Selçuk, 42031 Selçuklu, Konya, Turkey

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**Abstract:**  $\text{Cu}_2\text{SnS}_3$  (CTS) thin film has been produced for 30 sccm sulphur flux rate at 30 minutes annealing durations at 550 °C temperature. CTS thin film's crystalline structure has been investigated and crystalline size, lattice parameters, dislocation density and microstrain, crystalline number have also been determined. The CTS thin film's morphological and optical properties have been examined and thoroughly interpreted. Mo/CTS/CdS/AZO/Al solar cell has been modeled based on CTS thin film produced at the present work, using SCAPS-1D simulation program.  $V_{oc}$ ,  $J_{sc}$ , FF, conversion efficiency, and photovoltaic parameters have been determined depending on neutral defect density at the interface, coefficient of radiative recombination, Auger electron/hole capture's coefficient, and operation temperature of CTS solar cell. As a consequence of the simulation study, the ideal efficiency of CTS solar cell has been determined to be 3.72 % and all the data obtained in this study have been presented, interpreted, and concluded to be original results.

**Keywords:** CTS, solar cell, SCAPS-1D, simulation

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**1. Introduction**

The photovoltaic (PV) market is based on solar cells manufactured with Silicon (Si), Copper Indium Gallium Selenum (CIGS), and Cadmium Tellur (CdTe) materials. Some prominent disadvantages of these mentioned elements are the high cost of In, Ga, and Te and the high processing cost of Si as well as the toxicity of the Cd element. Some materials such as  $\text{Cu}_2\text{ZnSnS}_4$  (CZTS) have attracted great attention, which has properties such as low cost, easy to process, and being environmentally friendly. However, in recent years, since CZTS consists of many elements and its second phases are easily formed, research studies have been carried out on  $\text{Cu}_2\text{SnS}_3$  (CTS) material for use in PV field. CTS is a p-type semiconductor with band gap values ranging from 0.9 to 1.7 eV and a high absorption coefficient ( $>10^4 \text{ cm}^{-1}$ ) [1]. Due to different arrangements of atoms in a lattice structure of CTS, different phases such as  $\text{Cu}_4\text{Sn}_7\text{S}_{16}$ ,  $\text{Cu}_4\text{SnS}_4$ ,  $\text{Cu}_3\text{SnS}_4$  structure can also occur [2]. These phases can be considered a candidate for use as an absorber layer in solar cells.

The theoretically calculated efficiency of CTS solar cells is determined at about 30%. The reported highest power conversion efficiencies of CTS solar cell belongs to 6% Ge-doped CTS [3] and 5.24% Na-doped CTS [4] solar cells. Defects, voids, and second phases in CTS thin film cause some

limitations on efficiency. In order to overcome this problem, some parameters of technical and experimental apparatuses used in the thin film production are of great importance. Many techniques are described to achieve  $\text{Cu}_2\text{SnS}_3$  thin films, for instance, reactive radio frequency magnetron sputtering [5], co-evaporation [6], wet chemical process [7], and spray pyrolysis [8]. Nonetheless, merely a limited number of studies have been reported on sprayed  $\text{Cu}_2\text{SnS}_3$  materials [9]. In comparison to other methods, the Spin coating technique has numerous benefits including low production cost, easy deposition over large-area, and relatively simpler composition adjustment. Therefore, it is particularly more suitable for thin-film fabrication [10].

In recent years, simulation software used to calculate the efficiency of solar cells with the usage of layers forming solar cells has great importance. One of the most commonly used software in this field is SCAPS-1D (one-dimensional simulation software) only which among others calculates PV parameters of solar cell using physical parameters such as energy band gap, dielectric permittivity, the electron affinity of layers constructing solar cell, thin film thickness, the work function of contacts, etc [11, 12]. SCAPS-1D was developed at Gent University in the Department of Electronics and Information Systems. Depending on parameters such as operation temperature, Auger electron/hole capture coefficient, and interfacial defect density [13], PV parameters of solar cells can be calculated, and thus, a reliable prediction can be made on the performance of the solar cell.

In this study, CTS thin films have been grown for 30 sccm sulphur flux rate at 30 minutes annealing durations at 550 °C temperature. The structural, optical, and crystalline properties of thin film have been determined and interpreted. It is important to determine how the experimentally produced thin film will affect the efficiency by modelling it in the solar cell structure using the characteristic parameters of thin film. At this point, Mo/CTS/CdS/AZO/Al structure has been formed with the most ideal CTS thin film determined by using SCAPS-1D simulation program to show the effect of this thin film on the efficiency of CTS thin film solar cell. PV parameters of CTS solar cells have been calculated and their curves have been plotted, depending on temperature, Auger electron/hole capture coefficient, and interfacial defect density. It has been determined that PV performance of CTS solar cells depends on defects, recombination mechanism, and operation temperature. Thus, based on these parameters which significantly affect the efficiency, it has reached the conclusion that it is possible to obtain consistent interpretations of behaviour of solar cells. As a result, since CTS is a new material in solar cell applications, such a study on CTS solar cells with SCAPS program is very rare in literature, and it can be predicted that this study shed light on the experimental efficiency improvement studies of solar cells.

## 2. Materials and Methods

### 2.1. Experimental

CTS thin films have been fabricated on a glass substrate using a solution comprising 0.389 g copper(II) acetate ( $\text{Cu}(\text{CH}_3\text{COO})_2 \cdot \text{H}_2\text{O}$ ), 0.220 g tin(II) chloride dehydrate ( $\text{SnCl}_2 \cdot 2\text{H}_2\text{O}$ ), and 0.444 g thiourea ( $\text{CH}_4\text{N}_2\text{S}$ ) deposited under optimized conditions with different Sulphur flux rate and time. All chemicals are separately dissolved in a mixture of ethanol and glacial acetic acid for 6h at room temperature in magnetic stirring. Firstly, thiourea solution was slowly mixed into copper(II) acetate solution, then, tin(II) chloride dehydrate was poured into the thiourea/copper(II) acetate solution. Finally, obtained solutions were stirred at room temperature for 4h until a homogenous clear solution was obtained. To regulate pH values, a few drops of diethanolamine were added to the mixture solution for the final solution. The molar ratios of Cu/Sn/S elements in solutions were adjusted due to a ratio of 2/1/6. Thiourea has volatile nature at high temperatures [14]. Therefore, this component was added twice to avoid any possible loss of sulphur.

Before the deposition process, glass substrates were washed by boiling in sufficient quantities of a mixture of H<sub>2</sub>O, NH<sub>3</sub>, and H<sub>2</sub>O<sub>2</sub> at 105 °C, and then, in sufficient quantities of a mixture of H<sub>2</sub>O, H<sub>2</sub>O<sub>2</sub>, and HCl at 105 °C to eliminate any residual waste. Then, glass substrates were cleaned in deionized water for 3 min and later dried. After obtaining final solutions and cleaning of substrates, the obtained solution was deposited via spin coating at a rate of 1500 rpm for 63 s in air. Final solutions were deposited onto the glass substrate layer by layer, and each layer was preheated to 220 °C for 10 min. After this process, obtained films were annealed under 30 and 40 sccm (standard cubic centimeters per minute) in 10 % H<sub>2</sub>S + 90 % Ar atmosphere at 550 °C temperature in the furnace. CTS thin films were annealed under 30 sccm 10 % H<sub>2</sub>S + 90 % Ar atmosphere at 550 °C temperatures for 15, 30 and 60 min and 40 sccm 10 % H<sub>2</sub>S + 90 % Ar atmosphere at 550 °C temperatures for 15, 30 and 60 min, respectively. The obtained sample has been labelled and is demonstrated in Table 1 with Sulphur flux rate and time.

**Table 1.** Fabrication parameters for CTS film.

Thin films	Sulphur annealing temperature and time	Sulphur flux rate
CTS	550 °C for 30 min	30 sccm H <sub>2</sub> S: Ar

The effect of Sulfurization on the structural, morphological, optical, and photoluminescence properties of CTS thin film have been studied in this work. The crystalline properties of acquired CTS film have been studied by X-Ray Diffractometer (XRD) unit (Bruker D8 Advance) operated at 40 kV and 40 mA. XRD was set up with a range of  $\theta$ -2 $\theta$  in steps of 0.02° to analyse the structural and phase purity analysis of CTS thin film structure. In addition, obtained films were investigated by using Confocal Raman Microscope and the obtained results were analysed. The surface topology and EDX measurements of all obtained films were obtained by FEI Quanta 250 FEG Scanning Electron Microscopy (FEI Co., Eindhoven, Netherlands). Conclusions of transmittance, energy band gap, and Urbach energy of thin films were analysed by Shimadzu UV-3600 spectrophotometer (Shimadzu, Tokyo, Japan) between 300-1100 nm.

## 2.2. Numerical Modelling and Material Parameters

SCAPS-1D software calculates PV parameters ( $V_{oc}$ ,  $I_{sc}$ , FF, and  $\eta$ ) of solar cells using physical parameters such as dielectric permittivity, band gap, the electron affinity of semiconductor layers in solar cells, work function of contacts, etc [15]. This software, which is a package program, performs a calculation procedure based on the solution of the Poisson equation (Eq. (1)), hole and electron continuity equations (Eq. (2) and Eq. (3)) [16], respectively:

$$\frac{\partial}{\partial x} (\epsilon_0 \epsilon_r \frac{\partial \Psi}{\partial x}) = -q \left( p - n + N_D^+ - N_A^- + \frac{\rho_{def}}{q} \right) \quad (1)$$

$$-\frac{\partial J_p}{\partial x} - U_p + G = \frac{\partial p}{\partial x} \quad (2)$$

$$-\frac{\partial J_n}{\partial x} - U_n + G = \frac{\partial n}{\partial x} \quad (3)$$

where  $\epsilon_r$  and  $\epsilon_0$  are permittivity of semiconductor and vacuum, respectively,  $\Psi$  is electrostatic potential,  $N_A^-$  and  $N_D^+$  indicate densities of ionized impurities of acceptors and donors,  $n$  and  $p$  are carrier concentrations of electrons and holes, and  $\rho_{def}$  is charge density of defects,  $J_p$  and  $J_n$  indicate hole and electron current densities, respectively, and  $G$  is generation rate.

Calculation of PV parameters of optical devices such as p-n heterojunction solar cells, perovskite solar cells, and dye solar cells can be performed courtesy of SCAP-1D software.

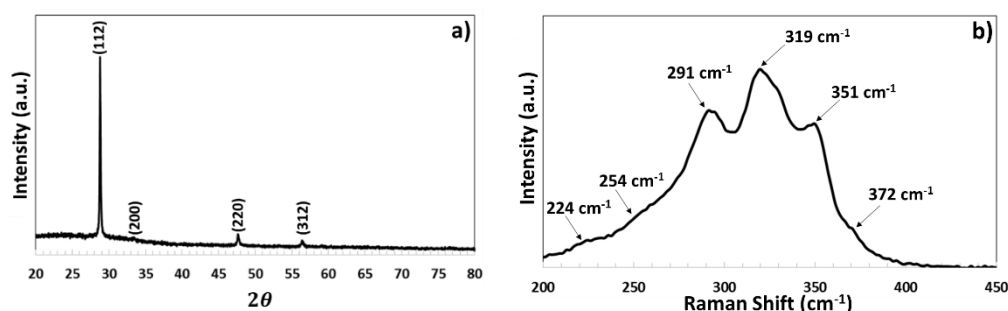
### 3. Results and Discussion

#### 3.1. XRD and Raman Analyses

CTS thin film has been formed in tetragonal  $\text{Cu}_2\text{SnS}_3$  crystal structures as seen XRD pattern and Raman spectrum in Figures 1a and 1b. (112), (200), (220) and (312) crystalline orientates in CTS thin film have been formed on  $2\theta = 28.8^\circ, 33.3^\circ, 47.6^\circ, 56.4^\circ$  angles, respectively. The crystal sizes of CTS films have been calculated by the Scherer equation:

$$S = 0.94\lambda/\beta\cos\theta \quad (4)$$

where  $S, \lambda, \beta$ , and  $\theta$  parameters are the size of crystalline, X-Ray wavelength, full-width at half-maximum (FWHM) of diffraction peak, and angle of Bragg diffraction, respectively. The main crystalline size of CTS was calculated to be 55.56 nm.



**Figure 1.** XRD pattern and Raman spectrum of CTS thin film

The micro-strain and dislocation density of CTS thin film [17, 18] were obtained by Eq. (5) and Eq. (6) as following:

$$\varepsilon = \frac{\beta\cos\theta}{4} \quad (5)$$

$$\delta = \frac{1}{D^2} \quad (6)$$

The microstrain ( $\varepsilon$ ) and dislocation density ( $\delta$ ), which express the formation of trap, vacancy, dangling bond, and defects in CTS thin film that negatively affect the development of the crystal structure.  $\varepsilon$  and  $\delta$  values have been determined to be  $0.65 \times 10^{-3}$  and  $3.24 \times 10^{16}$  lines/m<sup>2</sup>, respectively (as given in Table 2). The large crystal size leads to that there are few defects and traps in the grain boundary of thin film which ensures that  $\varepsilon$  and  $\delta$  are low. Thus, minority charge carriers in CTS thin film have a longer lifetime and this leads to the higher efficiency of solar cells produced based on the absorber layer.

The crystal number per unit surface area ( $N$ ) is calculated by Eq. (7),

$$N = \frac{T}{D^3} \quad (7)$$

where  $T$  is the thickness of CTS thin film.  $N$  value expresses the crystallization amount, which varies depending on the thickness and crystal size. The average thickness of CTS thin film has been measured to be  $\sim 1 \mu\text{m}$ .  $N$  values of thin film have been calculated as  $0.58 \times 10^{16} \text{ m}^{-2}$  (Table 2). The large crystal size relative to film thickness which causes the crystalline number to be somewhat small.

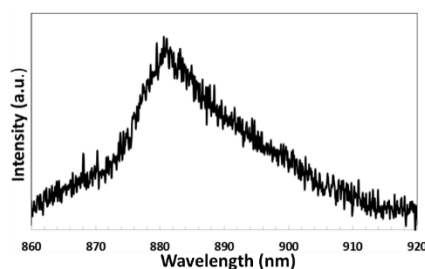
**Table 2.** Crystalline size, dislocation density, micro-strain, and crystalline number of CTS thin film

Sample	Crystalline Size (nm)	Dislocation density $\times 10^{16}$ (lines/m <sup>2</sup> )	Micro-strain $\times 10^{-3}$	Crystalline Number $\times 10^{16}$ (m <sup>2</sup> )
CTS	55.56	3.24	0.65	0.58

Raman spectrum in Figure 1b indicates that phase structures formed in CTS thin film in the 200-450 nm wavelength range. The monoclinic Cu<sub>2</sub>SnS<sub>3</sub> (254 cm<sup>-1</sup> [19], 291 cm<sup>-1</sup>[2], 372 cm<sup>-1</sup> [2]), tetragonal Cu<sub>2</sub>SnS<sub>3</sub> (319 cm<sup>-1</sup> and 351 cm<sup>-1</sup>[2]) and SnS phase (224 cm<sup>-1</sup>) formations have been occurred in CTS thin film. Due to dominant peaks on 319 cm<sup>-1</sup> and 291cm<sup>-1</sup>, it can be stated that CTS thin film is predominantly tetragonal phase structure which is compatible with the XRD pattern.

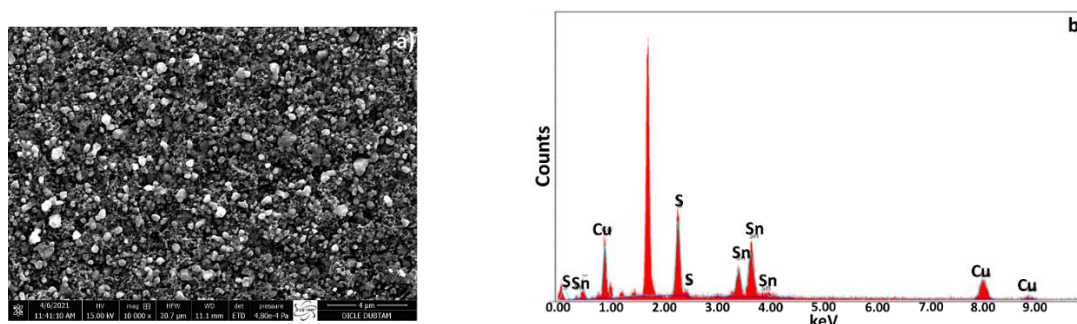
### 3.2. Photoluminescence Analyses

Photoluminescence (PL) is based on the principle that electrons are excited to upper energy levels by absorbing light incident on thin film, and then electron emits photons when it relaxes to a lower energy level. PL spectra of CTS thin film are presented in Figure 2. CTS thin film exhibits emission between 860 nm and 920 nm and PL has occurred at 1.40 eV (881 nm) under excitation. This energy is slightly above its band gap. Furthermore, PL formation of about 1.4 eV leading an increase in J<sub>sc</sub> and power conversion efficiency in the solar cell.

**Figure 2.** PL spectrum of CTS thin film

### 3.3. Morphologic and EDX Analyses

According to the SEM image in Figure 3a, CTS thin film consists of dense particles and particle size is a distribution between 300-500 nm indicating non-homogeneous particle size distribution.

**Figure 3.** SEM image and EDX spectrum of CTS thin film

As seen in the EDX spectrum given in Figure 3b and Table 3, CTS thin film is Cu-poor and Sn-rich. Copper vacancies ( $V_{Cu}$ ), which act like acceptor defects, enhance the p-type conductivity of CTS thin film and improve the efficiency of the solar cell. However, when Sn atoms occupy  $V_{Cu}$  vacancies [20, 21], Sn<sub>Cu</sub> donor defects form which can act as a recombination centre, and increase n-type

conductivity. In addition, the amount of elemental sulphur is high because the thin film is annealed under sulphur flux for a long time and at a high temperature.

**Table 3.** The atomic weight rates of elements in CTS thin film

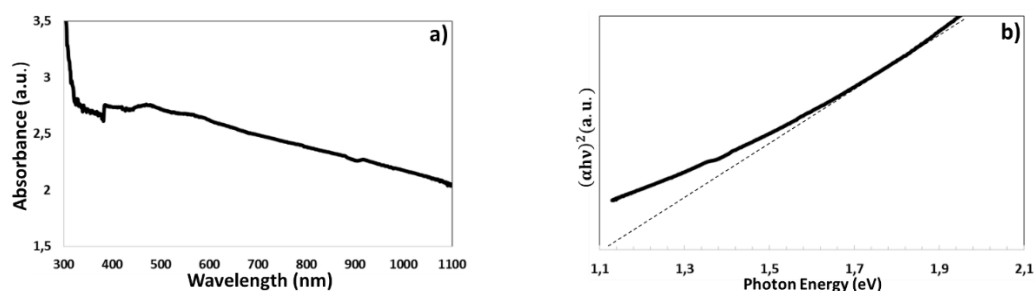
Sample	Cu(%)	Sn(%)	S(%)	Cu/Sn	S/metal
CTS	25.65	15.25	59.10	1.68	1.44

### 3.4. Optical Analyses

The light absorbance of CTS thin film is decreased slightly towards to near-infrared region, as shown in Figure 4a. However, it showed a similar absorbance in visible and near-infrared regions. Tauc equation denoted by Eq. (8) that is used to obtain band gap of thin film:

$$\alpha h\nu = A(h\nu - E_g)^{1/2} \quad (8)$$

where  $h\nu$  is photon energy,  $E_g$  is thin film energy band gap,  $A$  is a constant.  $E_g$  is obtained by a straight line of  $(\alpha h\nu)^2$  versus  $(h\nu)$  in Tauc plot in Figure 4b. CTS thin film's band gap has been determined to be 1.12 eV. This value proves that thin film absorbs a high number of photons in longer wavelength regions and is compatible with a band gap of  $\text{Cu}_2\text{SnS}_3$  given in the literature [22].

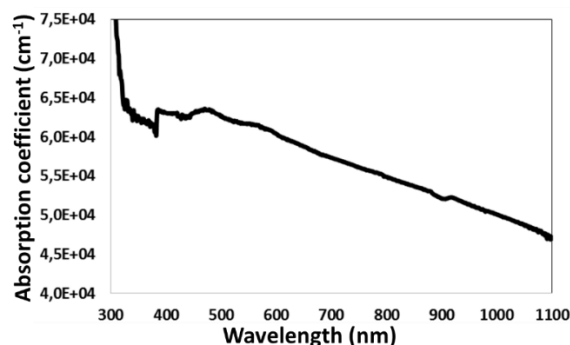


**Figure 4.** a) Absorption spectra and b) Tauc plot of CTS thin film

The thin film's absorption coefficient is determined by Eq. (9):

$$\alpha = 2.303(A/T) \quad (9)$$

$T$  is the thickness of thin film and  $A$  is the absorbance of material. As expressed in the spectrum sketched in Fig. 5, CTS thin film has an absorption coefficient greater than  $5.5 \times 10^4 \text{ cm}^{-1}$  in the visible region and this result is compatible with  $\text{Cu}_2\text{SnS}_3$  absorption coefficients reported in the literature [1]. It has been observed that the absorption coefficient decreases towards to near-infrared region.



**Figure 5.** Absorption coefficient spectrum of CTS thin film

### 3.5. SCAPS-1D Simulation Program

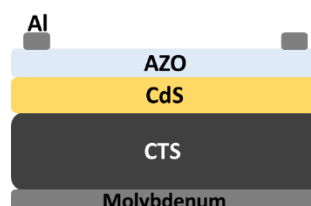
#### 3.5.1 Simulation of Mo/CTS/CdS/AZO/Al thin film solar cell

Absorber layers of solar cells, such as CTS, significantly affect power conversion efficiency. In many studies reported in the literature, only one layer of the solar cell was experimentally produced and the efficiency of the solar cell was determined by the physical parameters of that layer [15, 25, 26]. In this study, CTS thin film was determined to be the most ideal thin film depending on crystal structure and minimum defect conditions in CTS thin films.

**Table 4.** The physical parameters used in the modelling of Mo/CTS/CdS/AZO/Al solar cell

Layers	AZO [23]	CdS [24]	CTS [23]
Band Gap (eV)	3.3	2.4	1.12
Electron affinity (eV)	4.6	4.4	4.5
Dielectric permittivity (relative)	9	10	10
CB effective density of states (cm <sup>-3</sup> )	2.20x10 <sup>18</sup>	1.80x10 <sup>18</sup>	2.20x10 <sup>18</sup>
VB effective density of states (cm <sup>-3</sup> )	1.80x10 <sup>19</sup>	2.40x10 <sup>19</sup>	1.80x10 <sup>19</sup>
Electron/Hole thermal velocity (cm/s)	1.00x10 <sup>7</sup>	1.00x10 <sup>7</sup>	1.00x10 <sup>7</sup>
Electron/Hole mobility (cm <sup>2</sup> /Vs)	100/25	100/25	100/25
Shallow donor density (cm <sup>-3</sup> )	1.00x10 <sup>20</sup>	1.00x10 <sup>18</sup>	0
Shallow acceptor density (cm <sup>-3</sup> )	0	0	1.00x10 <sup>16</sup>
Thickness	200 nm	50 nm	1 μm
Contacts	Back Contact (Mo)	Front Contact (Al)	
Metal work function (eV)	5.00	4.08	
Surface recombination velocity of electrons (cm/s)	1x10 <sup>7</sup>	1x10 <sup>5</sup>	
Surface recombination velocity of holes (cm/s)	1x10 <sup>5</sup>	1x10 <sup>7</sup>	

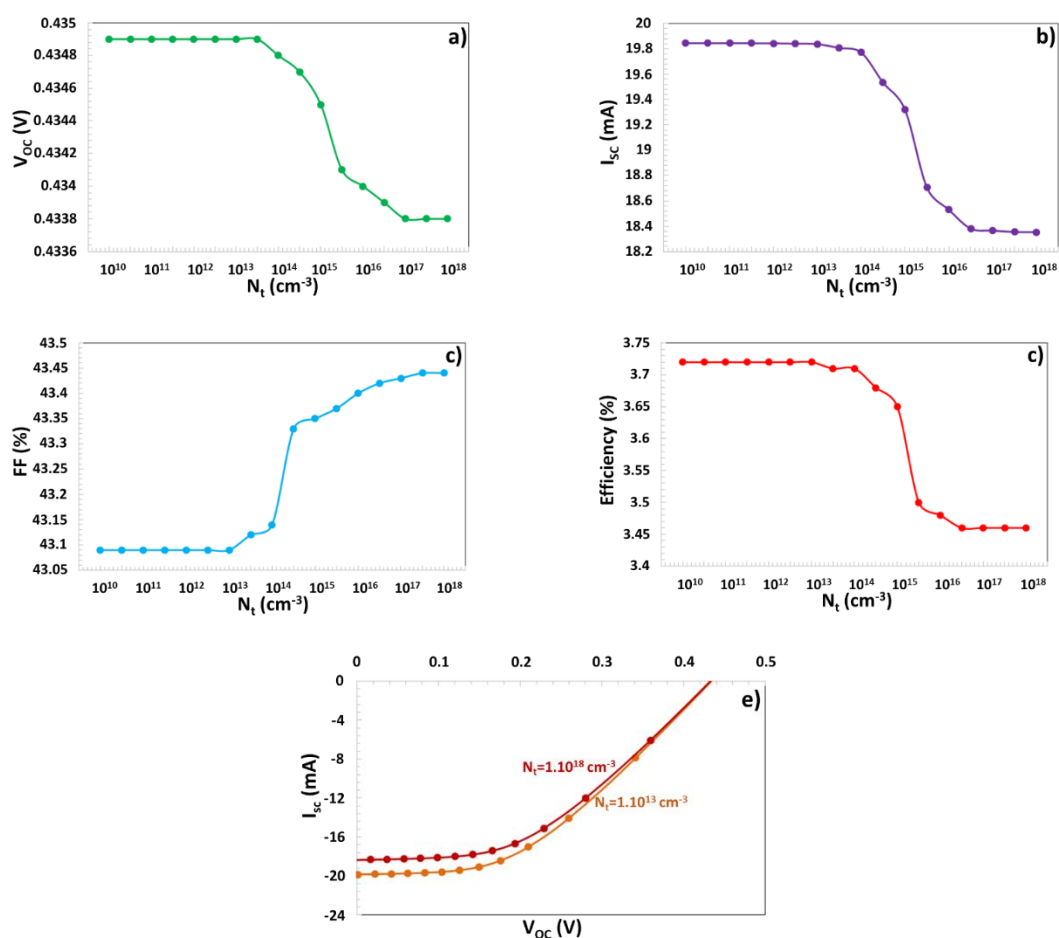
Therefore, we have formed Mo/CTS/CdS/AZO/Al solar cell structure based on CTS thin film absorber layer (in Figure 6), using SCAPS-1D program. The absorption coefficient spectrum file (shown in Figure 5) with 1 μm thickness and 1.12 eV band gap of CTS thin film was processed by SCAPS-1D simulation. Since Aluminium has a low work function, Al metal contact is preferred due to the possibility of exhibiting ohmic behaviour for the AZO semiconductor. We have calculated and interpreted PV performance depending on interface defect density, radiative recombination, Auger recombination, and operation temperature (parameters significantly change the efficiency) of Mo/CTS/CdS/AZO/Al the solar cell. Theoretically calculated results have been given below. Thus, by taking basic parameters of other layers for the simulated structures, the PV parameters of the solar cell are determined. This will provide a reliable and accurate path for the experimental operation of this type of solar cell. Physical parameters of layers forming CTS the solar cell in our model are given in Table 4.



**Figure 6.** Mo/CTS/CdS/AZO/Al modelled by SCAPS-1D simulation

### 3.5.2 The effect of defect density ( $N_t$ ) at the interface CTS/CdS of the solar cell

A high density of defect points can be localised at the interface between CTS and CdS layers leading to recombination centres [27]. Neutral defects can also occur at the interface of the second phase. The neutral defects acting as centres of Shockley-Read-Hall (SHR) recombination cause a certain decrease in the efficiency of the solar cell. These defects, located close to band edges, contribute to SHR recombination since the carrier is likely to return to its respective bands for shallow levels. Besides these, neutral defects can also be caused by lattice mismatch of CTS and CdS semiconductors in contact with each other [28, 29]. PV parameters of CTS solar cell versus interfacial neutral defect density (in  $10^{10}$  and  $10^{18}$   $\text{cm}^{-3}$ ) are given in Figure 7. According to these curves,  $V_{OC}$  and  $I_{SC}$  PV parameters of CTS the solar cell decreased after  $1.10^{13}$   $\text{cm}^{-3}$  of neutral defect densities.



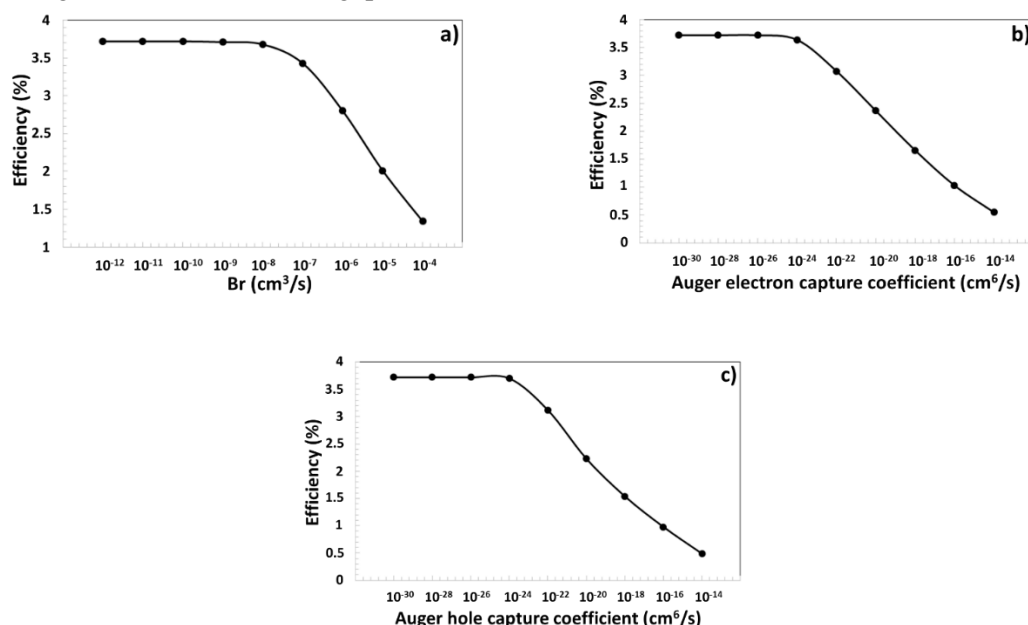
**Figure 7.** a)  $V_{oc}$ , b)  $I_{sc}$ , c) FF, d) Efficiency curves and e)  $I_{sc}$  depending on the interfacial defect density ( $N_t$  ( $\text{cm}^{-3}$ )) at CTS/CdS of the solar cell.

Power conversion efficiency (shown in Figure 7e) of the solar cell for  $1.10^{13}$   $\text{cm}^{-3}$  defect density is 3.72 %. As seen in Figure 7d, after a neutral defect density of  $1.10^{13}$   $\text{cm}^{-3}$ , there was a sudden drop in the efficiency of the CTS solar cell. It has been noticed that the efficiency of the solar cell has remained constant at 3.46 % between  $1.10^{17}$  and  $1.10^{18}$   $\text{cm}^{-3}$  of defect density [30]. As a result, neutral defect density should not be less than  $1.10^{13}$   $\text{cm}^{-3}$ . Therefore, it has been concluded that there is no reduction in power conversion efficiency.



### 3.5.3 Recombination mechanism for Mo/CTS-A2/CdS/AZO/Al solar cell

The recombination mechanism consists of three types of recombination radiative recombination, Auger recombination, and SRH recombination. These recombination mechanisms have a great influence on the PV performance of multilayer solar cells. In this study, the radiative recombination coefficient and Auger coefficient were evaluated. When an electron in the conduction band is transferred to the valence band, it emits a photon. The recombination of electrons and holes in this process is expressed as radiative recombination [31]. The efficiency spectra of the CTS solar cell depending on radiative recombination coefficient ( $Br$  ( $\text{cm}^3/\text{s}$ )) is given in Figure 8a and efficiency remains almost constant between  $10^{-12}$  and  $10^{-8}$   $\text{cm}^3/\text{s}$ , it drops abruptly with  $10^{-8}$   $\text{cm}^3/\text{s}$ . For efficiency not to decrease, the  $Br$  value must be less than  $10^{-8}$   $\text{cm}^3/\text{s}$ . Auger recombination is a non-radiative event, which has a large effect on small band gap semiconductors.



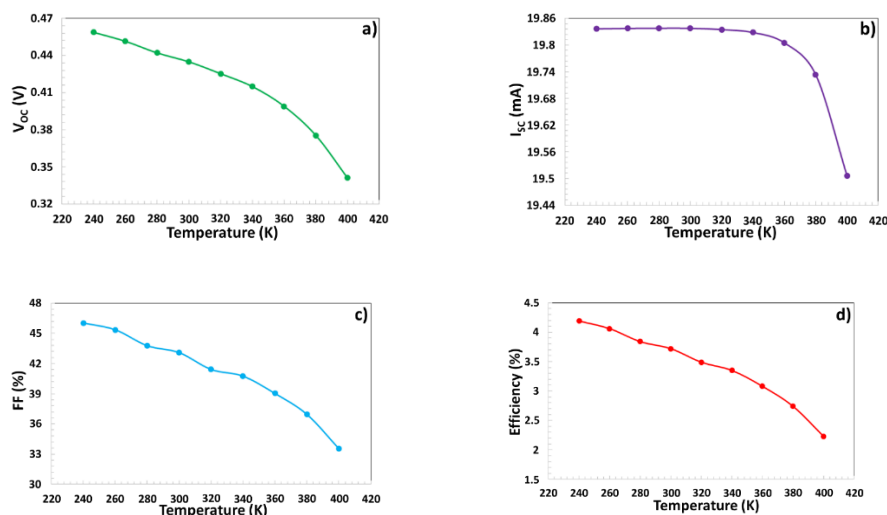
**Figure 8.** The efficiency curve of CTS solar cell depends on a) radiative recombination coefficient ( $Br$ ), b) Auger electron and c) hole capture coefficient

When an electron and hole recombine with excess energy, an electron rises to the conduction band, or the hole transitions deeper into the valence band, but no light is produced [32, 33]. This process is known as Auger recombination. As seen in Figure 8b and 8c, when Auger electron and hole capture coefficients increase from  $10^{-26}$  to  $10^{-14}$   $\text{cm}^6/\text{s}$  and  $10^{-24}$  to  $10^{-14}$   $\text{cm}^6/\text{s}$ , respectively, efficiency values decrease. Therefore, these values should not be exceeded in order to avoid a significant decrease in the efficiency of the solar cell.

### 3.5.4 The effect of the operating temperature on CTS solar cell

Operation temperature adversely affects the performance of solar cells due to PV characteristics based on operation temperature between 240 °K and 400 °K in Figure 9,  $V_{OC}$  and FF values of CTS solar cell decreases as operation temperature increases. So, with increasing operation temperature, the band gap of the semiconductor decreases. In other words, the crystal lattice of the thin film broadens and the interatomic bonds are weakened. Weak bonds between atoms express that very low energy is required to break a bond and take an electron from the conduction band. Thus, the recombination rate of electron-hole pair between conduction and valence band increases. It limits access of minority charge carriers to

the depletion region. Moreover, an increase in dark current causes an increment in leakage current and reduces the  $V_{OC}$  value [23, 34-36]. Furthermore, the energy of carriers increases even more and they become unstable as operation temperature increases. Therefore, carriers undergo recombination before they can reach the depletion region, this case reduces  $I_{SC}$  and  $V_{OC}$  values [36]. As a result, an increment in operation temperature deteriorates the performance of the solar cell. The efficiency of the solar cell was calculated to be 3.72 % for room temperature (300 K) [37-39].



**Figure 9.** Effect of the operating temperature on a)  $V_{OC}$ , b)  $I_{SC}$ , c) FF, and d) efficiency parameters of CTS solar cell

#### 4. Conclusion

CTS thin films were produced for 30 and 40 sccm sulphur flux rates in 15, 30, and 60 minutes annealing time durations at a constant 550 °C temperature. CTS thin film has been formed in tetragonal in  $Cu_2SnS_3$  crystalline structure. Crystalline size, dislocation density, microstrain, and the crystalline number of CTS structure have been calculated to be 55.56 nm,  $3.24 \times 10^{16}$  lines/m<sup>2</sup>,  $0.65 \times 10^{-3}$ , and  $0.58 \times 10^{16}$  m<sup>-2</sup>, respectively. CTS thin film consists of particles with dense and inhomogeneous size distribution. CTS thin film is Cu-poor and Sn rich, which has a band gap of 1.12 eV.

Mo/CTS/CdS/AZO/Al solar cell based on CTS layer was modelled using SCAPS-1D software.  $V_{OC}$  and  $I_{SC}$  PV parameters of CTS the solar cell were decreased with  $10^{13}$  cm<sup>-3</sup> of neutral defect density. Efficiency corresponding to this defect density is 3.72 %. Radiative recombination coefficient and Auger electron/hole capture recombination coefficient have been calculated: radiative recombination coefficient dropped abruptly beyond  $10^{-8}$  cm<sup>3</sup>/s value. For efficiency not to decrease, the  $B_r$  value must be higher than  $10^{-8}$  cm<sup>3</sup>/s. When Auger electron and hole capture coefficients increase from  $10^{-26}$  to  $10^{-14}$  cm<sup>6</sup>/s and  $10^{-24}$  to  $10^{-14}$  cm<sup>6</sup>/s, respectively, efficiency values decrease. As the operation temperature increases, the  $V_{OC}$  and FF of the solar cell decrease. CTS solar cell shows an efficiency value of 3.72 % at room temperature.

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### **Ethical Statements**

The author declares that this document does not require an ethics committee approval or any special permission. Our study does not cause any harm to the environment.

### **Conflict of interest**

The authors declare no conflict of interest.

### **Authors Contributions**

SYG carried out calculations and wrote the first draft of the manuscript. IC and SB carried out the experiments. HSK supervised the projects. All authors discussed the results and contributed to the final manuscript.

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