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Research Article

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Simulation of CIS/ZnO/TiO_2 Solar Cell and Optimization Using SCAPS

K. Hima[1], T.D. Subash[1] and Malathy Batumalay[2*]

[1]*VISAT Engineering College, Kerala, India*

[2]*INTI International University, Malaysia*

[*]Correspondence to:
Malathy Batumalay
INTI International University,
Malaysia.
E-mail: malathy.batumalay@newinti.edu.my

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Abstract

This paper proposes a CIS (copper indium selenide) based solar cell with an un-doped zinc oxide (ZnO), and titanium dioxide (TiO_2) as three layers and its performance was examined using a simulation program named SCAPS-1D software (Solar Cells Capacitance Simulator). Because of their affordable manufacturing prices and high conversion efficiencies, solar cells are extensively studied and used for power generation CIS based solar cells ($CuInSe_2$) are used since they are less expensive than silicon cells and uses thin sheet technology. In the visible range, ZnO is a highly conductive thin film with exceptional transparency. TiO_2 is a low cost and nontoxic photo catalyst. The ZnO layer thickness and temperature of solar cells were evaluated in depth based on the device structure and fabrication method. An efficient structure of CIS/ZnO/TiO_2 thin-film solar cell is obtained when the temperature is changed from 400 K to 150 K by adding an intrinsic layer of 2 micrometer in the structure. The ZnO layer thickness is changed from 0.001 micrometer to 1.5 micrometer and results are observed. Besides that, the C-V characteristics of the structure are observed.

Keywords

Copper indium selenide, Chalcopyrite, Titanium dioxide, Photovoltaic, SCAPS-1D

Introduction

The economic and social development of a country depends on its ability to obtain energy [1]. The primary goal of energy transformation is to increase energy access. A lot of energy is currently produced on a large scale using many sourcesincluding fossil fuels, wind turbines, etc. Yet, the fundamental issue is that continued use of energy-producing resources will result in a shortage of resources likefossil fuels. However, the continued use of fossil fuels due togreenhouse gas emission is bad for the environment. In addition to having a direct impact on agricultural activities andoverall health, access to electricity is crucial for achieving sustainable development goals [2].

Without generating electricity through sources that disturb the ecosystem, the energy deficit should be filled. Solarenergy is a good example of a renewable energy technology that can be used to satisfy this demand. The most significant source of energy which cannot be destroyed is solar energy.Solar cells have now been used as a remedy for energy shortage and to lessen the environmental issues brought on by the burning of fossil fuels.

The layers of semiconductor materials used to make photovoltaic devices are only a few microns thick comparedto crystal wafers that are hundreds of microns thick [2]. Furthermore, the development of flexible photovoltaic modules is made possible by the capacity to deposit films on thin substrates. By utilizing high throughput deposition methods, these developments can lower material andmanufacturing costs [2].

CIS (CuInSe$_2$) based solar cells have demonstrated strong photo conversion performance [3, 4]. It is a substance that is a part of the chain of chalcopyrite substances [5, 6]. CuInSe$_2$ based solar cells are desirable in the industrial and research domains due to their low material consumption,low manufacturing energy consumption, and low cost of substrates [6, 7]. This material can absorb the majority of input photons with just a few micrometers. In the visible spectrum, ZnO is a highly conductive thin film with outstanding transparency [8]. TiO$_2$ has high mechanical stability, excellent adhesion, and good transmission in the visible and infrared spectrum [9, 10]. TiO$_2$ is well recognized for more than 3 eV wide band gap and its variety of functions [9, 11]. In-depth research has been done on highly effective nanocrystalline TiO$_2$-based dye-sensitized solar cells as a viable low-cost option [1, 12].

Experimentation

Simulation using SCAPS

The simulation makes use of SCAPS, a program with a version 3.3.00 [2]. Open-circuit voltage (V_{OC}), short circuit current density (J_{SC}), fill factor (FF%), quantum efficiency (QE%), efficiency percentage, hetero junction energy band structure, etc. [12] can be calculated at various temperatures and in both light and darkness using this software.

In our paper we are taking each layer as uniform layer, and we are not introducing any defects. Thus, here the three layers CIS, ZnO, and TiO$_2$ are taken, and the solar cell is simulated. The SCAPS program computes concentrations, energy bands, currents, J-V characteristics, A-C characteristics, and spectral response at a specific working point (also with bias light or voltage) [12]. Left and right contact is given, and light is applied from right contact and voltage is given to left contact and right contact is grounded. Interfaces are also added. First the structure is simulated, and J-V characteristics and C-V characteristics are noted.

Table 1 lists the parameters for CIS, ZnO, and TiO$_2$ that were employed in the simulations [3]. The SCAP software's numerical portion is depicted in figure 1. The CIS/ZnO/TiO$_2$ solar cell structure that was built and employed in the SCAPS simulations is shown in figure 2. Analysis is done on the effects of ZnO layer thickness. The performance of thin film planar

Table 1: Parameters for CIS, ZnO, and TiO$_2$.

Parameter	CIS	ZnO	TiO$_2$
Thickness, d (μm)	2	0.200	2.00
Bandgap, Eg (eV)	1.040	3.300	2.260
Electronaffinity, EA (eV)	3.300	3.100	4.200
Relative permittivity	9	10	10
Valance band density of states (cm^{-3})	1.00E+19	1.00E+18	6.00E+17
Electron mobility	1.0E+2	1.00E+8	1.0E+2
Hole mobility	2.5E+1	1.000E+8	2.5E+1
Donor density, ND (cm^{-3})	0	1.0E+15	1.00E+17
Acceptor density, NA (cm^{-3})	1.0E+15	0	0
Electron thermal velocity (cm/s)	1.00E+7	1.00E+8	1.00E+7

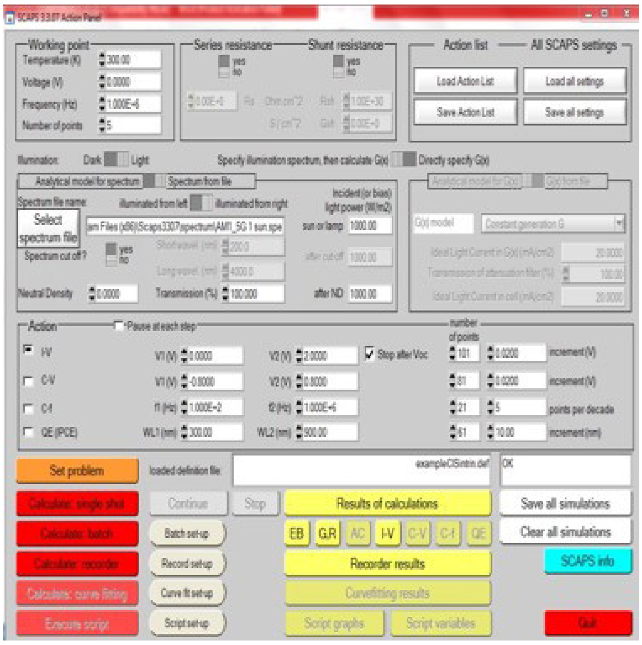

Figure 1: The numerical section of SCAP software.

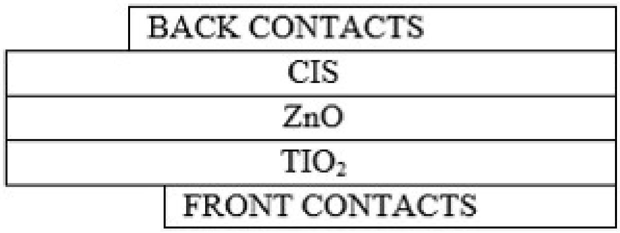

Figure 2: Schematic of CIS/ZnO/TiO$_2$ heterojunction solar cell.

CIS/ZnO/TiO$_2$ heterojunction solar cells at various solar concentrations andoperating temperatures were also evaluated by adding an inner layer.

Simulation of CIS/ZnO/TiO$_2$ heterojunction solarcell

Figure 3 presents simulated CIS/ZnO/TiO$_2$ heterojunction solar cell. Figure 4 presents the J-V characteristics of CIS/ZnO/solar cell. Observed V_{OC} = 0.455 V, J_{SC} = 35.82 mA/cm^2, FF = 77.27%, and module efficiency = 12.6%. Figure 5 presents C-V characteristics of CIS/ZnO/TiO$_2$ heterojunction solar cell.

Effect of thickness of ZnO layer

The ZnO layer thickness varies from 0.001 micrometer to 1.5 micrometer and the graph is observed. Figure 6 presents batch set up window. Figure 7 presents J-V characteristics of CIS/ZnO/TiO$_2$ heterojunction solar cell using batch setup. Here the short circuit current density reached up to 35.82 mA/cm^2 resulting in 12.6% power conversion efficiency.

Effect of adding intrinsic layer

An intrinsic layer of two micrometers is inserted between CIS and ZnO layer and simulated. Figure 8 presents solar cell layer of CIS/intrinsic/ZnO/TiO$_2$ heterojunctions. Figure 9 presents J-V characteristics of CIS/intrinsic/ZnO/TiO$_2$ heterojunction solar cell. From the J-V characteristics it can be observed that by adding an intrinsic layer of two

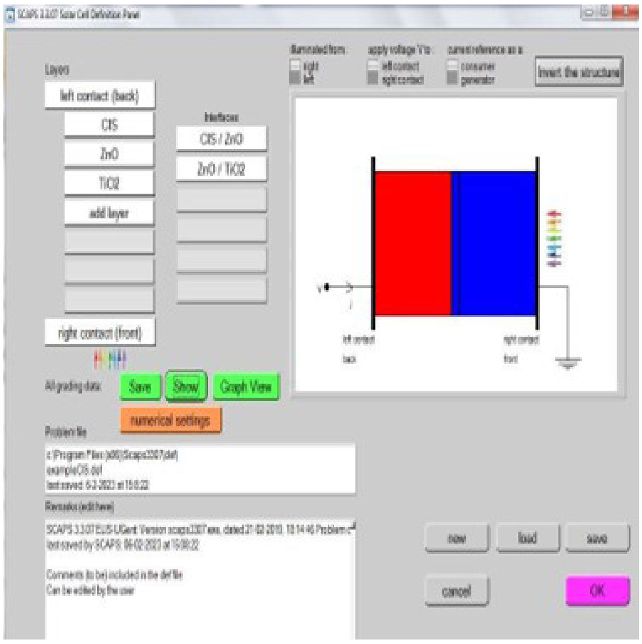

Figure 3: Simulated CIS/ZnO/TiO$_2$ heterojunction solar cell.

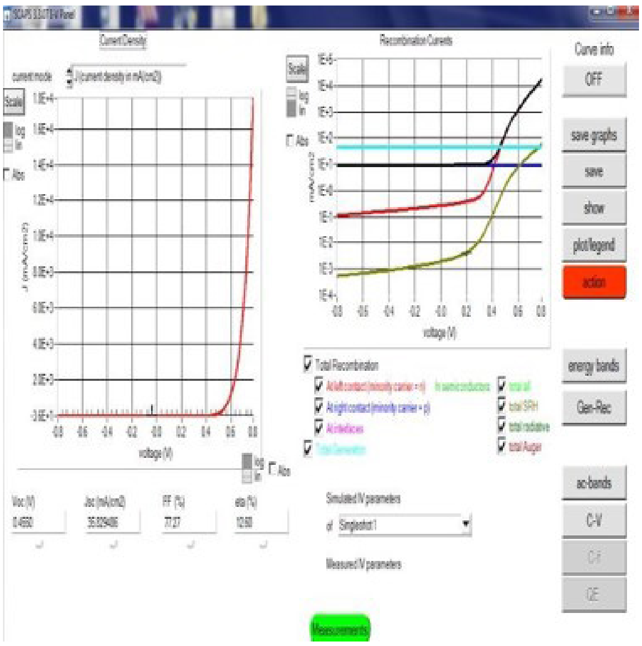

Figure 4: The J-V characteristics of CIS/ZnO/solar cell. Observed V_{OC} = 0.455 V, J_{SC} = 35.82 mA/cm^2, FF = 77.27%, and module efficiency = 12.6%.

micrometer thickness in between CIS and ZnO layer the efficiency increased from 12.6% to 12.93% where all other parameter values remain unchanged.

Effect of temperature variation

In this solar cell temperature is changed from 400 K to 100 K in seven steps (400 K, 350 K, 300 K, 250 K, 200 K, 150 K, and 100 K) and J-V characteristics is noted (Figure 10). From the J-V characteristics it can be inferred that efficiency increases from 12.93% to 15.12%. V_{OC} (V) vs temperature (K) graph is also plotted, and we found temperature and voltage varies linearly. By taking recorder set up V_{OC} vs temperature graph is plotted (Figure 11).

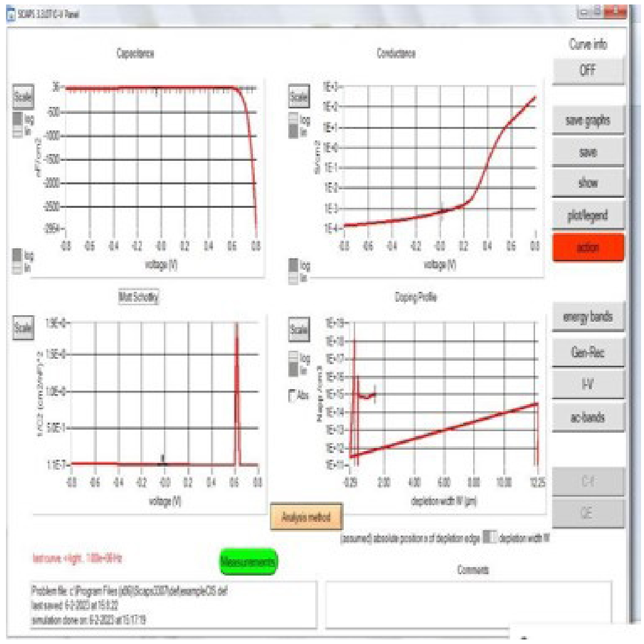

Figure 5: C-V characteristics of CIS/ZnO/TiO$_2$ heterojunction solar cell.

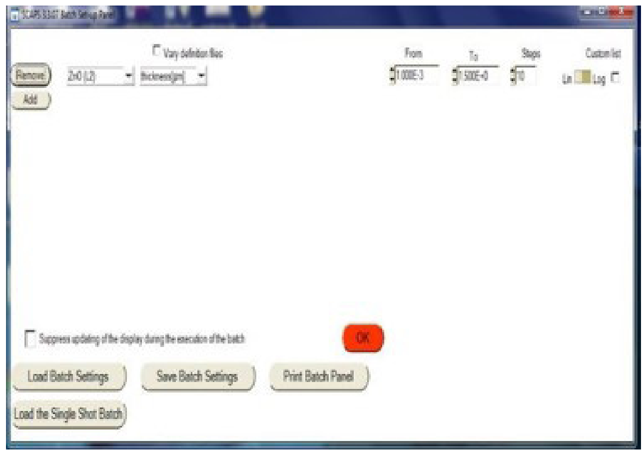

Figure 6: Batch set up window.

Effect of variation of left contact metal work function

Figure 12 presents left contact window. Figure 13 presents V_{OC} vs temperature graph. Here the left contact metal work function [6] is taken as 5 and again calculate the recorder we can observe that the voltage reaches saturation instead of straight line.

Without introducing additional defects simulation of the CIS/ZnO/TiO$_2$ heterojunction solar cells was performed. Variations in the ZnO layer's thickness are noted. The ZnO layer's shallow donor density was set at 1.000E+15 cm^3. The TiO$_2$ layer's shallow donor density was tuned at 1.000E+17 cm^3. In the CIS layer, the shallow acceptor densities were tuned at 1.000E+15 cm^3. In this construction, J_{SC} of up to 35.82 mA/cm^2 and a power conversion efficiency of 12.6% can be achieved. It can be concluded that by adding an intrinsic layer to thin-film planar CIS/ZnO/TiO$_2$ heterojunction structure having shallowdonor density and shallow acceptor densities as 1.000E+15 cm^{-3} efficiency can be enhanced.

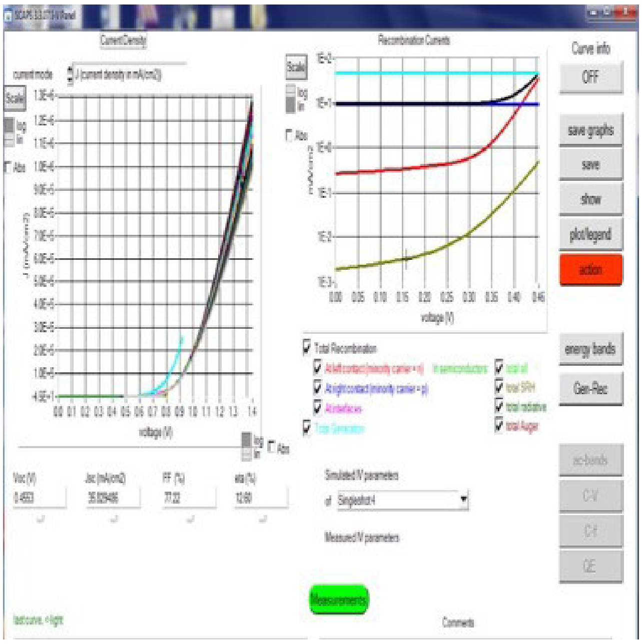

Figure 7: J-V characteristics of CIS/ZnO/TiO$_2$ heterojunction solar cell using batch setup.

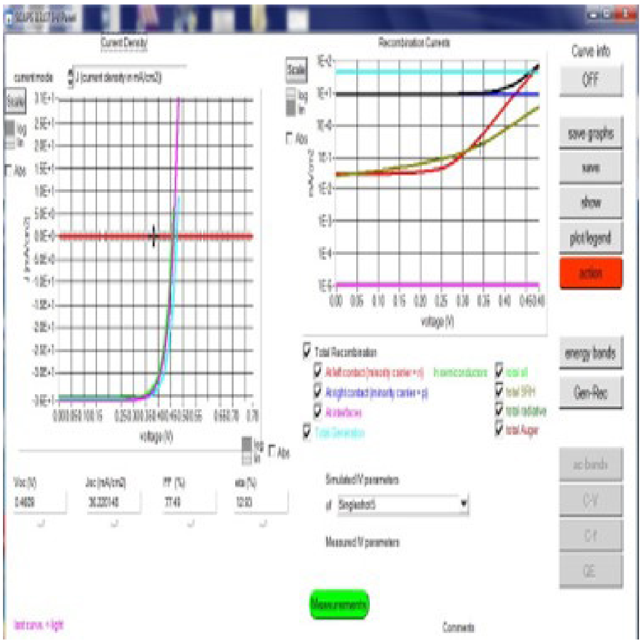

Figure 9: J-V characteristics of CIS/intrinsic/ZnO/TiO$_2$ heterojunction solar cell.

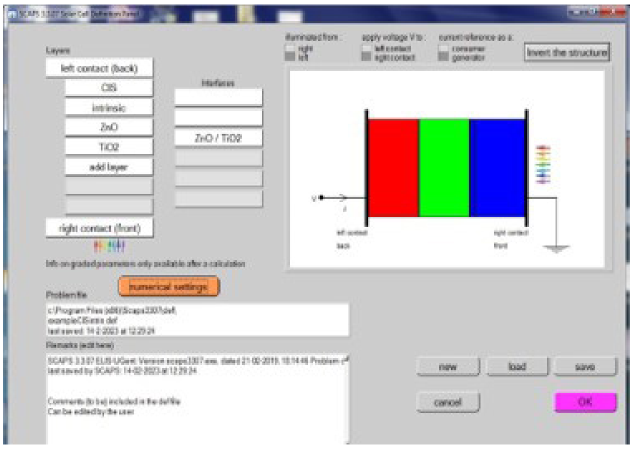

Figure 8: Solar cell layer of CIS/intrinsic/ZnO/TiO$_2$ heterojunctions.

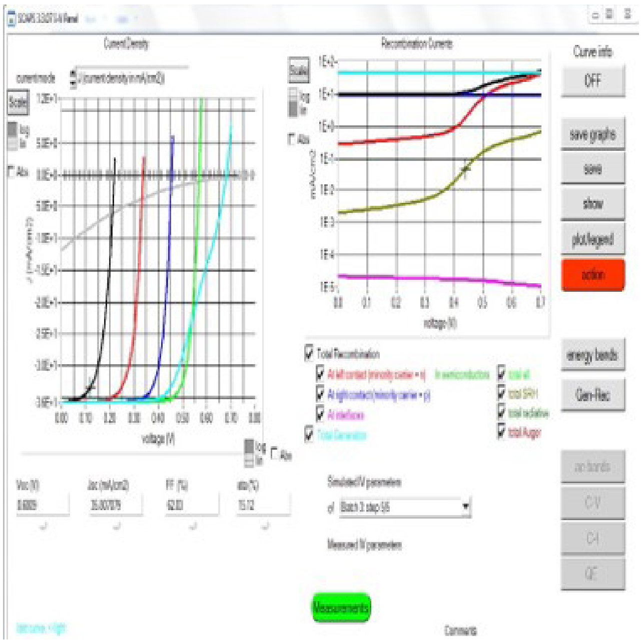

Figure 10: J-V characteristics of CIS/intrinsic/ZnO/TiO$_2$ heterojunctions by varying temperature. Observed V_{OC} = 0.6809 V, J_{SC} = 35.80 mA/cm^2, FF = 62.03%, and module efficiency = 15.12%.

Results and Discussion

The J-V characteristics in various cases of CIS/ZnO/TiO$_2$ heterojunction structure was observed. ZnO layer thickness is altered, and a graph is drawn. 12.6% efficiency is achieved. Thus, it has been found that here proposed solar cell's efficiency can be further increased to 12.93% by adding an intrinsic layer.

Conclusion

The effect of temperature and metal work function is also noted, and graph is plotted. The solar cell's efficiency again increases to 15.12% and thus we can conclude that an efficient CIS based solar cell is obtained.

Acknowledgements

None.

Conflict of Interest

None.

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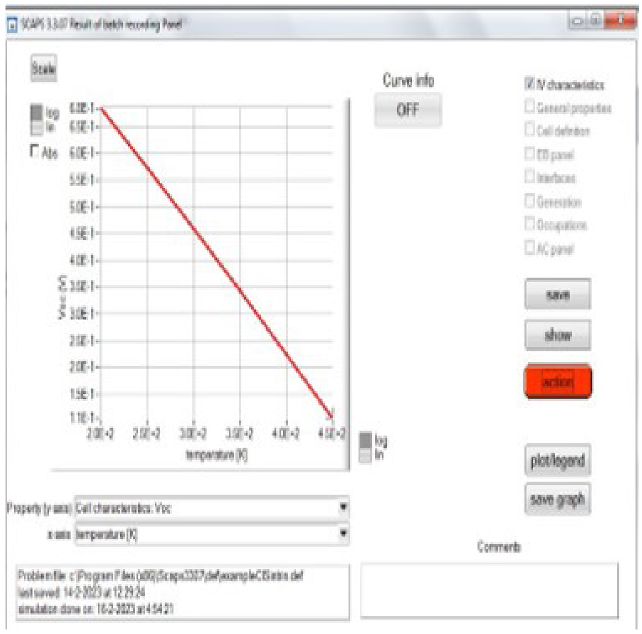

Figure 11: V_{OC} vs temperature graph.

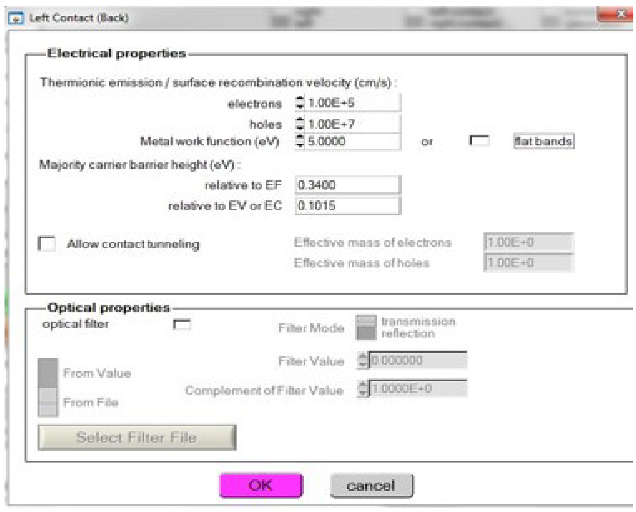

Figure 12: Left contact window.

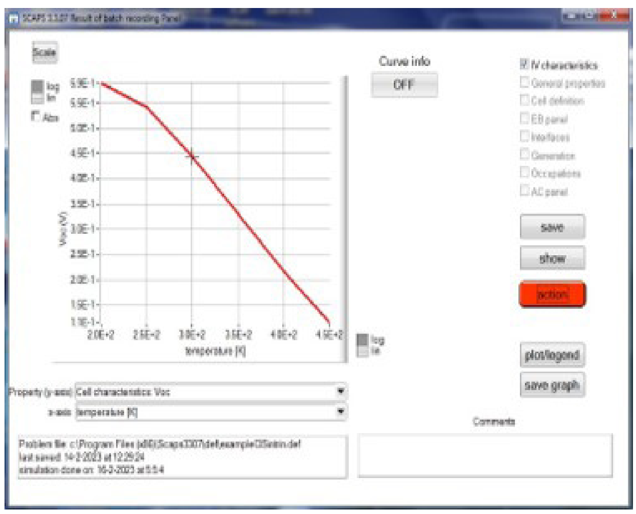

Figure 13: V_{OC} vs temperature graph.

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