Numerical Modelling Of The Effect Of Temperature And Thickness On The Electrical Properties Of Polycrystalline Semi-Conductor Solar Cells [CdTe and Cu(In,Ga)Se$_2$(CIGS)] Using One Dimensional Device Simulation.

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Abstract. A numerical simulation program SCAPS 1D (solar cell and capacitance simulator) was used in the simulation of CdTe and CIGS solar cells. We concentrated on the effect of temperature and thickness on the electrical properties of CdTe and CIGS solar cells and the agreement between the simulations and measurements was shown and discussed using SCAPS 3.3.00. The influences of temperature and thickness on CdTe and CIGS solar cells were investigated by I-V measurements. The simulated efficiencies for CdTe and CIGS solar cells at 300K were observed to be 16.03% and 16.54% which compare very well with the measured efficiencies 10.72% for CdTe and 15.96% for CIGS solar cell at same temperature. It was found out that as temperature and thickness increases from (200 – 400)K and (2 – 6)μm, efficiencies decrease from 18% to 10% for CdTe and 20% to 8% for CIGS from (250 – 400)K and (1 – 5)μm respectively. 

Keywords: SCAPS 1D, CdTe, Cu(In,Ga)Se$_2$, Numerical Simulation, Efficiencies $\eta$, Comparison of Simulation to Measurement.

1.0 Introduction

Solar energy is in abundance but only a little is used to directly power human activities. About 80%-85% of our total energy comes from fossil fuels. These resources are non-renewable, fast depleting, produce greenhouse gases and other harmful environmental pollutants [1]. Shifting the focus on renewable sources of energy is the ideal choice and solar power is by far the most prominent energy source owing to its versatility, inexhaustible and environmentally friendly features [1]. By covering 0.16% of Earth’s land with 10% efficient solar cells would provide 20TW of energy about twice of fossil fuel consumption of the world including numerous nuclear fission reactors [2].

Polycrystalline CdTe and CIGS are excellent candidates for stable, efficient and low cost solar cells which also have proven to be good choices as the base material for solar cells. The search for the ideal PV material is being actively pursued on many fronts [3]. However, efficiency is not the only parameter targeted by the solar cell industry; costs are also taken into account. The industrial manufacturing of solar cells aims to balance costs and efficiency during devices fabrication [4]. Numerical modeling of polycrystalline thin-film solar cells is an
important strategy to test the viability of proposed physical explanations and to predict the effect of physical changes on cell performance. In general, this must be done with only partial knowledge of input parameters. However, for consistent comparisons between laboratories, it is extremely useful to have a common starting point, or baseline [5]. There are several numerical solar cell simulation programs in use. The first solar cell program was developed by Mark S. Lundstrom as part of his PhD Thesis [6]. Numerical modeling is a necessity for the realistic description of thin-film PV devices [7]. In many cases numerical simulation of a thin film solar cell can lead to better insight into the details of physical operation. It can even give new insights to improve the technology [8]. However, the numerical treatment of various electronic effects present in polycrystalline thin film solar cells, which do not occur in standard crystalline Si solar cells, is explained using a numerical solar cell simulation tool, SCAPS (Solar Cell and Capacitance Simulator) [9].

**Figure 1:** Solar cell definition panel.

SCAPS has proven to be a reliable simulation tool by different groups that investigate thin film solar cells because originally it was developed for cell structures of the CuInSe$_2$ and the CdTe family. Several extensions however have improved its capabilities so that it is also applicable to crystalline solar cells (Si and GaAs family) and amorphous cells (a-Si and micromorphous Si) [10]. SCAPS solves model structures with up to 7 different layers, plus two contacts (figure 1). All kind of material parameters can be specified for each layer. SCAPS is able to calculate the relevant electro-optical parameters commonly carried out on thin film solar cells. These are not only the I-V characteristics, but also spectral response QE(λ) and the capacitance measurements C(V) and C(f), all these as a function of temperature [10]. SCAPS is developed and tested to simulate realistic situations, hence things can go wrong when simulating unphysical situations [11].
2.0 Theoretical Background

Most solar cell characteristics can be obtained from simple I-V measurements. (Figure 3) shows the I-V characteristics of a typical solar cell under forward bias and illumination. The short circuit current ($I_{sc}$) is the current through the solar cell when the voltage across the solar cell is zero. The open circuit voltage ($V_{oc}$) is the voltage across the solar cell when the current through the solar cell is zero and it is the maximum voltage available from the solar cell. The maximum power point ($P_{max}$) is the condition under which the solar cell generates its maximum power; the current and voltage in this condition are defined as $I_{max}$ and $V_{max}$ respectively. The fill factor (FF) equation (i) and the energy conversion efficiency ($\eta$) equation (ii) are metrics used to characterize the performance of the solar cell. The fill factor is defined as the ratio of $P_{max}$ divided by the product of $V_{oc}$ and $I_{sc}$. The conversion efficiency is defined as the ratio of $P_{max}$ to the product of the input light irradiance ($E$) and the solar cell surface area $A_c$ [12].

\[
FF = \frac{P_{max}}{I_{sc} V_{oc}} \quad \text{(i)}
\]

\[
\therefore \eta = \left( \frac{FF \times I_{sc} V_{oc}}{E \times A_c} \right) \quad \text{(ii)}
\]

(Figure 3: Typical I-V forward bias characteristics of a solar cell.)
The current density-voltage (J-V) measurement is common measurement technique used to investigate the characteristics of thin film through the current density-voltage (J-V) curve of thin films. From this curve the electrical properties of the thin films can be studied [13]. The material requirements of an efficient solar cell are determined by the basic steps involved in the conversion of sunlight to electric power [3].

3.0 Methodology

3.1 Material

SCAP-1D version 3.3.00 is a one dimensional solar cell device simulator, developed at Electronics and Information Systems (ELIS) University of Gent, Belgium. The simulator is freely available to the PV research community. The user can describe a solar cell as a stack of up to seven layers with different properties, such as thickness, optical absorption, and defect densities. It can then be used to simulate a number of common measurements: I-V, QE, C-V, C-f. SCAPS is a Windows-oriented program, developed with Lab Windows of National Instruments. We use here the Lab Window terminology of a ‘Panel’ (names used in other softwares are: a window, a page, an input, a pop-up...). SCAPS opens with the ‘Action Panel’ [10].

3.2 Simulation Procedure

This research work is computational which was carried out using a window oriented program that is, C-code. The program is made up of three categories of file: physics source code (discretized basic semiconductor equations), input and output files. The physics source code is the main source code which contains the routine for the actual computations. The input file contains data to be read into the main program at run-time. The output files keep the result of the computation.

The installation of the program code (SCAPS 3.3.00) in the computer was done successfully, which requires familiarity of the computer system. There are five (5) number of presets (dedicated panels) on the program, on which we run preset number (2), were we imputed (create/edit) solar cell structures by setting layer, interface and contact properties ideally, setting numerical presences and to save those to or load from definition files (figure 1). On preset number three (3), we indicated the circumstances in which to do the simulation (figure 4), that is, specify the working point (temperature K, Voltage V, frequency f and the illumination: light (one sun)/dark). We then used the temperature(K) menu on the action panel and that of the layer thickness (μm) on the solar cell definition panel to vary the temperature and the thickness respectively (figures 2 and 4), and in each case the reading of both the simulated and measured current-voltage characteristics where taken respectively.

![Figure 4: Setting the working point conditions, available on the action panel](image-url)
4.0 Results and Discussion

4.1 Results

In this section the results for the simulations of CdTe and CIGS solar cells are presented at various temperatures and thicknesses. Also, results/agreement for/between the simulated, theoretical (measured), and experimental results for CdTe and CIGS solar cells at 300K are presented.

4.1.1 Effect of Temperature (K) and Thickness (µm) on CdTe Solar Cells.

| Temperature(K) | Thickness (µm) | Voc (V)     | Jsc (mA/ cm²) | FF | η (%) |
|----------------|---------------|-------------|---------------|----|-------|
| 2.0000         | 200           | 4.8645V     | 23.900mA/ cm²| 0.16| 18.44%|
|                | 250           | 1.7626V     | 23.896mA/ cm²| 0.41| 17.71%|
|                | 300           | 0.8742V     | 23.891mA/ cm²| 0.75| 15.73%|
|                | 350           | 0.7208V     | 23.885mA/ cm²| 0.76| 13.14%|
|                | 400           | 0.6042V     | 23.882mA/ cm²| 0.73| 10.48%|
| 3.0000         | 200           | 4.7094V     | 24.122mA/ cm²| 0.16| 18.54%|
|                | 250           | 1.9696V     | 24.116mA/ cm²| 0.38| 17.94%|
|                | 300           | 0.9738V     | 24.108mA/ cm²| 0.69| 16.13%|
|                | 350           | 0.7434V     | 24.103mA/ cm²| 0.75| 13.43%|
|                | 400           | 0.6214V     | 24.102mA/ cm²| 0.70| 10.54%|
| 4.0000         | 200           | 3.9135V     | 24.183mA/ cm²| 0.20| 18.49%|
|                | 250           | 1.7635V     | 24.181mA/ cm²| 0.42| 17.77%|
|                | 300           | 0.9978V     | 24.108mA/ cm²| 0.67| 16.03%|
|                | 350           | 0.7525V     | 24.166mA/ cm²| 0.74| 13.37%|
|                | 400           | 0.6274V     | 24.159mA/ cm²| 0.69| 10.44%|
| 5.0000         | 200           | 3.1028V     | 24.201mA/ cm²| 0.25| 18.38%|
|                | 250           | 1.5419V     | 24.203mA/ cm²| 0.47| 17.45%|
|                | 300           | 0.9924V     | 24.198mA/ cm²| 0.66| 15.79%|
|                | 350           | 0.7568V     | 24.183mA/ cm²| 0.72| 13.21%|
|                | 400           | 0.6312V     | 24.166mA/ cm²| 0.68| 10.31%|
| 6.0000         | 200           | 2.4178V     | 24.205mA/ cm²| 0.31| 18.19%|
|                | 250           | 1.3663V     | 24.209mA/ cm²| 0.51| 17.10%|
|                | 300           | 0.9777V     | 24.206mA/ cm²| 0.66| 15.50%|
|                | 350           | 0.7586V     | 24.187mA/ cm²| 0.71| 13.01%|
|                | 400           | 0.6320V     | 24.164mA/ cm²| 0.67| 10.16%|
4.1.2 Effect of Temperature (K) and Thickness (µm) on CIGS Solar Cell.
Table 2: Simulated I-V parameters (V), (mA/ cm²), FF and eta (%) of single short obtained at various temperatures (K) and thicknesses (µm) for CIGS solar cell under illumination.

| Temperature (K) | 250 | 300 | 350 | 400 |
|----------------|-----|-----|-----|-----|
| Thickness (µm) | 1.0000 | 2.0000 | 3.0000 | 4.0000 | 5.0000 |
| Voc | 0.6933V | 0.7068V | 0.7111V | 0.7126V | 0.7130V |
| Jsc | 31.713mA/ cm² | 33.566mA/ cm² | 34.171mA/ cm² | 34.373mA/ cm² | 34.433mA/ cm² |
| FF | 0.81 | 0.82 | 0.84 | 0.84 | 0.82 |
| η | 17.84% | 19.49% | 20.00% | 20.16% | 20.20% |
| Voc | 0.5913V | 0.6071V | 0.6125V | 0.6145V | 0.6152V |
| Jsc | 31.659mA/ cm² | 33.423 mA/ cm² | 34.049mA/ cm² | 34.280mA/ cm² | 34.360mA/ cm² |
| FF | 0.78 | 0.79 | 0.79 | 0.79 | 0.79 |
| η | 14.64% | 16.06% | 16.54% | 16.71% | 16.76% |
| Voc | 0.4881V | 0.5055V | 0.5118V | 0.5143V | 0.5153V |
| Jsc | 31.401mA/ cm² | 33.029mA/ cm² | 33.654mA/ cm² | 33.906mA/ cm² | 34.002mA/ cm² |
| FF | 0.74 | 0.75 | 0.75 | 0.75 | 0.75 |
| η | 11.39% | 12.55% | 12.97% | 13.13% | 13.19% |
| Voc | 0.3848V | 0.4030V | 0.4101V | 0.4131V | 0.4145V |
| Jsc | 31.395mA/ cm² | 32.866 mA/ cm² | 33.480mA/ cm² | 33.750mA/ cm² | 33.867mA/ cm² |
| FF | 0.69 | 0.70 | 0.70 | 0.70 | 0.70 |
| η | 8.34% | 9.27% | 9.64% | 9.80% | 9.87% |
4.1.3 Simulation and Experimental Measurement of Current –Voltage Performance of CdTe Solar Cell.

Table 3: Simulated, Theoretical (measured), and Experimental I-V parameters: (V), (mA/cm²), FF and η (%) of single shot obtained at 300K and 4.0000µm for CdTe solar cell under illumination.

| CdTe       | Simulation | Theoretical/Measured[15] | Experimental[12][13] |
|------------|------------|--------------------------|----------------------|
| V_{oc} (V) | 0.9978     | 0.8220                   |                      |
| J_{sc} (mA/cm²) | 24.175   | 19.560000                |                      |
| FF         | 0.6645     | 0.6665                   |                      |
| η (%)      | 16.03%     | 10.7162003 = 10.72%      | (16-17)%             |

4.1.4 Simulation and Experimental Measurement of Current –Voltage Performance of CIGS Solar Cell.

Table 4: Simulated, Theoretical (measured) and Experimental I-V parameters (V), (mA/cm²), FF and η (%) of single shot obtained at 300K and 3.0000µm for CIGS solar cell under illumination.

| CIGS       | Simulation | Theoretical/Measured [5] | Experimental[14][15] |
|------------|------------|--------------------------|----------------------|
| V_{oc} (V) | 0.6125     | 1.0486                   |                      |
| J_{sc} (mA/cm²) | 34.048634 | 24.076433                |                      |
| FF         | 0.793      | 0.632                    |                      |
| η (%)      | 16.54%     | 15.95581811088 = 15.96% | (16-19)%             |

3.3.3 The IV- Curve under Illumination and Darkness

Figure 5: Simulated and Theoretical (Measured) (Open Symbols/Boxes) I-V Characteristics of CdTe at 300K under Illumination and Dark, W_{CdTe}=4µm, Theoretical Measured Efficiency η = 10.72%.
4.2 Analysis of Result

Tables 1 and 2, summarizes the simulated I-V parameters $J_{sc}$ (mA/cm$^2$), $V_{oc}$ (V), FF and $\eta$ (%) of single shot obtained at various temperatures and thicknesses for both CdTe and CIGS solar cells under illumination, where the CdTe solar cell happened to be at its best with open-circuit voltage, short-circuit current density, fill factor and efficiency of 0.9978V, 24.108mA/cm$^2$, 0.67, and 16.03% at 300K and 4.0000µm respectively. Likewise for CIGS solar cell: 0.6125V, 34.049mA/cm$^2$, 0.79, and 16.54% at 300K and 3.0000µm respectively. This is because SCAPS working temperature is 300K at default and most semiconductor modeling is done at 300K since it is close to room temperature and a convenient number. However, solar cells are typically measured almost 2 degrees lower at 250C (298.15K). In most cases the difference is significant (only 4mV of $V_{oc}$) and both are referred to as room temperature. Occasionally, the modeled results need to be adjusted in the measured results [16]. And since the fill factor (FF) is inversely proportional to the product between short circuit current density and open circuit voltage, these parameters remain almost constant for the whole series [17]. Therefore, CdTe and CIGS had fill factor of 0.67 and 0.79 at 300K respectively. All these simulation results will give some important guides for feasibly fabricating higher efficiency CdTe and CIGS solar cells.

The electrical power conversion efficiencies $\eta$ were observed to decrease as temperature increases. This can be attributed to the shift in the I-V characteristic curves of a typical polycrystalline solar cell with increase in temperature. The energy conversion efficiency will have a peak as the solar cells thickness is reduced due to two opposing factors; The $V_{oc}$ increases and the $I_{sc}$ decreases with decreasing cell thickness which is due to a shorter optical path length [19]. More so, solar cell performance decreases with increasing temperature, fundamentally owing to increased internal carrier recombination rates / increase dark current, caused by increased carrier concentration. Both the electrical efficiency and power output of a solar cell module depend linearly on the operating temperature. The effect of temperature on the electrical efficiency of a solar cell can be obtained by using the fundamental equation (i.e. equation ii). As
such, the operating temperature plays a central role in the solar cells (CdTe and CIGS) conversion process. Both the electrical efficiency and, hence, the power output of the solar cells depend linearly on the operating temperature decreasing with solar temperature [20].

Too small thickness of the absorbing layer in solar cell based CdTe and CIGS lead to a lower value of photocurrent, while too thick absorbing layer leads to a large series resistance and increase in material consumption and, consequently, the cost per unit of power produced [18]. However, the increases of the buffer layer thickness only reduce the cell performances. The optimum thickness of the absorber layer was about 3 μm, a value from which the efficiency has no significant increase. The increase of the absorber band gap reduces the optical absorption, which was reflected in the reduction of the photocurrent density. Accordingly the open circuit voltage increases as a result to the linear variation with the band gap. The compromise between these two phenomena would be a band gap of 1.55 eV which is the optimum value for obtaining a high efficiency of about 25%. All these optimization results give helpful indication for a feasible fabrication process.

Resulting I-V output (T=300K) from simulation and theoretical measurements of the solar cells, using Tables 3 and 4, parameters are shown in Figures 5 and 6. Light and dark I-V curves showed a reasonable superposition where the simulated efficiencies for CdTe 16.03% and 16.54% for CIGS are close to the theoretical (measured), and experimental efficiencies, which are (CdTe=10.72% and CIGS = 15.96%), (CdTe=16-17% and CIGS = 16-19%) respectively. All these simulation results will give some important guides for feasibly fabricating higher efficiency polycrystalline solar cells.

However, in this research work, the optimum energy conversion efficiencies at 300K for both simulation and measurement, generated their maximum values as shown in Tables 3 and 4, which is reasonably good when compared with work of [5]. Numerical modeling of CIGS and CdTe solar cells: setting the base line, with efficiencies 16.4% and 17.7% for CdTe and CIGS solar cells at the same temperature range (300K). Similarly, the numerical modeling efficiencies obtained are in close agreement with the experimental efficiencies obtained by [21] and [22], where CdTe solar cells recorded experimental efficiency of about 16%-17%; while [23] and [24] reported efficiency cells (16%-19%) for CIGS solar cells respectively. The efficiency results obtained was also found to compare to that obtained by [25], where CdTe had efficiency of 16.4% and CIGS 18.8% both at 300K. The cells in reference had a somewhat higher V_{oc} due to band gap grading in space charge region. Consequently, a link between the characteristics of these cells and the material parameters was established. This procedure helped improving the performances of the cell and can lead to a better insight in the internal physical operation of a solar cell which agrees with each other.

5 Conclusion
CdTe and CIGS Solar Cells were successfully simulated at various thickness and temperature using SCAPS 33.00 in which the electrical properties such as J_{sc} and V_{oc} are very important parameters and happened to be at its best with short circuit current and open circuit voltage of 24.175(mA/cm²), 0.9978(V) and 19.560000(mA/cm²), 0.8220(V) under illumination for both simulated and measured respectively. It was observed that thickness and temperature directly affect the electrical properties of CdTe and CIGS solar cells. This is because at various
temperature and thickness of the solar cells under illumination, \( J_{sc} \) and \( V_{oc} \) can no longer work efficiently as temperature and thickness increases as the case may be. The decrease in \( \eta \) with thickness can be attributed to the possible increases in the volume of the crystal defects with increase in the thickness of the solar cell materials. It was shown that it may be necessary to control the thickness of the layer and temperature precisely in order to improve the efficiency.

The efficiency values obtained are in close agreement with the experimentally reported values in the literature [12-15]. Taking the case of CdTe: The simulation measurements (i.e this work), theoretical (measurements) and experimental values in % are; 16.03%, 10.72% and 16%-17% and for CIGS solar cells; 16.54%, 15.96% and 16%-19% respectively. The novelty of our work is its ability to produce the achieved accuracy considering the little computational effort it requires. Therefore, the CdTe and CIGS solar cells are considered as promising future source of excellent stable, efficient and low-cost solar power. Numerical modeling of these solar cells provided a way of analyzing device operation and can be used as a design aid.

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